Titles and Astracts

Nihan Acar, Florida State University
Investigation of Optimal Antibiotic Timing in Disinfecting Bacterial Population
Several important diseases like Tuberculosis are caused by bacterial biofilms. Many of these diseases can not be treated with standard antibiotic therapy. Although there are multiple mechanisms that bacteria use to evade treatment, phenotypic tolerance is one of the most novel. Among the bacteria within a biofilm, persisters are a subpopulation which are tolerant to antibiotics and knowing more about them is very critical and helpful.

This talk specializes on minimizing the susceptible and persister bacteria concentration using Optimal Control Theory in batch culture. We investigate the optimal timing for the application of antibiotic and refreshing the nutrient using mathematical tools and having the Poincare Map.

Orhan Akal, Florida State University
Employing Convolutional Neural Network to Segment Lymph Nodes
MatConvNet is a Matlab toolbox of Convolutional Neural Network(CNN) that is a state of the art tool to be used for image processing.

In this study MatConvNet is employed to segment Lymph nodes, while processing computerized tomography (CT) scans of patients. The end result of this study is that we'll be able to segment out Lymph nodes with the help of MatConvNet, once a physician points a single pixel inside the Lymph node. This study will reduce the workload of a technicians/physician who has to go through CT scans and spend time to do is by hand, as well as, this study will enable to get a quantified measure of from a hospital visit to another how much the Lymph node got bigger or smaller.

Orhan Akal, Florida State University
Sustainable Equilibrium in a Stock Market: Agent-Based Modeling with Evolutionary Game Theory Applied to Traders
This study employs an Agent-Based Model with Evolutionary Game Theory. First, we utilize a stock market simulation with four heterogeneous trader types: Momentum, contrarian, long term and speculative traders. They have deterministic decision rules, and they are given realistic trading conditions such as wealth constraints and learning behaviors. Their interactions are applied to a simulated stock market where we were able to replicate the quasi-random dynamic behavior of an actual stock market. Each trader also has the ability to change his/her trader type based on his/her past trading performance and its competitors past performance. In the long run equilibrium, long term traders dominate the stock market; the number of momentum and contrarian traders remain relatively low. In terms of relative total wealth, however, speculators hold almost half of the entire wealth that is invested in the stock market simulation.

Secondly, we focus on understanding the behavior of the stock market traders by utilizing an evolutionary game theory model. We allow each trader type to have his/her own strategy to make trading decisions in the stock market to maximize wealth. Each trader tries to maximize his/her payoff by changing the trading strategies with the consideration of learning and wealth constraints.

However, each trading strategy will incur two types of costs: time value of money and transaction costs. We predict a variety of realistic trading strategies that may be found in a market in equilibrium.

Alessandro Alla, Florida State University
Model order reduction for the control of parametrized PDEs via dynamic programming equations
We investigate infinite horizon optimal control problems for parametrized partial differential equations. We are interested in feedback control via dynamic programming equations. Since it is well-know that its numerical approximation suffers from the curse of dimensionality, we propose to apply parametric model order reduction techniques to make the approach computationally feasible. The idea is to construct low-dimensional subspaces with suitable information on the control problem, for which the dynamic programming equations can be solved efficiently by well-known techniques. Furthermore, we employ parameter partitioning techniques to be able to construct surrogate models with only 4-5 basis functions in each subregion. Numerical examples will illustrate the effectiveness of the proposed method.

Hamed Amini, University of Miami
Systemic Risk and Central Clearing Counterparty Design
We examine the effects on a financial network of multilateral clearing via a central clearing counterparty (CCP) from an ex ante and ex post perspective. The CCP is capitalized with equity and a guarantee fund and it can charge a volume-based fee. We propose a CCP design which improves aggregate surplus, and reduces banks' liquidation and shortfall losses. We characterize the CCP's equity, fee and guarantee fund policies that reduce systemic risk and are incentive compatible for banks. A simulation study based on real market data shows that central counterparty clearing can reduce systemic risk and improve banks' utility. This is joint work with Damir Filipovic and Andreea Minca.

Harbir Antil, George Mason University
Fractional Operators with Inhomogeneous Boundary Conditions
In this talk we will introduce new characterizations of fractional Laplacian to incorporate nonhomogeneous boundary conditions. We will discuss the well-posedness of the problem and we will derive a priori error estimates.

Feng Bao, The University of Tennessee at Chattanooga
Hierarchical Optimization for Neutron Scattering Problems
We present a scalable optimization method for neutron scattering problems that determines condence regions of simulation parameters in lattice dynamics models used to t neutron scattering data for crystalline solids. The method uses physics based hierarchical dimension reduction in both the computational simulation domain and the parameter space. We demonstrate for silicon that after a few iterations the method converges to parameters values (interatomic force-constants) computed with density functional theory simulations.

Johnna Barnaby, Florida State University
A Mathematical Approach to the Immune Response Following Treatments for Prostate Cancer
Prostate cancer is the second most common cancer in men. While initially treatments are promis-

ing, as the cancer progresses treatments become less and less effective. Androgen ablation therapy is a treatment used in early stages of prostate cancer. However, the cancer usually recurs and is resistant to this initial treatment. New treatments have been developed, such as immunotherapy, which use the patients own immune system to target the tumor. New evidence points to using a combination of these two treatments. To test this hypothesis we have begun developing a mathematical model of the immune response after the administration of androgen ablation.

Philip Boehner, Florida State University
Computational framework for evolution and nucleosynthesis studies of astrophysical objects
The chemical composition in the evolution of stellar plasma is one of the most critical components of computational models in astrophysics. We aim to construct the framework to support such computations in the context of multi-dimensional stellar evolution studies. A number of challenges arise from the fact that two different types of discrete representations of data are used in these computations. Our hydro simulations are performed on an adaptive Eulerian mesh, where we introduce passively advected Lagrangian tracer particles to continuously interpolate the thermodynamic quantities of the plasma for use in post-processing their initial isotopic abundances with a realistic set of isotopes. Thermodynamic trajectory information is output on a per-particle basis, but only once the fractional change of the density or temperature reaches a user-defined threshold, resulting in highly irregular data output. This data is buffered between checkpoint times to reduce computational cost of tracer particle output and to synchronize thermodynamic trajectory results with restart times. Following the post-processing stage, we map the more complete isotopic abundance distributions from the particles to the hydro domain using a monotonized variant of the linear Shepard's method.

We demonstrate the application of the newly-developed framework using the cellular detonation problem. We discuss the improvements to the efficiency of the thermodynamic trajectory information output from our hydro simulation as well as preliminary results with more realistic chemical compositions. Future applications of this framework will be within explosive phenomena in astrophysics including core-collapse and thermonuclear supernovae.

Tyler Bolles, Florida State University
Linear Water Waves Over Variable Depth and Singular Flow Around Corners
This talk introduces the widely used mathematical model of small amplitude water waves in the context of variable water depth. Lacking exact methods for obtaining solutions to arbitrary water depth, we consider gluing together solutions for separate, constant depths. This method is semi-analytical, using numerical methods only for the inversion of a block tri-diagonal coupling matrix. Our contribution to this classic problem is an insight relating the convergence rate of the eigenfunction expansion for the velocity potential to the bottom geometry. After being partitioned to piece-wise constant segments, the bottom exhibits sharp corners allowing for singularities in the irrotational velocity. Quantitative bounds on the convergence rates are provided through theorems relating the smoothness of a function to the asymptotic decay rate of its Fourier coefficients and conclusions are supported by numerical evidence.

Cameron Browne, University of Louisiana at Lafayette
Minimizing reproduction number in virus model with periodic combination antivirals

We derive formulas and threshold dynamical properties of the basic reproduction number for a within-host virus model with periodic combination drug treatment. We show that the phase difference between drug dosages may critically affect the reproduction number and asymptotic dynamics of the model. In particular, our main results establish that reproduction number is minimized for out-of-phase drug combinations and maximized for in-phase combinations, in the cases where drug efficacies are sinusoidal perturbations and for the case of piecewise constant "bang-bang" efficacies.

Valerie Bullock, Florida State University
Dynamic neuron networks with Fitzhugh-Nagumo nodes
Firing patterns of intricate neuron networks generate a wide range of animal behaviors. Several factors including network architecture, neuron connection strength, and signal propagation speed determine the nature of firing patterns. As a low-dimensional model of neural firing, the Fitzhugh-Nagumo system is a tractable choice for the graph nodes of a dynamic network that models neural computation. We discuss differences between dynamic neuron networks with Fizghugh-Nagumo nodes on small graph motifs that arise from various modeling choices such as the choice to include signal propagation delays. We also discuss a case study of calibrating a dynamic network to publicly available data on neuron networks.

Lukas Bystricky, Florida State University
Using Boundary Integral Equations To Model Rigid Body Motion
Boundary integral equations (BIEs) can be used to efficiently model the movement of particles suspended in a Stokesian fluid. This talk will review the theory and implemenation of BIEs applied to modeling a 2D suspension of rigid particles. Results will be shown which demonstrate the applicability of the model to estimate rheological parameters, such as effective viscosity.

Jesse Canfield, Los Alamos National Laboratory
Modeling wildfire with HIGRAD/FIRETEC
It is shown through numerical simulations of grass fires that the initial length of the ignition line affects forward rate of spread (ROS). HIGRAD/FIRETEC was utilized to model grass fires and understand the effect that ignition line length has on these fires. Finger shaped structures emerged in the combusting fuels, upstream of the fire front. The fingers correlated with counter-rotating vortex pairs in the gas-phase above them. It was also shown that increasing ignition line length does indeed increase forward ROS, an expected result supported by previous investigations. Results are presented that suggest physical reasons why a spreading grass fire develops flanks that move forward slower than the front of the fire.

A gas-phase mixture model was derived for the planetary boundary layer (PBL), where fires and other phenomena occur. The model partitions the state variables with Dalton's law of partial pressures and thermal equilibrium. This model was then coupled to HIGRAD and its efficacy was assessed for two scenarios. The first case was to numerically spin-up a moist unstable PBL. The second case simulated an idealized thermal plume loaded with gaseous combustion products. The heat source to the plume is shut off after some time and the relative mass of the combustion products to air causes the plume to fall back down on itself and spread outward in a density current.

Roger Pacheco Castro, Florida State University

Karst Flow Model Validation at Laboratory Scale for Coupled Discrete Continuous Models
Karst flow modeling is difficult due to the high heterogeneity of karstic aquifers. The heterogeneity is caused by the presence of fractures and conduits product of the dissolution. Different conceptual models have been proposed in the literature to overcome the natural complexity of karst aquifers in flow modeling. The coupled discrete-continuum approach conduits are conceptualized as discrete pipes and are linked to the porous media by an exchange term or a boundary condition. This kind of approaches has the advantage of integrating the information available for the conduits. We are interested in the validation of couple discrete-continuum models. The validation is performed by comparing the results of the model simulations with laboratory data for heads and flow rates under different configurations for the conduit geometry and boundary conditions. Two coupled discrete-continuum models are evaluated. The first one is the one implemented in the software MODFLOW CFP1 and the second one is known as the Darcy-Stokes model with Beaver-Joseph boundary condition. The laboratory experiment consist of sandbox filled with porous media coupled with a pipe simulating a conduit. Preliminary results showed that MODFLOW CFP1 is able to reproduce flow rates however heads in the porous media are overestimated. Our results will provide strong support on the validity of coupled discrete continuum models for real scale applications.

Serdar Cellat, Florida State University
A New Family of Shape Metrics to Improve Shape Classification
Study of shapes has been increasingly important in evolutionary and developmental biology. Identifying shape similarities and dissimilarities within and across populations is a fundamental problem in the field of evo-devo biology. In quantifying shape differences between populations, one must introduce a shape metric where the differences(distance) between shapes can be measurable. In this study, we extend the notion of shape distance using a new family of shape metrics. We also introduce a learning criteria that differentiates different groups in the optimal form. We use Monte Carlo optimization methods in learning process.

Qingshan Chen, Clemson University
Convergence and error analysis of staggered finite volume methods on unstructured meshes
Traditionally, analysis of finite difference finite volume (FDFV) schemes has been hard, because these methods are not based on variational formulations. Error analysis to establish the convergence rate of these numerical schemes has been particularly challenging, when FDFV discretizations of some high-order differential operators are not even consistent. In recent works, we have developed a new framework, based on external approximations of functional spaces, to address these challenges. In this talk, we will demonstrate how this framework can be employed to establish the convergence of a staggered FDFV for the classical incompressible Stokes problem. We will also show that, actually, consistency in low order differential operators, coupled with the external approximation framework, can produce error estimates that improve upon existing results.

Yue Chen, Auburn University at Montgomery
Monitoring depth profile of residual stress via Rayleigh-wave dispersion
We study the inverse problem on inferring depth profile of near-surface residual stress in a weakly anisotropic medium by boundary measurement of Rayleigh wave dispersion if all other relevant material parameters of the elastic medium are known. The solution of the problem is based on the direct problem to determine dispersion curves for Rayleigh waves propagating in various directions

when the material parameters,texture coefficients,and initial stresses are given. We can infer the depth profiles of the residual stresses which are good approximations to the real ones.

James Cheung, Florida State University
Boundary Condition Approximation for Lagrange Finite Elements by Polynomial Extension
Curved domains pose a great problem to high order finite element methods because the accuracy of a numerical solution ultimately depends on how well the discrete domain approximates the continuous domain. As such, the majority of the higher order finite element codes utilize some sort of coordinate transformation to fit a polygonal mesh to the curved domain up to an acceptable order of accuracy. While these methods can recover optimal theoretical accuracy for the underlying approximation space, they are often difficult to implement. In this talk, we present a new approach to recovering optimal accuracy for higher order finite elements with Lagrange elements for Dirichlet and Neumann problems for scalar elliptic PDE on curved domains. Instead of cumbersome coordinate transforms, we utilize a simple Taylor series to extend the underlying polynomial approximation space to approximate the given boundary condition on the curved boundary. This approximation allows us to retain our polygonal mesh, while at the same time, achieve optimal accuracy.

Evan Cresswell, Florida State University
Computational Model for Local Calcium Dynamics in Astrocytes
Several contemporary studies show that astrocytes, a type of glial cell, are fundamental to several neural functions ranging from metabolic support to higher cognition such as recollection memory. This has resulted in the introduction of astrocytic dynamics into neural modeling. Most cellular function in the astrocyte is triggered by an increase or decrease in calcium concentration within the cytosol. Previous work considered astrocytic dynamics by representing calcium concentration as a point source or a completely spatial model in the cell. We now know, more than ever, that the role of the astrocyte takes many different perspectives. This work, which is inspired by in vivo recordings of astrocytes in the ferret visual cortex, puts forward a novel approach to modeling the different levels of astrocytic calcium activity in the astro-neural system. In the model, we introduce a compartmentalized astrocyte with the purpose of understanding intra-cellular calcium dynamics. Compartmentalizing the astrocyte's cytosol into the soma and individual branches captures the effect of the local dynamics while still holding on to the analytical power of ODE's. With this model we investigate the interaction between local and global cellular dynamics within the astrocyte in response to neural activity. This allows us to better understand the effect that astrocytes can have on both individual neurons and populations of neighboring neurons.

Nathan Crock, Florida State University
New Analysis Techniques for New Imaging Techniques
The neuron doctrine has been a foothold for all neuroscientists as we ascend in our understanding of the brain. It revolutionized our knowledge of neuronal dynamics and our ability to study and diagnose diseases and disorders. Several contemporary studies show that astrocytes are more fundamental to many neural functions than previously believed. An "astrocyte doctrine" as one might call it, is sorely missing. With the advent of two-photon microscopy we are able to peer deeper into the complex inner workings of astrocytes. Studying this rich data may bring us closer to understanding their governing processes, but to do so requires the utilization of more sophis-

ticated analysis techniques. Here we present a new method aimed at shining light on the rules governing intracellular calcium dynamics of astrocytes, which is believed to be their mechanism for communication. We employ state of the art denoising techniques, compute the flow of calcium throughout the cell using Farneback's optical flow algorithm, and measure the flux of calcium in and out of different compartments of the cell.

Ana-Maria Croicu, Kennesaw State University
Optimal Control Applied to Anthrax Transmission in Animal Populations
Anthrax is an infectious disease that is known to infect both humans and animals. It turns out that Anthrax outbreaks occur periodically in animals. A vaccine against the Anthrax disease was developed long time ago. The purpose of this research is to identify an optimal vaccination regime based on the classical optimal control theory. For this goal, the Anthrax disease is considered for two special cases: herbivore and carnivore populations.

John Cummings, University of Tennessee
Modeling and Simulation of Microstructural Evolution in Organic Photovoltaic Thin Films
Organic Photovoltaics (OPVs) are popular alternatives to traditional silicon based solar cells which have numerous advantages, but lack currently in their power conversion efficiency. When constructing the OPV thin film active layer, a volatile solvent is mixed with multiple polymers and allowed to evaporate, resulting in the active layer of the OPV device. In an effort to further understand these devices, we develop a thermodynamically consistent model for the time evolution of the microstructure of the active layer in the OPV, resulting in a quaternary Cahn-Hilliard equation which is solved using a Full Approximation Scheme (FAS) multigrid method.

Angie Davenport, Florida State University
A Seasonal Matrix Model for Growth of Lycium carolinianum in Coastal Marshes
In this presentation we will discuss the proposed models that can provide valuable insight into the ecosystem that encompasses the Aransas National Wildlife Refuge (ANWR) and the migrating Whooping Crane, Grus americana. A stage-based model of Lycium carolinianum, the Carolina Wolfberry, was created to understand its importance in the survival of the Whooping Crane. Lastly this model will be simulated with the program, NetLogo, in order to test its application specifically to the ANWR area.

William Dewar, Florida State University
A Multiphase Model of Deep Oil Spills in the Ocean
The 2010 Deep Water Horizon (DwH) Oil spill in the Gulf of Mexico has generated renewed interest in point source, sustained, buoyant convection within the physical oceanography community. The problem is fundamentally one in multiphase fluid mechanics as the spill consisted of oil and gas released in sea water, requiring the development and use of a multiphase approach. Such modeling is rare in oceanography, although relevant applications of the method are increasing in number. Multiphase problems are notoriously computationally demanding, and this holds for the DwH setting. The fluid dynamics are intrinsically nonhydrostatic and the fast, convective velocities that are generated combined with the need for fine resolutions result in very restrictive time steps. In addition, simulations must be run for long times (i.e. several days) and to be useful, model time must be faster than real time. We describe development of a model meant to address these issues, as well

as to examine the dynamics of the convection. The model equations involve an arbitrary number of phases, including gas, with the primary restriction that the gas is considered as a dispersed phase. Perhaps the most surprising discovery is that planetary rotation emerges as a dominant effect on the nature of the convective plume, in spite of parametric settings that suggest otherwise. The structure of our current best DwH simulation is described.

Atanaska Dobreva, Florida State University
Sensitivity analysis applied to models for hair growth and disease
The organs that produce hair, called hair follicles, are known to constantly cycle through stages of growth, regression, and rest. Alopecia areata is an autoimmune disease which disrupts the growth stage, making it much shorter than normal, and this results in hair loss. We will first present a model that describes how the disease develops over time in a small cluster of homogeneous cycling follicles. The model joins a system capturing the hair cycle with equations that reflect the behavior of autoreactive immune cells. Next, we will present our results from using sensitivity analysis to determine which processes play the most important role in relation to the dynamics of autoimmune components as well the duration of hair growth in healthy and alopecia-affected follicles.

Sepideh Ebadi, Florida State University
Bacterial Persistence, Mathematical Model, Experimental Validation and Parameter Estimation
Bacterial infections cause many chronic diseases such as tuberculosis, meningitis and pneumonia. These diseases may not respond to treatment with antibiotics. Bacteria evade antibiotics using a variety of tolerance mechanisms such as modifying their genotypic or phenotypic expression. They can also protect themselves in structured communities referred to as biofilms. In order to outsmart the bacteria we must have a better understanding of these tolerance mechanisms. The focus of this study is on the dynamics between phenotypes. Understanding the changes in the persistent bacterial population before and after antibiotic challenge is of primary importance for creating treatment methods. In this research we intend to bridge the gap between experimental and theoretical/mathematical models and to deliver brighter intuitions to experiments that describe several current hypotheses regarding phenotypic expression. Finding the best applicable set up to eliminate the bacteria by comparing our theoretical model against experimental data, is our main goal. This will then be used to develop and quantify treatment methods.

Ahmed Elshall, Florida State University
Numerical Daemons of Monte Carlo based Bayesian Model Evidence Estimators
Bayesian multimodel inference is increasingly being used in geoscience.Estimating Bayesian model evidence (BME) is of central importance in many Bayesian multimodel analysis such as model selection, optimal experimental design, model averaging, simulation-optimization and other. BME is the overall probability of the model in reproducing the data, accounting for the trade-off between the goodness-of-fit and the model complexity. Yet estimating BME is challenging, especially for high dimensional problems with complex sampling space. Estimating BME using the Monte Carlo numerical methods is preferred, as the methods yield higher accuracy than semi-analytical solutions (e.g. Laplace approximations, BIC, KIC, etc.). However, numerical methods are prone the numerical demons arising from underflow of round off errors. Although few studies alluded to this issue, to our knowledge this is the first study that illustrates these numerical demons. We show that the precision arithmetic can become a threshold on likelihood values and Metropolis acceptance ratio,

which results in trimming parameter regions (when likelihood function is less than the smallest floating point number that a computer can represent) and corrupting of the empirical measures of the random states of the MCMC sampler (when using log-likelihood function). We consider two of the most powerful numerical estimators of BME that are the path sampling method of thermodynamic integration (TI) and the importance sampling method of steppingstone sampling (SS). We also consider the two most widely used numerical estimators, which are the prior sampling arithmetic mean (AS) and posterior sampling harmonic mean (HM). We investigate the vulnerability of these four estimators to the numerical demons. Interesting, the most biased estimator, namely the HM, turned out to be the least vulnerable. While it is generally assumed that AM is a bias-free estimator that will always approximate the true BME by investing in computational effort, we show that arithmetic underflow can hamper AM resulting in severe underestimation of BME. TI turned out to be the most vulnerable, resulting in BME overestimation. Finally, we show how SS can be largely invariant to rounding errors, yielding the most accurate and computational efficient results. These research results are useful for MC simulations to estimate Bayesian model evidence.

Arash Fahim, Florida State University
Model risk and constrained optimal transportation
In a multi-dimensional data, the approximation of marginal distributions is much more accurate than the joint distribution of the data. In financial context, the distribution of quoted asset price at each time is usually easy to obtain with high accuracy; however the distribution of the whole time series of asset price usually requires several assumption and usually narrows down to a choice of a model, bases on computational discretion. This increases the exposure to the risk of choosing a model which does not match the data at its best. We study the model risk in the context of option pricing and relate it to the constraint optimal transportation theory.

Zachary Feinstein, Washington University in St. Louis
An extension of the Eisenberg-Noe network model with fire sales
In this talk we will consider an extension of the Eisenberg & Noe (2001) model of financial contagion to include fire sale externalities from multiple illiquid assets. By allowing for multiple illiquid assets, institutions may have a choice in how they delever in a fire sale. Mathematical results on existence and uniqueness of clearing payments and prices will be given. Special emphasis will be placed on a game theoretic equilibrium liquidation strategy.

Antigoni Georgiadou, Florida State University
Automated Parameter Fitting in Stellar Evolution
Computer modeling is extensively used to probe structure and evolution of stars and planets. In particular, these computations allow astrophysicists to connect the star formation process to astronomical observations of stellar objects. Because stellar evolution is a highly complex process, matching the initial conditions to the observed objects requires substantial effort and expert knowledge. Typically probing parameter space of this problem is done using a trial-and-error approach, which is inefficient, incomplete and prone to bias. Our aim is to identify the key model parameters, their most probable values, and their observationally-constrained ranges in an automated way. We formulate a suitable constrained optimization problem, and combine select global optimization methods with stellar evolution code, MESA. For example, we use the Controlled Random Search method coupled with the MESA code in order to account for the evolutionary behavior and

physics of average mass stars and white dwarfs. By combining those stellar evolution models with constrained optimization we can account for optimal progenitor models. Such optimal progenitor models can be used as initial conditions for multidimensional computer simulations that will provide input data to future core-collapse supernova explosion models.

Scott Goodrick, USDA Forest Service
Operational fire behavior prediction models in the U.S. Forest Service
Quantitative fire behavior predictions became a reality for the U.S. Forest Service in 1972 with what is now referred to as the Rothermel spread model. This semi-empirical model related the forward spread of a fire to a relatively small set of fuel, weather and terrain related variables. While this model is limited in the range of fire phenomena it can describe, it has become the cornerstone of all operational fire behavior prediction tools used by the U.S. Forest Service. This presentation examines the strengths and weaknesses of this model with a view towards how its use has evolved over the past 45 years. Using this historical overview as a starting point, we will also explore some of the model's limitations that need to be addressed in developing the next generation of operational fire behavior prediction tools.

Ayşe Gör, Bilecik Şeyh Edebali Universitesi
Rank of Elliptic Curve
Elliptic Curve Cryptography (ECC) is an approach to public-key cryptography based on the algebraic structure of elliptic curves over finite field. Elliptic curves are applicable for encryption , digital signatures pseudo-random generators and other task. They are also used in several integer factorization algorithms based on elliptic curves that have applications in cryptography, such as Lenstra elliptic curve factorization.

This study gives a general survey of rank of elliptic curves over the field of rational numbers. Also this study gives proof of all rational points of elliptic curves is commutative group, includes discussion of the Birch and Swinnerton-Dyer Conjecture,the Parity Conjecture,rank of elliptic curves over Q in families of quadratic twists and way to search for elliptic curves of large ranks.

Shu Gu, Florida State University
Recent progress in homogenization of Stokes systems
Over the past three decades, a penalization method has been used in the study of incompressible Navier-Stokes equation in porous media, by adding a penalty term on the velocity defined on the volume of porous body. In the case of porous with a periodic structure and of size order $O(\varepsilon)$, this penalty method may be viewed as homogenization of Stokes systems with rapidly oscillating periodic coefficients. In this talk, we will discuss our recent results in quantitative homogenization of Stokes systems, including uniform interior and boundary regularities as well as the convergence rates results.

Mansoor Haider, North Carolina State University
Fast algorithms for integral equation models of viscoelasticity in biological soft tissues
Viscoelasticity is an important energy dissipation mechanism in modeling the mechanics of biological soft tissues. Several examples of viscoelastic continuum models relevant to biomechanical deformation in articular cartilage will be presented. These models are formulated at both the

macroscopic (tissue) scale and the microscopic (cellular) length, and give rise to integral equation formulations that are solved numerically. In each case, techniques for accelerating solution of the computational models will be presented and discussed in the context of the associated applications.

Daozhi Han, Indiana University
Second order methods for computing phase field fluid models
In this talk, we present second order accurate, unconditionally stable numerical methods for solving Cahn-Hilliard type fluid models, including Cahn-Hilliard-Navier-Stokes equations and Cahn-Hilliard-Darcy equations. These methods are shown to be uniquely solvable, mass-conservative, and satisfy discrete energy laws.

Matthew Hancock, Florida State University
Lung nodule malignancy classification using diagnostic image features
To determine the potential usefulness of quantified diagnostic image features as inputs to a Computer-aided Diagnosis (CAD) system, we investigate the predictive capabilities of statistical learning methods for classifying nodule malignancy, utilizing the Lung Image Database Consortium (LIDC) dataset, and only employ the radiologist-assigned diagnostic feature values for the lung nodules therein, as well as our derived estimates of the diameter and volume of the nodules from the radiologists' annotations. We calculate theoretical upper bounds on the classification accuracy that is achievable by an ideal classifier that only uses the radiologist-assigned feature values, and we obtain an accuracy of 85.74($\pm$1.14)% which is, on average, 4.43% below the theoretical maximum of 90.17%. The corresponding area-under-the-curve (AUC) score is 0.932($\pm$0.012), which increases to 0.949(0.007) when diameter and volume features are included, along with the accuracy to 88.08($\pm$1.11)%. Our results are comparable to those in the literature that use algorithmically-derived image-based features, which supports our hypothesis that lung nodules can be classified as malignant or benign using only quantified, diagnostic image features, and indicates the competitiveness of this approach. We also analyze how the classification accuracy depends on specific features, and feature subsets, and we rank the features according to their predictive power, statistically demonstrating the top four to be spiculation, lobulation, subtlety, and calcification.

Mario Harper, Florida State University
Highly Parallel Motion Planning Using Monte Carlo Techniques in Applied Robotics
A key difficulty of motion planning is the computational cost of searching for an optimized trajectory. This is particularly true in the case of online planning on a field robotic platform where the computational time and power is severely limited. This research shows some preliminary results of simple exploration using a Monte-Carlo based optimization approach to find a sub-optimal but feasible trajectory. This research also uses a novel approach of sampling the control space. This allows us to remove the difficulty of using an inverse kinematic model to invert positional space into the controllable parameters of the robotic platform.

Corey Harris, Florida State University
The Chern-Mather class of the multiview variety
The multivew variety associated to a collection of N cameras records which sequences of image points in PP^{2}N can be obtained by taking pictures of a given world point x in PP^3 with the cameras. In order to reconstruct a scene from its picture under the different cameras it is important

to be able to find the critical points of the function which measures the distance between a general point u in PP^2N and the multiview variety. In this paper we calculate a specific degree 3 polynomial that computes the number of critical points as a function of N. In order to do this, we construct a resolution of the multiview variety, and use it to compute its Chern-Mather class.

Xiuxiu He, Georgia State University
Substrate Curvature Regulates Cell Migration
Cell migration is essential in many aspects of biology. Many basic migration processes including adhesion, cytoskeletal polymerization, contraction, and membrane protrusion and tension, have to act in concert to regulate cell migration. At the same time substrate topography modulates these processes. In this work, we study how substrate curvature at micron-meter scale regulate cell motility. We developed a 3D mechanical model of single cell migration and simulated migration on curved substrates with different curvatures. The simulation results show that cell migration on concave surfaces is more persistent than on convex surfaces. We further calculate analytically the cell shape and the protrusion force for cells on curved substrates. We show that while cells spread out more on convex surfaces than on concave ones, the protrusion force magnitude in the direction of migration is larger on concave surfaces than on convex ones. These results offer a novel biomechanical explanation to substrate curvature regulation of cell migration: geometric constrains bias the direction of the protrusion force and facilitates the persistent migration on concave surfaces.

Thi Thao Phuong Hoang, University of South Carolina
Global-in-time domain decomposition methods for linear advection-diffusion equations
We consider nonoverlapping domain decomposition methods for solving heterogeneous advection-diffusion problems in which different time steps can be used in different parts of the domain. First order operator splitting is used to treat differently the advection equation and the diffusion equation. A discrete multidomain problem is formulated where separate transmission conditions for the advection equation and for the diffusion equation are derived. Two types of domain decomposition methods are studied: one is based on a generalization of the Steklov-Poincaré operator to time-dependent problems and one is based on the optimized Schwarz waveform relaxation (OSWR) method in which Robins transmission conditions are used to accelerate the convergence of the method. For each method, a discrete space-time interface problem is derived and nonconforming time grids are employed to adapt to different time scales in the subdomains. Numerical results in 2D for both academic problems and more realistic prototypes for simulations for the underground storage of nuclear waste are presented.

Hua Huang, Florida State University
Indirect combustion noise generation in a supersonic nozzle
When jet engine operates with afterburner on, lots of fuel get dumped to the afterburner, and these hot blobs form entropy wave. Entropy wave consists of density and temperature fluctuation. When these hot spots were carried by the meanflow to downstream, pressure fluctuations are generated. In this study, a broad band entropy wave source model based on measured temperature fluctuation spectra is designed and implemented. The indirect combustion noise generation process of hot spots passing a transonic nozzle is numerically investigated. A fourth-order accurate Dispersion-Relation-Preserving scheme is adopted. With an incoming entropy wave of 5% fluctuation intensity, an intense noise of 170dB is generated when entropy wave pass the shock.

Downstream of the shock,two humps are observed in the spectra and these two humps are expected to be irritated by duct mode. This study indicates a significant sound will be generated when entropy wave pass a transonic nozzle and the presence of shock further amplifies this phenomenon.

Ray Huffaker, University of Florida
Diagnosing and Reconstructing Real-World Hydroclimatic Dynamics from Time Sequenced Data
There are increasing calls to audit decision-support models used for environmental policy to ensure that they correspond with the reality facing policy makers. Modelers can establish correspondence by providing empirical evidence of real-world dynamic behavior that their models skillfully simulate. We present a pre-modeling diagnostic frameworkbased on nonlinear dynamic analysisfor detecting and reconstructing real-world environmental dynamics from observed time-sequenced data. Phenomenological (data-driven) modelingbased on machine learning regression techniquesextracts a set of ordinary differential equations governing empirically-diagnosed system dynamics from a single time series, or from multiple time series on causally-interacting variables. We apply the framework to investigate saltwater intrusion into coastal wetlands in Everglades National Park, Florida, USA. We test the following hypotheses posed in the literature linking regional hydrologic variables with global climatic teleconnections: (1) Sea level in Florida Bay drives well level and well salinity in the coastal Everglades; (2) Atlantic Multidecadal Oscillation (AMO) drives sea level, well level and well salinity; and (3) AMO and (El Nio Southern Oscillation) ENSO bi-causally interact. The thinking is that salt water intrusion links ocean-surface salinity with salinity of inland water sources, and sea level with inland water; that AMO and ENSO share a teleconnective relationship (perhaps through the atmosphere); and that AMO and ENSO both influence inland precipitation and thus well levels. Our results support these hypotheses, and we successfully construct a parsimonious phenomenological model that reproduces diagnosed nonlinear dynamics and system interactions. We propose that reconstructed data dynamics be used, along with other expert information, as a rigorous benchmark to guide specification and testing of hydrologic decision support models corresponding with real-world behavior.

Caitlin Hult, University of North Carolina at Chapel Hill
Modeling nucleosomal DNA in living yeast
The genome in living yeast cells is a highly dynamic system where entropic interactions and nuclear confinement drive the formation of domains of high chromosomal interaction, known as topologically associating domains. We investigate dynamic organization and territory formation of all 16 chromosomes in living yeast cells during interphase, using coarse-grained, entropic polymer chain models. We are interested in determining the mechanisms, such as packaging molecules that create loops within chromatin fibers, that govern inter- and intra-chromatin fluctuations and induce global features of the entire genome as well as more localized features of the nucleolus. The Bloom lab measures specific DNA sites in specific chromosomes using live cell fluorescence microscopy. Our goal is to identify the sufficient biological and biophysical assumptions necessary to reproduce the experimental data, from which we aim to shed insights into dynamics and structure that are beyond current experimental resolution.

Monical Hurdal, Florida State University
Conformal Brain Mapping
Computationally unfolding and "flattening" the surface of the brain from magnetic resonance imag-

ing (MRI) data is of great interest to neuroscientists in order to reveal the underlying folded tissue. These brain maps are subsequently used in studies that compare healthy brains to those with various disorders including depression, schizophrenia, or Alzheimer's disease. However, most of the current brain maps are computed usinguse ad hoc approaches that are specific to a particular laboratory or their software.

In this presentation, we will discuss some of the mathematical methods we are using to to create quasi-conformal maps of the brain. We will discuss how we construct these maps using the method of circle packing and we will show some of the areas where we are applying our methods. Additionally, we will present some of our current research using conformal invariants.

Melanie Jensen, Tulane University

Antibody-mediated immobilization of virions in mucus

In recent years, particle tracking experiments have provided new insights into interactions between our immune system and foreign bodies like viruses and bacteria. Sam Lai (UNC-Chapel Hill, Pharmacy) and collaborators have demonstrated that certain types of antibodies have the capacity to essentially immobilize Herpes virions and it is believed that a similar effect will be true for HIV. Because antibodies are too small to be directly observed in these experiments, the physical mechanism underlying this effect remains unclear. Using particle tracking data for Herpes, we construct a multi-scale model assuming linear rates to describe the dynamics of virions in a mucosal medium in varying exogenous antibody concentrations.

First, we develop a classification system for the data based on the trajectories of the visions that correspond to Brownian and stationary motion. While the antibody-mucin dynamics and the virion-antibody-mucin dynamics occur on different time scales, we model both interactions with continuous-time Markov Chains in order to compute the stationary distribution of virion immobilization. To specify our model with the data, we use identifiability analysis to set mathematically optimal and biological feasible parameter values. Finally, we compare theoretical immobilization times with observed immobilization times to determine if the virion-antibody-mucin dynamics can be approximated using linear rates.

Lili Ju, University of South Carolina

A conservative nonlocal convection-diffusion model and asymptotically compatible finite difference discretization

In this talk we first propose a nonlocal convection-diffusion model, in which the convection term is constructed in a special upwind manner so that mass conservation and maximum principle are maintained. The well-posedness of the resulting nonlocal model and its convergence to the classical, local convection-diffusion model are established. A quadrature-based finite difference discretization is then developed to numerically solve the nonlocal problem and is shown to be consistent and unconditionally stable. We also prove that this numerical scheme is asymptotically compatible, that is, the approximate solutions converge to the exact solution of the corresponding local problem when the horizon and the grid size go to zero at arbitrary speed. Consistent error orders are carefully derived to illustrate the effect of the nonlocal convection term. Some numerical experiments are also performed to validate the theoretical results.

Gokberk Kabacaoglu, University of Texas

Stable and accurate low-resolution simulations of two-dimensional vesicle flows
Vesicles, which resist bending and are locally inextensible, serve as experimental and numerical proxies for red blood cells. Vesicle flows, which are governed by hydrodynamic and elastic forces, refer to flow of vesicles that are filled with and suspended in a Stokesian fluid. In this work we present algorithms for stable and accurate low-resolution simulations of the vesicle flows in two-dimensions. We use an integral equation formulation of the Stokes equation coupled to the interface mass continuity and force balance. The problem poses numerical difficulties such as long-range hydrodynamic interactions, strong nonlinearities and stiff governing equations. These difficulties make simulations with long time horizons challenging, especially at low resolutions. We develop algorithms to control aliasing errors, correct errors in vesicles area and arc-length, and avoid collision of vesicles. Additionally, we discuss several error measures to study the accuracy of the simulations. Then we closely look at how accurate the low-resolution simulations can capture true physics of the vesicle flows.

Ruian Ke, North Carolina State University
Modeling the mechanistic action and predicting the impact of an immunotherapeutic DART molecule in HIV shock and kill strategies
HIV eradication studies have focused on the shock and kill strategies to induce HIV expression in latently infected cells using latency reversing agents (LRAs). However, minimal clearance of latently infected cells is achieved under LRA treatments. This points towards the need to combine LRAs with immunotherapeutics that boost immune mediated killing. HIVxCD3 DART molecules are bispecific antibody-based constructs that facilitate binding of cytotoxic effector T cells to cells expressing HIV antigen. In ex vivo studies, HIVxCD3 DART molecules effectively redirect cytotoxic T cells to kill latently infected cells following latency reversal by an LRA, vorinostat.

Here, we constructed mathematical models to gain a quantitative understanding of the mechanistic action of HIVxCD3 DART molecules. We estimated key parameters, including the rate of DART molecule-mediated killing of HIV-expressing cells from ex vivo data, and found that when effector cell concentration is sufficiently high, the rate of killing is close to the estimated death rate of productively infected cells in vivo, suggesting that HIVxCD3 DART molecules represent promising immunotherapeutics for future HIV eradication studies. We further incorporated the estimation into within-host meta-population models to explore its potential therapeutic impacts on the HIV latent reservoir in vivo. Our model serves as a quantitative tool for evaluating combination strategies involving LRAs and immunotherapies.

Karina Khazmutdinova, Florida State University
Natural Ventilation in Caves with a Single Opening
Speleothems, mineral deposits from limestone caves, contain valuable information for understanding ancient and recent climates. Air ventilation within caves influences the speleothem growth rates, thus, understanding of air exchange rates is important for an accurate paleoclimate reconstruction. Previous cave ventilation models have produced the results by combining cave measurements and mathematical models of heat exchange. Here we developed an analytical model to simulate air ventilation patterns within the cave by only using outside climatology and physical parameters of the limestone. We established baseline parameters necessary for modeling the airflow into and out of the caves with a single opening. Ventilation within the cave is governed by heat transfer through

the ground and natural convection. Combined with simple first-order CO2 and Radon-222 mass balances, the model predicts net CO2 and Radon-222 concentrations in the cave and shows an excellent agreement with in situ measurements.

Mikhail Khenner, Western Kentucky University
Model and computation of graphene island growth
Graphene, a two-dimensional layer of carbon atoms arranged in a honeycomb lattice, holds a promise of becoming the material of choice in advanced nanoelectronic technologies. The 2010 Nobel Prize in physics was awarded for extraction of graphene "from a piece of graphite such as is found in ordinary pencils", and for discovery of some of graphene's extraordinary electronic properties. In this talk I will present a nonlinear free-boundary model for graphene island growth on the copper surface. The model consists of (i) two partially coupled diffusion-type PDEs that describe evolution of the concentrations of the carbon atoms and dimers on the section of the copper substrate that is not yet covered by the growing island, and (ii) an ODE for the position of the island edge that is coupled to the concentration fields at the edge. Analytical map onto a fixed interval and the transformation enabling the clustering of the computational grid points near the island edge will be described. Computations of the edge speed on Cu surfaces of various crystallographic orientations will be presented; also, the contributions provided by atoms and dimers attachments to the edge will be discussed.

Ahmet Kilniç, Florida State University
A Mathematical Model of Cerebral Cortical Folding Development
All large mammalian species including humans have a cerebral cortex—the brain's outer folded layer. A number of biological hypotheses have been proposed to explain the process of the formation of the brain's folding patterns. Among these hypotheses, a biomechanical one claims that axonal tension forces between highly interconnected cortical areas are the principal force for cortical folding development. In a recent tension-based model, the deformation of a two-dimensional semi-circular domain representing the cerebral cortex was analyzed through the theory of linear elasticity (S. Kim, PhD Thesis, Florida State University, 2015). The coupled partial differential equations for elasticity were implemented computationally using the finite element method. Kims simulation results use plausible tissue elasticity, and domain size parameters for the brain and the degree of folding across simulation results was compared using a gyrification index measure.

In this presentation, Kims model is analyzed in terms of both theoretical and practical points of view, and some of the simulation results are reproduced. We will discuss ways of improving this model to make it more biologically relevant, including using the theory of non-linear elasticity instead of the theory of linear elasticity.

Hyunju Kim, North Greenville University
Implicitly enriched partition of unity mapping method for numerical solutions of fourth order partial differential equations containing singularities
Using Partition of unity (PU) functions with at-top, B-spline functions are modified to satisfy boundary conditions of the fourth order equations. Since the standard isogeometric analysis(IGA) as well as the conventional FEM have limitations to deal with fourth order equations containing singularities, we consider two enrichment methods (explicit and implicit) in the framework of the

p-, the k, and the h-refinements of IGA. We demonstrate that both enrichment methods yield good approximate solutions, but explicit enrichment methods give large (almost singular) matrix condition numbers and face integrating singular functions. Because of these limitations of external enrichment methods, we extensively investigate implicit enrichment methods (mapping methods) that virtually convert fourth order elliptic problems with singularities to problems with no influence of the singularities. EEffectiveness of the proposed mapping method extensively tested to one-dimensional fourth order equation with singularities. The mapping method is extended to the two-dimensional cases and test it to fourth order partial differential equations on a cracked disk and an L-shaped domain.

Yongje Kim, University of Central Florida
Probabilistic Sinkhole Hazard Model of East Central Florida
A number of sinkhole events have emerged at various locations in East Central Florida (ECF) and the consequences of its occurrence would lead to loss of property and human lives. Increasing concerns for the potential risk of sinkholes have raised the necessity of developing a sinkhole hazard map for the region. A sinkhole hazard can be assessed as the probability of occurrence accounting for time, location, and magnitude. The objectives of this study are 1) to develop a methodology of assessing the sinkhole hazard for ECF within a geographic information system (GIS) environment, and 2) to compare and verify sinkhole hazard maps generated by the probabilistic model with existing data. In this study, a quantitative methodology considering three variables (i.e. time, space, and magnitude) is presented to assess the sinkhole hazard in ECF. A standard statistical technique to derive a multivariate model is not appropriate because hazard variables can be interdependent. A Copula-based joint statistical model is used to determine the possible correlation among the components and predict the probability of sinkhole hazard. The probabilistic sinkhole map for ECF would provide useful information on future sinkhole hazard in order for decision makers to develop proper sinkhole mitigation strategies.

Dennis Kriventsov, Courant Institute
A Local-Nonlocal Transmission Problem
I will discuss the solutions to some elliptic equations which change abruptly across a smooth interface. The main equation of interest, motivated by applications to atmospheric dynamics, is local on one side of this interface and nonlocal on the other, and features a critical nonlinear drift term. The major difficulty of the problem stems from a lack of scale invariance caused by the different orders of the different principal terms. While the existence of weak solutions follows from standard methods, the continuity of them across the interface requires a careful investigation of the scale dependence. The main results are a De Giorgi-Nash-Moser type continuity theorem, an in-depth analysis of the nonlocal analogue of the transmission condition satisfied by the frozen-coefficient equation, and a perturbative result for sufficiently smooth interfaces.

Ming-Jun Lai, University of Georgia
Max-Norm Estimate for Bivariate Spline Solutions to Second Order Elliptic Partial Differential Equations in Non-divergence Form
The convergence of the bivariate spline solution to the solution of the second order elliptic PDE in non-divergence form in the maximum norm is presented in this paper. Mainly, the L_∞ norm of the spline projection in the Sobolev space $H_0^2(\Omega) \cap H_0^1(\Omega)$ is shown to be bounded, where Ω is

a polygonal domain. With the boundedness of the projection, one can establish the error of the spline solution to the weak solution in the L_∞ norm. Several remarks are given to explain how to extend the ideas of the proof for other linear elliptic PDEs.

James Lanterman, University of Georgia
Construction of Hermite interpolatory cubic Wachspress functions on rectangles
Generalized barycentric coordinates (GBCs) have seen application recently through the development of polygonal splines. While polygonal splines have some advantages over traditional splines in some situations, one of their biggest drawbacks are their inability to enforce smoothness across adjacent polygons. In this talk we'll detail a construction of smooth functions on rectangles using Wachspress coordinates - specifically, a collection of cubic Wachspress functions. The functions built are locally supported and have properties well-suited to Hermite interpolation.

Ryan Learn, Florida State University
Sensitivity studies of mixing in astrophysical plasmas
Motivated by recent studies of mixing in explosive stellar phenomena, we consider the dependence of mixing due to the Kelvin-Helmholtz instability on the problem dimensionality, Mach number of the flow, and the density and velocity structure near the fluid interface. We use a high-resolution finite-volume approach, and perform a series of simulations in 2D and 3D in Cartesian geometry. We use both Godunov type hydro solvers as well as a set of flux-vector splitting algorithms of the AUSM family. We analyze the growth of the instability as a function of time and assess the performance of various methods for this problem. Preliminary results for the viscous are presented, along with the results of various solvers in the low-Mach number regime. This regime is of particular importance during evolutionary stages leading up to explosions. We find substantial dependence of the evolution and morphology of the Kelvin-Helmholtz instability on the method of numerical flux calculation in the low-Mach number regime, with some of the AUSM family solvers displaying nonphysical oscillations emanating from low-velocity areas of the fluid flow. These oscillations result in a checkerboard-type pattern that eventually overcomes and suppresses the Kelvin-Helmholtz instability. More sophisticated AUSM type solvers do not display such artifacts, and provide good agreement with our Godunov type solvers for the linear evolution phase of the KHI.

Eitan Lees, Florida State University
The Electroneutrality Constraint in Peridynamic Modeling
The conservation of mass in multi-component ionic systems leads to the Nernst-Planck equation. To solve for the concentrations as well as the potential an additional constraint of electroneutrality is introduced. We developed a simple 1D peridynamic model for reaction and diffusion in multicomponent ionic solutions, which describes the classic "liquid junction potential" problem in electrochemistry . When contact is initiated between two electrolytic solutions with different ion compositions via a permeable membrane, an electric field is induced which adjusts transport of the charged species across the membrane until a stable concentration and potential profile is established. We impose electroneutrality using the nonlocal counterparts of the charge conservation and Gauss's law, and discuss their relationship with the condition of strict electroneutrality. We consider the relative merits of two methods, and reflect on their suitability for general problems like corrosion. We show that low levels of concentration lead to numerical instabilities when using charge conservation that do not arise using Gauss's law.

Hongwei Li, Shandong Normal University

Unconditionally energy stable linear schemes for a diffuse interface model with Peng-Robinson equation of state

In this talk, we discuss numerical solution of a diffuse interface model with Peng-Robinson equation of state, that has been widely used to describe the real state of hydrocarbon fluids in the petroleum industry. Due to the strong nonlinearity of the source terms in this model, how to design appropriate time discretizations to preserve the energy dissipation law of the system at the discrete level is a major challenge. Based on the "Invariant Energy Quadratization" approach, we develop a first and a second order time stepping schemes, where the resulted temporal semi-discretizations lead to linear systems with symmetric positive definite spatial operators at each time step, and thus can be efficiently solved. We also rigorously prove the unconditional energy stabilities of both schemes. Various numerical simulations in two and three dimensional spaces are presented to illustrate accuracy and stability of the proposed linear schemes.

Jian Li, Florida State University

Eliminating dental biofilms with the less viscous fluid

Biofilms are gel like groups of microorganism in which bacteria stick to each other through a self-produced matrix of extracellular polymeric substance (EPS). It have been widely shown that a large amount of microbial infections in the body involve biofilm. Dental plaque is one of examples in which is an oral biofilm attaches to the teeth, and consists of many species of both bacteria and fungi. In this paper, we implement a multiphase model to simulate the dynamic of the mixture of water and biofilm during the plaque removing process. The projection method will be applied to numerically solve the model which is a system of partial differential equations.

Shiying Li, Vanderbilt University

Adaptive Algorithms using Splines on Triangulations with Hanging Vertices

Adaptive approximation of functions is tested using polynomial splines on triangulations with hanging vertices and indicates improved efficiency as compared to ordinary triangulations. Algorithms for generating data structures needed for triangulations with hanging vertices are also developed. Adaptive mesh generation algorithms using the finite element method(FEM) for solving a model problem involving a second order elliptic PDE are also discussed. Numerical examples using different a posteriori error indicators are given.

Yun Ling, University of Waterloo

Computationally Efficient Inference for Particle Tracking Data

Passive microparticle rheology techniques give researchers easy access to volumes of particle trajectory data to study their dynamical properties. While key scientific quantities of interest such as mean squared displacement (MSD) can be estimated in a model-free setting, likelihood-based inference via parametric models can increase precision by an order of magnitude or more. However, realistic stochastic models often must include several "nuisance parameters" to account for signals corrupted by drift or measurement error, thus considerably complicating parameter calibration. Moreover, naive computations of the likelihood function scale as $\mathcal{O}(N^3)$ in the number N of observations per trajectory. Here, we show how a statistical technique called Profile Likelihood can effectively eliminate many nuisance parameters from popular particle trajectory models, thus considerably simplifying numerical calibrations. Moreover, we introduce the "SuperGauss" software library, which can reduce computational complexity from $\mathcal{O}(N^3)$ to $\mathcal{O}(N \log^2 N)$. An application is presented to the de-noising of dynamic localization error in subdiffusive particle trajectories.

Xinfeng Liu, University of South Carolina
Multi-scale and stochastic modeling of HER2 signaling for cancer tumor growth
HER2-signaling pathways are often activated with apparently conflicting responses such as apoptosis, proliferation, growth arrest, differentiation, and senescence, depending on the cell type and the duration and strength of the stimulus. NFkB is a family of dimeric transcription factors that regulates cell division, apoptosis and inflammation. In close integration with experiments, we have developed a system of equations based on mass action kinetics to describe the dynamics of HER2 signaling pathway. Our preliminary results through computational exploration reveal that there is a positive feedback from the downstream NFkB to regulate IL1, which correlates nicely with experimental observations.

Yongjin Lu, Virginia State University
Uniform stability to a non-trivial equilibrium of a nonlinear fluid structure interaction subject to viscoelastic damping
We consider uniform stability to a non-trivial equilibrium of a nonlinear fluid-structure interaction, where the interface is assumed to be static. The coupled dynamics is governed by a PDE system coupling Navier-Stokes equation with a wave equation. FSI considered here could model the dynamics of a structure submerged in viscous non-compressible fluid and has wide applications ranging from aerospace engineering, civil engineering, medicine and environmental sciences, etc. Uniform stability to a non-trivial equilibrium of FSI is obtained by implementing a viscoelastic damping on the structure and a fully supported interior feedback on the fluid.

David Mandel, Florida State University
Model Robustness and Sensitivity in Finance
Global sensitivity analysis is a widely used tool for modelers in the physical sciences and engineering; however, it has seen only limited use in financial modeling. I will discuss global sensitivity analysis based on Sobol' sensitivity indices, and through an application to short rate models I will introduce an approach to quantify the robustness of a model using randomized sensitivity indices. Results from weather derivatives pricing will be presented as a further application of model robustness.

Jorge Martinez, Florida State University
Shape Analysis Framework of Nucleosome Positioning
DNA-histone complexes, also known as nucleosomes, occupy each chromosome of a multitude of eukaryotic species. Nucleosome positioning, histone modifications, and general nucleosome make-up are the underlying factors in affecting gene transcription, thus, understanding how nucleosomes are distributed can advance the understanding how genes are expressed can equate to understanding the actual proteins that code for them. Nevertheless, the full comprehension to which nucleosomes are arranged in DNA remains elusive.

To solve the problem, we use the density interpretation of the nucleosome positioning. In the density setting, we propose a new computational approach to capture changes in density shapes between conditions. We test the hypothesis that this change is correlated to differential gene expression between same conditions. The model utilizes the new Square Root Velocity Function Framework for shape analysis.

Matthew McCurdy, Florida State University
Small Darcy Number Asymptotics of the Coupled Navier-Stokes-Darcy System
Fluid flow at the interface of a conduit and porous media can be an area rich in ecological diversity, a region of importance for agriculture, and can be involved in numerous environmental phenomena (sinkholes, karst aquifers, etc.). When coupling fluid flow between a conduit and porous media, obvious choices for governing equations are Navier-Stokes for the free flow and Darcy for the porous medium. To solve the coupled system, three interface conditions are required. Two of the interface conditions are relatively agreed upon; conservation of mass and the Beavers-Joseph-Saffman-Jones conditions are both widely used and accepted by the scientific community. However, there is debate about the third condition concerning whether or not to include a dynamic pressure term for the balance of the normal forces across the interface. We analyze the coupled system and by looking at the small Darcy number asymptotics, we discuss differences in the solutions determined by both choices for the third interface condition.

Joseph McKenna, Florida State University
Glucose oscillations can activate an endogenous oscillator in pancreatic islets
Pancreatic islets manage elevations in blood glucose level by secreting insulin into the bloodstream in a pulsatile manner. Pulsatile insulin secretion is governed by islet oscillations such as bursting electrical activity and periodic calcium entry in beta-cells. In this talk, we demonstrate that although islet oscillations are lost by fixing a glucose stimulus at a high concentration, they may be recovered by subsequently converting the glucose stimulus to a sinusoidal wave. We predict with mathematical modeling that the sinusoidal glucose signal's ability to recover islet oscillations depends on its amplitude and period, and we confirm our predictions by conducting experiments with islets using a microfluidics platform. Our results suggest a mechanism whereby oscillatory blood glucose levels recruit non-oscillating islets to enhance pulsatile insulin output from the pancreas. Our results also provide support for the main hypothesis of the Dual Oscillator Model, that a glycolytic oscillator endogenous to islet beta-cells drives pulsatile insulin secretion.

Andrew McMillan, Florida State University
A Pseudo-Spectral Method Approach to the Differentially Heated Rotating Annulus
The differentially heated rotating annulus is a benchmark problem in atmospheric modeling. With the outer layer of the annulus heated and with a cooler core, the annulus models the differential heating that occurs between the Earth's equator and the respective poles. It is widely accepted that the observed, experimental flows are representative of the large-scale flows that are seen in the Earth's atmosphere. There are a number of observable flow transitions for differing rotation values, but this investigation is centered on the chaotic instability that occurs once the annulus is rotated and reaches some critical rotation speed. For very low rotation speeds, the annulus undergoes a concentric heating pattern, but once the rotation speed eclipses some critical value, the instability takes on an undetermined sinusoidal pattern. Then, for a second critical rotation speed, the sinusoidal pattern transitions into chaos. The current investigation takes a numerical approach by

analyzing a coupled Navier-Stokes system and assuming a Lagrange polynomial expansion. Then, coupling the Pseudo-Spectral Method with a new resampling method, the hope is to solve the resulting eigenvalue and eigenvector problem more efficiently. This proposed work will ultimately serve as the initial conditions for the dynamical case.

Clay Mersmann, University of Georgia
Spline Solutions of the Maxwell Equations
The Maxwell equations are a system of first-order PDEs that describe all classical electromagnetic phenomena. We review common formulations of these equations for numerical study, and present a simple potential formulation for our spline analysis. In contrast with common finite element schemes, our spline solutions have an arbitrary degree of global smoothness; thus, we can obtain an accurate approximation of the electric and magnetic field quantities in question.

We conclude with some preliminary numerical results, including a computation of the electric field arising from a shielded microstrip.

David Miller, Florida State University
Bugs on a Surface
The bugs on a square problem considers N ordered bugs in a plane that continuously move in the direction of their neighbor. We extend this classic problem to N bugs on closed curves and surfaces. This extension makes it possible for bugs to not collapse to a point, but instead they can form a closed rotating loop. We show how the dynamics depend on both the geometry, the number of bugs, and the bugs initial condition.

Evan Milliken, University of Florida
Probability of Extinction in Metapopulation Models of Infectious Salmon Anemia virus
Infectious Salmon Anemia virus (ISAv) causes Infectious Salmon Anemia in a variety of finfish including Atlantic salmon (L. Salmo salar). This disease has impacted most salmon producing countries and has had a devastating effect on the salmon culture industry. In previous work, deterministic models of an ISAv infectious were proposed and studied. Analysis indicated that whenever the basic reproduction number was above the threshold value of 1, the disease would invade and persist if introduced in small numbers. However, in small numbers, individuals in infectious classes are subject to random fluctuations not captured by deterministic models. Markov chain models are proposed that capture these fluctuations, but the complexity of these systems makes analysis difficult. Multitype branching process models are proposed to approximate the probability of extinction of the Markov chain models. Strengths and weaknesses of these approximations are discussed.

Mahsa Mirzargar, University of Miami
On Evaluation of Ensemble Forecasts Calibration Using the Concept of Data Depth
Various generalizations of the univariate rank histogram have been proposed to inspect the reliability of an ensemble forecast or analysis in multidimensional spaces. Multivariate rank histograms provide insightful information about the misspecification of genuinely multivariate features such as the correlation between various variables in a multivariate ensemble. However, the interpretation of patterns in a multivariate rank histogram should be handled with care. The purpose of this paper is to focus on multivariate rank histograms designed based on the concept of data depth and

outline some important considerations that should be accounted for when using such multivariate rank histograms. In order to generate correct multivariate rank histograms using the concept of data depth, the datatype of the ensemble should be taken into account to define a proper pre-ranking function. We demonstrate how and why some pre-ranking functions might not be suitable for multivariate or vector-valued ensembles and propose pre-ranking functions based on the concept of simplicial depth that are applicable to both multivariate points and vector-valued ensembles. In addition, there exists an inherent identifiability issue associated with center-outward pre-ranking functions used to generate multivariate rank histograms. This problem can be alleviated by complementing the multivariate rank histogram with other well-known multivariate statistical inference tools based on rank statistics such as the depth-versus-depth (DD) plot. Using a synthetic example, we show that the DD-plot is less sensitive to sample size compared to multivariate rank histograms.

Hadi Mohammadigoushki, Florida State University
Flow of wormlike micelles past a falling sphere
Flow of a wormlike micellar solution past a falling sphere is considered. A combination of particle tracking, particle image velocimetry and microscopy is used to obtain detailed information on the flow of wormlike micelles around the falling sphere. Beyond a critical threshold, a sphere never reaches a terminal velocity and instead exhibits oscillatory motion in the axial direction. By systematically varying sphere density, sphere size, temperature, and concentration of surfactant and salt over a wide range of inertia and elasticity, we propose a suitable criterion to separate different modes of sphere motion. We also show that the spheres with roughened surfaces fall faster than smooth spheres. In the direction perpendicular to the sphere motion, there is no difference between the velocity of the fluid for smooth and roughened spheres. However, in the axial direction and in the wake of the sphere, roughened spheres tend to generate a larger negative wake. More importantly and in contrast to the smooth spheres, we find that the surface of the roughened spheres is covered by numerous micro-bubbles. The presence of such micro-bubbles may potentially reduce the drag at the surface of roughened spheres and eventually lead to higher falling velocities.

Raymond Morie, Florida State University
Modeling Cortical Folding Patterns on a Growing Oblate Spheroid Domain
Many of the mechanisms involved in brain development are not definitively understood. This includes the mechanism by which the folds of the cerebral cortex, called gyri and sulci, are formed. This research adopts the Intermediate Progenitor Model, which emphasizes genetic chemical factor control. This model is based on a hypothesis that activation of radial glial cells produces intermediate progenitor cells that in turn correspond to gyral wall formation. In previous work, Toole and Hurdal (Computers and Mathematics with Applications, 66:16271642, 2013) developed two biomathematical models that use a Turing reaction-diffusion system on a prolate spheroid domain. These models examined the effect that different domain growth functions had on cortical folding pattern formation. In this research, we modify those models to utilize an oblate spheroid domain. By analyzing the role of various parameters, we seek to use this modified domain to model diseases such as holoprosencephaly and ventriculomegaly, which alter the shape of the lateral ventricle.

James Moseley, West Virginia University
The Agglomeration Model: The Fixed Problem II
Agglomeration of particles in a fluid environment is an integral part of many industrial processes

and has been the subject of scientific investigation. One model of the fundamental mathematical problem of determining the number of particles of each particle-size as a function of time for a system of particles that may agglutinate during two particle collisions uses the coagulation or Smoluchowskis equation. With initial conditions, it is called the Discrete Agglomeration Model. Several problems have been associated with this model allowing progress to proceed separately. To facilitate this progress, in this paper we develop and solve the Fixed Agglomeration Problem and establish the Fundamental Agglomeration Problem for all cases of the autonomous quadratic kernel.

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

Lin Mu, Oak Ridge National Laboratory
DG-IMEX Stochastic Galerkin schemes for Linear Transport Equation with Random Inputs and Diffusive Scalings
We consider the linear transport equation under diffusive scaling and with random inputs. The method is based on the generalized polynomial chaos (gPC) approach in the stochastic Galerkin (SG) framework. Several theoretical aspects will be addressed. A uniform numerical stability with respect to the Knudsen number , and a uniform in error estimate is given. For temporal and spatial discretizations, we apply the implicit-explicit (IMEX) scheme under the micro-macro decomposition framework and the discontinuous Galerkin (DG) method. We provide a rigorous proof of the stochastic asymptotic-preserving (sAP) property. Extensive numerical experiments that validate the accuracy and sAP of the method are conducted.

Andrew Nevai, University of Central Florida
Feral cat population dynamics
Feral cat populations cause ecological destruction and spread many diseases in places that people live. Here, we describe a mathematical model for their population dynamics. The gender-based model includes kittens, adult females and adult males. A net reproduction number R_0 distinguishes between population extinction ($R_0 < 1$) and population persistence ($R_0 > 1$). This is joint work with J. Sharpe (UCF).

Jay Newby, University of North Carolina, Chapel Hill
Pixels to predictions: a unified framework for mechanistic modeling and image analysis of particle motion in micron scale environments
Particle tracking of microscopic species is widely employed to infer biophysical transport properties and to validate prospective species transport models. “Particles” include viruses, bacteria, bacteriophages, passive or active microbead probes, and drug carrier nanoparticles. The major bottlenecks in application of predictive mathematical models to micron-scale living systems are low data throughput (manual conversion of videos to an ensemble of position time series) and the

inability of 2D particle tracking to capture rapidly diffusing, low SNR species for sufficiently long duration. I will present a new deep learning algorithm that automates the conversion of 2D and 3D raw videos and makes feasible, for the first time, 3D particle tracking of sub-micron species at low SNR, for which 2D particle tracking has been futile. The artificial neural network enables sufficient data for Bayesian model selection and parameter estimation of these important transport processes. I will discuss two ongoing collaborations that illustrate the application of automated particle tracking: (1) flagellar-mediated active motion of Salmonella in visco-elastic biogels; and (2) intracellular visco-elastic micro domains in multinucleate fungal cells.

Calistus Ngonghala, University of Florida
Understanding poverty dynamics from an epidemiological perspective
The rural poor rely heavily on their immediate natural environment for subsistence and suffer high morbidity and mortality due to infectious diseases. We develop and use coupled epidemiological-economic models to show how interactions between epidemiological processes and economics can create reinforcing feedbacks associated with poverty traps, characterized by a stable, low level, equilibrium; or multiple stable equilibria in epidemiological-economic space. These models are calibrated from country-level data and analyzed over the feasible parameter space to explore qualitative and quantitative properties of different regimes of economic development and human health. All the models exhibit three possible regimes corresponding respectively to a globally stable wealthy/healthy equilibrium, a globally stable poverty equilibrium, or bistability. Our analysis indicates that bistability emerges as a common property of generalized disease-economic systems for about a fifth of the feasible parameter space and that the overall proportion of parameter space leading to poverty is larger than that resulting in wealthy/healthy development. Global sensitivity analyses show that epidemiological parameters in the form of disease transmission and recovery rates are the most consistently important determinants of long-term wealth and health dynamics. Combined, these models provide a general framework for deeper theoretical and empirical explorations of the effects of health care on cycles of poverty and disease.

Nguyet Nguyen, Youngstown State University
Hidden Markov Model for Stock Trading
Hidden Markov model (HMM) is a signal prediction model, assuming a given number of hidden states that govern the Markov chain of observations. While HMM has been used to predict economic regimes and stock prices, we propose to use HMM for predicting the monthly prices of the S&P 500 (and other stocks as well) and then trading the index. First, we use four criteria, including the Akaike information, the Bayesian information, the Hannan-Quinn information, and the Bozdogan Consistent Akaike Information to evaluate the HMMs with two, three, and four hidden states. Of them, the four-state HMM is determined to be the best. We then use this optimal HMM to predict monthly close prices of S&P 500. We use the out-of-sample R-square, the utility gain, and some other error estimators to test the HMM predictions against the simple average model, the exponential average model, and the historical average model. Finally, we use the predicted prices to trade S&P 500, showing that HMM outperforms the competitive models in predicting and trading stocks.

H. Reed Ogrosky, Virginia Commonwealth University
Modeling and identification of planetary-scale rainfall events in the tropical atmosphere
Rainfall and clouds, i.e. convection, in the tropics occur on many temporal and spatial scales.

Increasing our understanding of tropical convection is essential due both to its large economic and societal impacts in the tropics as well as its close connections to events in the midlatitudes and beyond. In this talk I will discuss some recent work on modeling two planetary-scale patterns of convection seen in the tropics: the Madden-Julian oscillation (MJO) and the Walker circulation. Particular attention will be given to the challenges in using observational data to develop estimates of the forcing functions used in each model. It will be shown that the model results agree remarkably well with observed events and accurately capture typical event lifetime, propagation characteristics, frequency, intermittency, and strength. This agreement is found using a data analysis technique based on solutions to the shallow water equations frequently used in studying the tropical atmosphere. Additional applications of the data analysis method will also be discussed, including identifying the MJO in observational data.

Ashish Pathak, University of Massachusetts Dartmouth
A fully Eulerian fictitious domain method to study interaction between moving structures and two-phase fluid flows
A fully Eulerian method is developed to study two-way interaction between moving structures and two-phase fluid flows. To resolve three phases in an Eulerian mesh, a novel minimization based scheme is proposed. This scheme uses volume-of-fluid (VOF) information available in the neighborhood of a three-phase cell to construct an error function, which is minimized in order to obtain the interface orientation. A 3D geometric toolbox based on convex polyhedrons, developed in this study, provides the building blocks to the proposed three-phase reconstruction scheme. The toolbox is further employed to compute the volume fluxes of individual phases out of a three-phase cell. Canonical problems were used to test the accuracy of the reconstruction method.

The three-phase reconstruction scheme and 3D geometric toolbox were integrated into a Navier-Stokes solver to develop a fully Eulerian fictitious domain method. Here, the structure and the two fluids are represented by two VOF scalars. Special schemes were used to ensure numerical stability, enabling the solver to handle arbitrarily high density, and avoiding artificial interfacial deformation. A multigrid preconditioned conjugate gradient method was developed to accelerate the Poisson equation solution, which is characterized by high condition number in high density ratio flows. The FSI method was used to study problems involving free-surface piercing structures. Benchmark problems were employed to validate the proposed FSI algorithm.

Chaoxu Pei, Florida State University
A hierarchical block structured space-time spectral element method for incompressible flows
A new hierarchical space-time spectral element method has been developed for simulating incompressible flows. The novel hierarchical adaptive mesh strategy is to prescribe the highest order spectral elements on the coarse adaptive levels, and progressively reduce the order by a factor of two on finer levels. On the hierarchical adaptive spectral element grid, a novel multigrid preconditioned BiCGSTAB algorithm is developed for the variable density projection equation. In the smooth regions, the grid is not adapted and the solution is obtained in the highest order spectral elements, while in the non-smooth parts, the grid is adapted as detected by an indicator function and the order is progressively reduced by a factor of two. We report the performance of the present method on the thin shear layer problem which was also tested by Brown and Minion. (Performance of under-resolved two- dimensional incompressible flow simulations.)

Sirani M. Perera, Embry-Riddle Aeronautical University
Self Recursive Radix-2 Fast DCT Algorithms
Fast Fourier Transform (FFT) can be seen in a quite diverse field in applied mathematics and electrical engineering. The FFT is used compute Discrete Fourier Transform (DFT) and its inverse efficiently. The Discrete Cosine Transform (DCT) is the real versions of DFT. DCT and Inverse DCT (IDCT) have been popular in recent decades due to their applications in image compression, digital video technology, and high efficiency video coding.

In this talk, we will observe a hybrid of polynomial arithmetic and matrix factorization techniques to factor DCT matrices having self-contained, sparse, and scaled orthogonal matrices. Once the factorization is established we analyze the arithmetic complexity and elaborate numerical results. The presented DCT and IDCT algorithms attain the lowest multiplication complexity for the transform matrix sizes $n \geq 8$. Furthermore, the language of signal flow graph representation of digital structures is used to describe these DCT algorithms. Finally, image compression results are presented based on these algorithms.

Adam Perez, University of Central Florida
Study of Florida's sinkhole mechanism by a physical hydrogeological model
Florida is underlain with soluble bedrock composed of limestone and dolomite. Over geological time this soluble bedrock goes through a geomorphic process to produce what is known as karst terrain. Sinkholes are a feature of all kart terrain and are produced by the process of the overburden eroding down into conduits formed within the soluble bedrock. In Florida the two types of sinkholes which pose a hazard are the cover-subsidence and cover-collapse. A relationship of the susceptibility to sinkhole formation in Florida has been linked to hydrogeological and geotechnical conditions. In this study, a physical simulation of cover-subsidence and cover-collapse sinkholes was conducted and behaviors of groundwater and soils were monitored during the entire sinkhole simulation. A physical model incorporating both an unconfined and confined aquifer with constant head controls and water level sensors was constructed to investigate the hydrogeological parameters involved in sinkhole formation, which includes head difference between the aquifers and the overburden composition and thickness. Characteristics of the cover-subsidence and cover-collapse mechanisms and their qualitative relationship to shear strength of the overburden were established in this study.

Giorgi Pertaia, University of Florida
Fitting normal mixtures with tail constraints
Normal mixtures models are used in financial applications dealing with heavy tail distributions. We have suggested a new CVaR distance between distributions. The CVaR distance is a convex function w.r.t. weights. Weights of normal mixture are found by minimizing CVaR distance between the mixture and the target distribution. We suggested convex constraints on the weights assuring that tail of mixture is as fat as the original distribution. We have conducted a case study demonstrating efficiency of the suggested approach.

Maria Poole, Florida State University
Modeling HCV Interactions with p53 in Hepatocytes: Implications for Carcinogenesis
Infection with Hepatitis C virus (HCV) has reached epidemic proportions; it is one of the least

tested for, but often one of the most dangerous silent killers among American men. Individuals with chronic HCV infection, without access to treatment, are at high risk for developing Hepatocellular Carcinoma (HCC), a liver cancer that is rapidly fatal after diagnosis. The unnerving part about this cancer is that because it can escape immune defenses, patients can be living with this virus for more than 30 years without any symptoms; the subsequent development of liver cancer goes unnoticed for years. The overarching goal in my research is to understand how that happens.

There is strong experimental evidence that shows virus protein can directly interact with the p53 pathway, thereby modulating its action by preventing p53 from mediating cell death and contributing to carcinogenesis. Once p53 is mutated by the virus protein, the infected individual has a higher chance of developing cancer. Unfortunately, the mechanism of interaction between p53 and the virus protein remains to be elucidated. That is why a mathematical model of the virus/cancer progression is needed. I will use biochemically-motivated mathematical modeling to describe p53 regulation within the cell and its interactions with the HCV virus core protein. Specifically, I will be using mass action kinetics to translate (proposed and known) chemical reactions within the infected hepatocyte which will result in a system of coupled non-linear ordinary differential equations (ODEs). Experimental data obtained from an exhaustive literature survey will be used to estimate the various parameters involved. My strategy will be a combination of simulation and analysis to study properties of the solutions of the dynamical system. The model will also be based on previously published models of p53 regulation; but it will include virus core protein-p53 interactions, which has not been done before. The goal of this research is to use mathematical modeling to understand the p53 interaction with infected hepatocytes and the eventual development of cancer.

Elbridge Gerry Puckett, University of California, Davis
A Study of Interface Tracking and Capturing Algorithms for Computing A Fundamental Instability in the Earth's Mantle
Seismic imaging of the mantle has revealed large and small scale heterogeneities in the lower mantle; specifically structures known as Large Low Shear Velocity Provinces (LLSVP) below Africa and the South Pacific. Most interpretations propose that the heterogeneities are compositional in nature, differing in composition from the overlying mantle, an interpretation that is consistent with chemical geodynamic models. The LLSVPs are thought to be very old, meaning they have persisted throughout much of Earth's history. Numerical modeling of persistent compositional interfaces presents challenges, even to state-of-the-art numerical methodology, since even basic models of LLSVPs involve modeling both the RayleighBnard instability balanced against an instability at the compositional interface. There are two non-dimensional parameters in this problem, the Rayleigh number Ra and the Buoyancy number B. I will describe a study of four alternative algorithms for computing solutions of a basic model of LLSVPs: an interface tracking method and three interface capturing methods. All of these algorithms have been implemented in the open source Finite Element Code ASPECT, which is designed to model convection in the Earth's mantle. Our computational results span the entire range of possible regimes: from pure thermal convection with no chemical buoyancy at B = 0, to small chemical buoyancy in which the latter flow is maintained but with organized kinematic mixing of the compositions at $B = 0.1$ and 0.2, to unsteady flows that greatly enhance the kinematic mixing at $B = 0.3$ and 0.4, to a regime in which the compositional buoyancy does not prevent a significant vertical displacement of the compositional boundary but there is relatively little mixing between the compositional layers and

the structure resembles that of LLSVPs at $B = 0.5$ and 0.6, to a chemical stabilizing buoyancy that is sufficiently strong to block vertical flows between the upper and lower layers at $B = 0.7$ to 1.0.

Edward Qian, PanAgora
The Triumph of Mediocrity: A Case Study of "Naïve Beta"
In contrast to factor-based "smart beta", diversification-based "smart beta" assumes that, seemingly "naively", all investments are just average or the same in some dimension. The four possible dimensions: portfolio weight, expected return, risk-adjusted return, and risk contribution, lead to four "nave beta" portfolios respectively: equal-weight, minimum variance, maximum diversification, and risk parity portfolios. In this paper, we show how these four portfolios outperform the capitalization-weighted S&P 500 index due to their sector differences and especially, the index's aggressive shifts into specific sectors. Among the three "naïve beta" portfolios that use risk inputs as part of their portfolio construction, both minimum variance and maximum diversification portfolios tend to be highly concentrated in certain sectors. We develop an analytic framework based on a partitioned correlation matrix, modeling sectors as two groups (mostly defensive versus cyclical). The results shed light on material differences between the risk parity and optimized portfolios in their level of diversification across the sector and stock dimensions. Empirical examples of sector and stock portfolios within the universe of the S&P 500 index show the triumph of "naïve beta" over the index, which suffers from strong sector biases and ill-timed allocation shifts.

Zihua Qiu, Northwestern Polytechnical University
A sliding-mesh interface approach to spectral difference method on unstructured grids for simulating vortex-induced vibrations
We report our recent development of a 2D solver of compressible Navier-Stokes equations by using the high-order spectral difference (SD) method using flux interpolating functions in Raviart-Thomas spaces(SD-RT).

Our SDRT method is designed for unstructured grids with a mixture of triangular and quadrilateral elements. Furthermore, we implement a non-uniform sliding-mesh approach based on this 2D SDRT solver. Our sliding method creates straight non-uniform dynamic mortars on sliding-mesh interfaces to couple a translating and deforming domain with a stationary domain. To verify the spatial order of accuracy of the non-uniform sliding-mesh SDRT method, both inviscid and viscous flow cases are tested. We are able to demonstrate that the sliding-mesh method preserves the high-order accuracy of the SDRT method. This sliding-mesh SDRT method is being applied to simulate vortex induced vibration(VIV) problems.

Bryan Quaife, Florida State University
Eroding bodies in a Stokesian fluid
Erosion of solid material by flowing fluids plays an important role in shaping many objects in nature. For example, erosion of a porous media can be be used to describe groundwater flow. I will describe a high-order and fast method that couples a boundary integral equation method with erosion equations to simulate the erosion of multiple bodies in a Stokesian fluid.

Petronela Radu, University of Nebraska-Lincoln
Properties and convergence analysis for state-based Laplacians

Inspired by the state-based theory of peridynamics we introduce a new nonlocal version of the Laplacian, labeled a state-based Laplacian. We study properties of this double integral operator and show its connections with the single-integral nonlocal Laplacian and with the classical Laplacian. We also derive rates of convergence with respect to the radius of the interaction horizon for each of the two kernels of the operator.

Pablo Raúl Stinga, Iowa State University

How to approximate the fractional Laplacian by fractional powers of the discrete Laplacian

We use the solution to the semidiscrete heat equation in combination with the language of semigroups to define and obtain the pointwise formula for the fractional powers of the discrete Laplacian on a mesh of size $h > 0$. It is shown that solutions to the continuous fractional Poisson equation $(-\Delta)^s U = F$ can be approximated by solutions to the fractional discrete Dirichlet problem $(-\Delta_h)^s u = f$ in B_R, $u = 0$ in B_R^c. We obtain error estimates in the strongest possible norm, namely, the L^∞ norm, under minimal natural Hölder regularity assumptions. Key ingredients for the analysis are the regularity estimates for the fractional discrete Laplacian, which are of independent interest. The results presented are joint work with Ó. Ciaurri and J. L. Varona (Universidad de La Rioja, Spain), L. Roncal (BCAM, Spain) and J. L. Torrea (Universidad Autnoma de Madrid, Spain).

David Robinson, Florida State University

A Simple Empirical Fire Line Model

Wildfires are complex multi-scale systems and accurate simulations that capture observed behavior require large amounts of computational time. We propose a new method that represents the fire front as a closed curve with a normal velocity that is related to the heat flux and advective terms. By representing the closed curve with spectral methods and using a well-developed method for maintaining an equidistributed mesh, a large number of time steps can be taken. The goal is to capture fire line behaviors that have been observed in other models and experiments, but with a much smaller computational cost. The talk will consist of an overview of the model, preliminary results, and the fire line traits the model should be capable of replicating.

Kelvin Rozier, Georgia State University

Modeling the Physiological Effects of β2-adrenoceptors in Mouse Ventricular Myocytes

The β1- and β2-adrenergic receptors play a significant role in cardiac cell function. Upon stimulation with an agonist, the effects of β1-adrenoceptors are, in general, stronger than those of β2-adrenoceptors in multiple species. In mice, under normal (control) conditions, the effects of β2-adrenergic receptors are negligible. However, in some specific physiological states, the effects of β2-adrenoceptors can be revealed. To find the physiological conditions under which β2-adrenoceptors play important roles, we developed a mathematical model that includes both β1- and β2-adrenergic signaling systems. The model describes biochemical reactions that govern the signaling systems, how the target proteins (ion channels, ion transporters, and contractile proteins) are modulated upon stimulation of both β1- and β2-adrenergic receptors, separate stimulation of β1-adrenergic receptors and separate stimulation of β1-adrenergic receptors. We found from simulations that the application of agonist isoproterenol does not cause notable effects upon separate stimulation of β2-adrenergic receptors. The effects of β2-adrenoceptors are revealed with an additional inhibition of inhibitory G protein Gi or upon inhibition of phosphodiesterases of type 3 and 4.

Jeremy Sauer, National Center for Atmospheric Research

Numerical Investigations into the Influence of Atmospheric, Topographic, and Fuel Aggregation Conditions on Fire Behavior

Influencing factors in wildland fire behavior include atmospheric flow conditions, complex topography, and numerous aspects of fuels such as spatial distribution and species or lifecycle properties. With the continued development of large-eddy simulation (LES), and coupled physics based fire behavior models, the simulation and analysis of fire fronts and fire behavior are contributing to new understanding. This knowledge helps fire mitigation personnel and policy makers by asking increasingly sophisticated questions about what influences fire behavior. When is fire beneficial or healthy for local ecology? What factors increase danger to lives and property? What strategies are effective in achieving desirable outcomes with respect to fire events. This talk presents a high-level overview of several efforts wherein LES and physics-based fire behavior models aimed to target real world complexity in the numerical investigations of fire behavior.

Patrick Schambach, Kennesaw State University

Mathematical Analysis of Tumor Growth Models Combining Chemotherapy and Immunotherapy

Ordinary differential equations have been already used to generate numerous mathematical models of tumor growth. Usually several specific populations are used to model the spread of cancer cells. The purpose of our study is to examine two cancer treatment methods, chemotherapy and immunotherapy, with the goal of optimizing treatment methods.

Michael Schneier, Florida State University

Reduced Basis Methods and Their Application to Ensemble Methods for the Navier Stokes Equations

The definition of partial differential equation (PDE) models usually involves a set of parameters whose values may vary over a wide range. The solution of even a single set of parameter values may be quite expensive. In many cases, e.g., optimization, control, uncertainty quantification, and other settings, solutions are needed for many sets of parameter values. We consider the case of the time-dependent Navier-Stokes equations for which a recently developed ensemble-based method allows for the efficient determination of the multiple solutions corresponding to many parameter sets. The method uses the average of the multiple solutions at any time step to define a linear set of equations that determines the solutions at the next time step. To significantly further reduce the costs of determining multiple solutions of the Navier-Stokes equations, we incorporate a proper orthogonal decomposition (POD) reduced-order model into the ensemble-based method.

Richard Schugart, Western Kentucky University

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 time-course 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.

Ian Seim, University of North Carolina
Uncovering signals in bronchoalveolar lavages from patients with cystic fibrosis
As part of the AREST project, we study bronchoalveolar lavages from patients with cystic fibrosis as well as from those suffering unrelated, acute lung problems in an attempt to characterize unique rheological properties of lung mucus in pediatric and adult patients with cystic fibrosis. As a result of the procedure, these samples are diluted to highly varying degrees by a buffer solution, which presents a challenge in identifying the most clinically relevant portions of the samples. Due to low volume limitations and the need to characterize heterogeneity, we probe these samples using microbead rheology. Using maximum likelihood estimation with advection-diffusion models, we characterize each particle path with a pair of rheological parameters, creating a two-dimensional distribution for each sample that reflects the varying degrees of heterogeneity due to dilution and the nature of lung mucus and cystic fibrosis itself. It is necessary to extract the most clinically relevant portions of these distributions to effectively compare groups of patients and understand disease progression. Using principal components, we define several regions of interest and calculate proportions of samples that fall outside of them, corresponding to domains in our parameter space most closely aligned with pathological mucus. Among the four patient groups studied, we find a strong statistical difference between the two adult groups, and a weaker but significant difference between the pediatric groups.

Pablo Seleson, Oak Ridge National Laboratory
Anisotropic bond-based peridynamic models
The peridynamics theory of solid mechanics is a nonlocal reformulation of classical continuum mechanics, suitable for material failure and damage simulation. Originally, this nonlocal theory was presented as the bond-based peridynamic theory, for which the material response of an isotropic medium is limited by a fixed Poisson's ratio. To overcome this limitation, the state-based peridynamics theory was developed. Applications in peridynamics to date cover a wide range of scientific and engineering problems; however, the majority of those applications employ isotropic material models. Only recently, a limited number of anisotropic peridynamic models were proposed. In this talk, we will first survey the different classes of anisotropic material models in classical linear elasticity, and we will present general anisotropic bond-based peridynamic models. We will show a classification and a hierarchy of those models, and we will discuss their relation to classical elastic models as well as their modeling restrictions.

Kyle Shaw, Florida State University
Accounting for alignment and sequence quality in likelihood calculations

Population genetics analyses depend on the variable sites in the data-set. Modern sequencing methods are not perfect and include sequencing errors. Commonly, sequences are reported with quality scores. Often, these quality scores are discarded by analysis methods for population genetics models. We developed a method that can take aligned data and these quality scores as input. These quality scores inform the likelihood calculation of the sequence uncertainty. We also use the Poisson-Indel process to take into account gaps in the alignment. Taking into account sequencing quality scores and alignment uncertainties improve the inference of population model parameters.

Kourosh Shoele, Florida State University
Flow-induced vibration of piezoelectric membrane energy harvester
We report numerical studies on energy harvesting by self-sustained oscillations (flutter) of flexible piezoelectric membranes. Immersed boundary technique with explicit description of fluid, solid and electric systems as well as their coupling is developed to investigate the electrical energy harvesting efficiency of the piezoelectric structures. Our results show that an inverted configuration of the piezoelectric membrane with the fixed trailing-edge and free leading-edge can amplify the flag deflection over a wide range of wind speeds where there is lock-on between the flag flutter and the intrinsic wake shedding phenomenon. The state with large, symmetric flutter is identified as being most promising for energy harvesting, occurs when there is a match between the timescales of flutter and the intrinsic time-scale of the piezoelectric circuit. The simulations are used to examine a simple scaling law that could be used to predict the energy harvesting performance of such devices. Three dimensional effects are explored and the relation between the aspect ratio of the flag and the level of electrical power generation by the piezoelectric system is examined. Finally, the numerical predictions are tested with a series of experiments at a tabletop wind tunnel where high-speed videography confirms good agreement between numerical simulations and experimental observations.

Chad Sockwell, Florida State University
A Novel Normal Inclusion Modeling Strategy for Vortex Pinning in Two-Band, High-Temperature Superconductors
New high-temperature superconductors give great promise to a new generation of superconducting electronics, free of electrical resistance, which is made feasible by higher critical temperature values. Modeling and simulating a process known as vortex pinning is crucial in preserving the resistance free properties of these materials. Unfortunately, many of these materials are what is known as two-band superconductors making the conventional modeling strategy for vortex pinning unsuitable. In this paper, a novel strategy to model vortex pinning in two-band superconductors is presented and simulations of the material magnesium diboride are shown to validate this strategy

Chad Sockwell, Florida State University
Conservative Properties and Performance of Exponential Integrators for Nonlinear Conservation Laws
Current Climate models use explicit schemes in time over implicit schemes. This provides a reduction in computational cost but severely restricts the size of the time step that can be taken in a simulation. Recently, exponential integrators have been developed that provide explicit-type schemes, while relaxing time step restrictions. This is an attractive property for climate modeling simulations that must simulate to a time horizon of the order of millennia, while being restricted

to time steps of the order of minutes to hours. This problem is further complicated by the fact that the time step size restriction is dependent on the spatial resolution as well. As the simulation grid is made finer, to resolve smaller effects, the allowable time step size becomes even smaller. Exponential integrators provide an explicit-type scheme while avoiding the time step size restriction. Although it seems clear that exponential integrators provide an advantage over explicit methods, the conservation properties of the exponential integrators are still not clear. In this work, we aim to show through analysis and computations that a family of exponential integrators possess conservation properties when applied to non-linear conservation laws and the shallow water equations

Xiaoyu Song, University of Florida

Computational modeling of multi-physical processes in unsaturated porous geological materials

Geological materials are porous media that have a spatially varying internal pore structure. Computational modeling plays an increasingly important role in studying the multi-physical processes in porous geological materials. In this talk, we first discuss the essential components of unsaturated soil mechanics - the effective stress concept and soil-water characteristic curve, and the challenges and engineering applications of computational modeling of unsaturated fluid flow and deformation in geological materials. Secondly, we present the continuous porous media theory and its mathematical formulation and numerical implementation via the mixed finite element method. Thirdly, we present a recent study on strain localization and progressive failures in a solid-water-air system via stabilized lower-order mixed finite elements as well as its implications in geotechnical and geoenvironmental engineering practice. We highlight the challenges of computational modeling of failures triggered by coupled hydro-mechanical processes in unsaturated soils. We also discuss the need to formulate and implement non-local multi-physical models in the effort to understand the fundamental triggering mechanism of geohazards (sinkholes triggered by fluctuations of groundwater table, levee erosion, etc.)

Inmaculada Sorribes, Florida State University

Overcoming Chemotherapy Resistance in Glioblastoma Multiforme

Glioblastoma is by far the most common and most malignant of glial tumors. With standard treatment, the median survival of adults diagnosed with high-grade gliomas is only 12 14.6 months.

The advancements in treatments have been minimal in the last 20 years, and even the current treatments, such as chemotherapy, are not effective due to resistance. Chemotherapy resistance depends on multiple cell repair mechanisms which are controlled by specific enzymes. The hypothesis is that the inhibition of such enzymes will enhance chemotherapy repair.

To test our hypothesis I will present a sub-cellular model of chemotherapy repair, which will be included into an age-structured population model. The model will be completed with TMZ pharmacokinetics and pharmacodynamics.

Jacob Spainhour, Florida State University

Computational Geometry in Public Policy

Every ten years, the current members of state legislatures undergo a process of redistricting, in which congressional districts are drawn to accurately reflect changing demographics. However, this process has become entangled with partisan politics, leading to divisions that intentionally leave entire populations unrepresented. Where these politicians are prone to manipulating the system in their favor, a computer will be objective in providing an accurate representation. This project involves the creation of software to perform this task of dividing a given state into areas with regular shapes and similar populations. The program is written in Python code, and uses an algorithm based on the mathematical concept of a centroidal Voronoi tessellation (CVT). In general, this process repeats essentially two steps. Random generator points are created, each being used to create a subsection containing every point closer to it than any other generator. The centers of these subsections are computed, which then become generators for the next iteration. This process is repeated many times, and results in an ideal subsection distribution. This process is adapted for districting purposes by accounting for varied population densities, allowing the districts to also have similar populations after several iterations. The code itself is both portable and malleable, allowing it to be adapted to other situations involving a CVT.

Mark Sussman, Florida State University
A finite volume moment of fluid method for approximating solutions to the diffusion equation for systems consisting of many (> 2) materials
A new finite volume numerical method will be presented for approximating solutions to the diffusion equation. The diffusion coefficient is allowed to be piecewise continuous in which jumps can occur between different material regions. The material regions are delineated by the piecewise continuous multimaterial moment of fluid (MOF) reconstructed interface.

The motivation for our new method is in being able to numerically simulate flows that occur in phase change and materials processing applications. The moment of fluid reconstruction enables the accurate reconstruction of any number of materials in a computational cell. Furthermore, as illustrated in a recent article by Jemison, Sussman, and Shashkov, one can introduce "twin" materials in order to capture thin filamentary regions. The features of the MOF method together with our new finite volume method will allow one to efficiently simulate diffusion processes even when thin thermal layers, or thin material regions exist.

Liang-Hsuan Tai, Florida State University
Trend and seasonal effect estimation under random time warpings
The problem of estimating trend and seasonal effect using time-series data has been studied over the past fifty years, albeit using a single observation. In this talk, we study the problem of estimating these components from functional data, i.e. multiple observations (curves), in situations where seasonal effects exhibit arbitrary time warpings across different observations. Rather than assuming pre-aligned curves, or using an off-the-shelf alignment method, we take a model-based approach where we estimate the trend and the seasonal effects, while performing alignments over the seasonal effects at the same time. More precisely, we solve for the maximum likelihood estimates of trend and seasonal effects, and the seasonal time warpings, using a Coordinate Descent method. We study the performance of these estimators using bootstrap and calculate confidence bands for the estimated quantities. This framework is demonstrated using experiments involving synthetic data and two real data (Berkeley Growth Velocity and U.S. electricity price).

Meliheh Shaban Tameh, Florida State University
Fractional shifted Legendre tau method for linear and nonlinear variable order FPDEs : Klein-

Gordon Equations
While some other methods have been applied to fractional linear and nonlinear Klein-Gorden PDEs, reaching a desirable accuracy is still of more interest. In this paper, the operational matrices of fractional order shifted Legendre functions (FSLFs) are derived and combined with Tau method to convert the fractional order differential equations having variable coefficients to a system of solvable algebraic equations. Here, we focus on linear and nonlinear fractional Klein-Gorden PDEs to show the performance of the application derived operational matrices on linear and nonlinear problems appeared in science and engineering, as well as simulation of dynamics systems. Our numerical results confirm how we are capable of dealing with nonlinear cases in FPDEs.

Jing Tian, University of South Florida
On the emergence of the Navier-Stokes-alpha model for channel flows
In this talk, we concentrate our consideration to a restricted class of fluid flows. With the hypothesis that the turbulence described by the NS-alpha is partly due to the roughness of the walls, we present the transition from the Navier-Stokes equations into the Navier-Stokes-alpha model by introducing a Reynolds type averaging.

Xiaochuan Tian, Columbia University
On energy-based coupling strategies of nonlocal and local models
Multiscale models for materials with fractures or defects involve local interaction where classical models work well and nonlocal interaction where defects display. In this talk, we present two types of energy-based coupling methods that combines nonlocal models and local models. The first idea comes from peridynamics model with a heterogeneous nonlocal horizon(interaction length). By allowing a smooth change of horizon from nonzero to zero, we effectively have a seamless coupling of nonlocal and local models. Another idea is borrowed from the quasicontiumm method in the atomistic-to-continuum coupling which leads to a way to get a well-posed model that passes the patch test.

Ihsan Topaloglu, Virginia Commonwealth University
Flow-induced vibration of piezoelectric membrane energy harvester
Height-constrained nonlocal interaction energies and congested aggregation models, which formally can be considered as gradient flows of these energies, have recently appeared not only in models of collective behavior such as biological swarming and pedestrian crowd motion but also in simple nonlocal geometric shape optimization problems. In these models the inclusion of a height constraint on admissible functions poses significant challenges both analytically and numerically. In order to overcome these we consider a regularization of the energies by including a highly degenerate diffusion term and approximate the height-constrained model by the unconstrained ones. Justifying our approach analytically in the context of Gamma-convergence we implement this scheme numerically in two dimension, and compute gradient flows via particle approximations. This is a joint project with Katy Craig.

Necibe Tuncer, Florida Atlantic University
Identifiability issues in multiscale immune-epidemiological models
In this talk, I will present a mathematical model that links immunological model and epidemiological model. This model allows us to understand dynamical interplay of infectious diseases at two

different scales; immunological response of the host at individual scale and the disease dynamics at population scale. Once the host is infected, it triggers the immune response which produces anitgen-specific antibodies to clear the pathogen. The pathogen and antibody levels are often monitored in laboratory experiments. But how can we use the data generated in the laboratory experiments to estimate the parameters of the immunological model. Clearly, the parameters of the within-host immunological model has an effect of the epidemiological characteristics of disease such as reproduction number and prevalence. I will present the identifiability issues in parameter estimation of the immunological model.

Yuying Tzeng, Florida State University
Time Series Simulation with Randomized Quasi-Monte Carlo Methods
Quasi-Monte Carlo methods are designed to produce efficient estimates of simulated values but the error statistics of these estimates are difficult to compute. Randomized quasi-Monte Carlo methods have been developed to address this shortcoming. In this paper we compare quasi-Monte Carlo and randomized quasi-Monte Carlo techniques for simulating time series. We use randomized quasi-Monte Carlo to compute value-at-risk and expected shortfall measures for a stock portfolio whose returns follow a highly nonlinear Markov switching stochastic volatility model which does not admit analytical solutions for the returns distribution. Quasi-Monte Carlo methods are more accurate but do not allow the computation of reliable confidence intervals about risk measures. We find that randomized quasi-Monte Carlo methods maintain many of the advantages of quasi-Monte Carlo while also providing the ability to produce reliable confidence intervals of the simulated risk measures. However, the advantages in speed of convergence of randomized quasi-Monte Carlo diminish as the forecast horizon increases.

Mehdi Vahab, Florida State University
A coupled level set and moment of fluid method for phase change problems
We are presenting a numerical method to model multiphase systems. An enhanced coupled level set (LS) and moment of fluid (MOF) method is developed to consider phase change phenomena such as solidification and boiling. A level set reinitialization method is introduced to reset the level set functions to the numerically exact distance functions to the reconstructed piecewise linear multimaterial interfaces. This procedure also create a robust estimate for evaluation of normal vectors and curvature to evaluate surface tension forces near multimaterial regions. Additionally, the level set functions are used to make a better estimate for slope optimization of the MOF reconstruction, which specifically avoid convergence to local minima for problems in cylindrical coordinates. The numerical tests show that the enhanced method is advantageous compared to previous CLSMOF implementations in the sense of producing significantly less flotsam, convergence in cases with notable surface tension forces, and conservation properties.

Hans-Werner van Wyk, Auburn University
Localizing Uncertainty with Multiscale Gaussian Markov Random Field Models
The high computational cost of stochastic simulations involving partial differential equations (PDEs) with uncertain input parameters is often attributable to a combination of two bottlenecks: i) the steep cost of evaluating sample paths and ii) the complexity of the underlying parameter space. In this talk we relate both of these problems to the computational mesh, by using Gaussian Markov random fields to model the spatially varying input parameters for a simple PDE. This allows us to

exploit readily available local dependency information of the parameter field in conjunction with standard finite element error estimates to identify spatial regions that contribute statistically to the error in the computed quantity of interest. These estimates can then be used to inform spatial mesh refinement.

Matthew Villemarette, Florida State University
Maximally Preserving Finite Difference Schemes for the Allen-Cahn Equation using Operator Splitting
The Allen-Cahn equation is an important PDE in phase field modeling. Used originally to describe binary alloys undergoing spinodal decomposition, it has now been applied to model tumor growth, flock migration and many other physical processes. One of the important properties of the solutions of these equations is the maximum principle, conserving the mass / volume fraction of a concentration over time. We design finite difference schemes using operator splitting to directly preserve the maximum principle by integrating the diffusion and potential parts independently in time. Numerical simulations verifying the accuracy of the method and the ability to preserve the maximum principle, spinodal decomposition, etc. are carried out to ensure the validity of the scheme.

Hong Wang, University of South Carolina
Fast numerical methods for nonlocal models
In recent years nonlocal models are emerging as powerful tools for modeling challenging phenomena in many applications, including anomalous diffusion processes in transport problems and elasticity problems with evolving discontinuities in displacement fields. However, nonlocal models generate numerical methods with dense matrices that have significantly increased memory requirement or computational complexity. Moreover, due to the impact of the singular kernels in the integral operators in nonlocal models, the evaluation and assembly of the stiffness matrices can be very expensive. We go over the recent developments of fast and accurate numerical methods for nonlocal models, by exploring the structure of the stiffness matrices.

Jilu Wang, Florida State University
Convergence analysis of time discretization for stochastic time-fractional PDEs subject to additive space-time white noise,
In this work, we consider the stability and convergence of numerical approximation of solutions of the stochastic time-fractional PDE

$$\partial_t \psi - \Delta \partial_t^{1-\alpha} \psi = f + \dot{W},$$

where $\partial_t^{1-\alpha}\psi$ denotes the Caputo fractional time derivative of order $1-\alpha \in (-1,1)$ and $\dot{W}$ space-time white noise. The stochastic time-fractional equation is discretized by a backward Euler convolution quadrature in time for which the sharp error estimate

$$\mathbb{E}\|\psi(\cdot, t_n) - \psi_n\|_{L^2}^2 = O(\tau^{1-\alpha d/2})$$

is established for $\alpha \in (0, 2/d)$, where d denotes the spatial dimension, ψ_n the approximate solution at the nth time step, and $\mathbb{E}$ the expectation operator. The results cover both subdiffusion and diffusion-wave cases in one-dimensional spatial domains and, for the subdiffusion case, multi-dimensional domains. Numerical examples are presented to illustrate the theoretical analysis.

Qi Wang, Beijing Computational Science Research Center
University of South Carolina
Energy quadratization: a new strategy for developing linear, energy stable numerical schemes for dissipative systems
I will discuss the nascent technique for developing linear, energy stable numerical schemes for dissipative partial differential equation systems derived from an variational principle and the generalized Onsager principle. The dissipative system possesses a mathematical structure that can be exploited to yield a linear, high order energy stablke numerical scheme. We will demonstrate the idea using a multiphasic field theory and a generalized hydrodynamic theory for liquid crystal polymers.

Qi Wang, Beijing Computational Science Research Center
University of South Carolina
Modeling and simulation of active liquid crystal flows
Active liquid crystals belong to the class of active matter, in which energy input at the molecular level drives the system away from its equilibrium state. In this talk, I will present a continuum theory for flows of active liquid crystals and then discuss some numerical techniques for discretizing the governing partial differential equations. Then, I will present some numerical results for active liquid crystal flows in a couple of confined geometry. Various patterns and structures due to spontaneous flows will be contrasted with the flow driven structures.

Xiaoming Wang, Florida State University
An energy stable decoupled scheme for the Navier-Stokes-Darcy system
We consider the Navier-Stokes-Darcy system which models coupled free flow with porous media flow. Such kind of systems is of great importance in a variety of applications such as the study of hyporheic zone. The system enjoys an energy law when equipped with the Beavers-Joseph and the Lions interface boundary conditions. We present a novel first-order in time numerical scheme that decouples the Navier-Stokes solver from the Darcy solver while maintaining the energy stability.

Sergiusz Wesolowski, Florida State University
Functional Data Analysis Framework for Next Generation Sequencing Experiments
Sequencing-based methods to examine fundamental features of the genome, such as gene expression and chromatin structure have been challenging due to the scale and nature of these data. Drawing sound inferences from such experiments relies on appropriate mathematical methods that can capture the complexity of the structure of the underlying biological processes.

In this talk we describe a new statistical shape analysis framework based on Square Root Slope Functions to analyze Illumina sequencing experiments. The new approach uses the Poisson point process filtering to interpret the experimental output as functions over reference genome. We propose a new generative model and equip it with an equivalent of a Fisher test for functional data and a functional noise removal procedure. We show that it is capable of detecting new activity patterns in genomic data that are not possible to detect by state of the art methods.

The performance of our approach is evaluated on RNA-seq data in exon level differential gene expression problem and DNA-seq data in detection of nucleosome positioning changes. In both cases we have shown that our model detects new biologically meaningful differential patterns.

Timothy Wessler, University of North Carolina
Modeling Antibody-Mucus-Pathogen Kinetics
Many viruses and bacteria are able to move freely through mucus, yet mucus is an invaluable protective barrier against foreign pathogens and particulates. Experiments demonstrate that even a pathogen with absolutely no affinity to mucus can become trapped in a mucus network with the presence of antibodies (Ab). Ab and mucus work cooperatively to trap pathogens by an Ab attaching to a pathogen on one side and to mucus on the other, tethering the pathogen to the mucus via the Ab. Our research models the attachment/detachment of Ab as pathogens move through mucus, generating many unexpected yet important insights into the design of antibodies, and offering a promising approach to protecting against foreign pathogens.

Bin Xu, Florida State University
Simulating spring hydrograph recession and karst parameters estimation with multiple reservoirs
Karst aquifers can be described into two systems, conduit systemconduit networkand matrix systemfissured and pores. Conduit system with a fast and turbulent flow is clearly different from the matrix system with a slow and laminar flow pores, and the water from matrix system is drained by conduit system. It is difficult to accurately characterize the karst systems with heterogeneous media. During the recession of karst systems, the recession limb of a spring hydrograph can reflect the two systems with different hydraulic parameters. To simulate the karst aquifer, we propose a multiple reservoirs model, the matrix system conceptualized as one reservoir and conduit system conceptualized as a set of serial small reservoirs. This study also introduces an approach to fit a storage-outflow model for each segment indicating a small reservoir and then average the parameter estimates. Matching strip method was used to analyze the matrix system. The above methods facilitate best global model selection and effective porosity estimation for the karst catchment.

Feifei Xu, University of North Carolina at Chapel Hill
Modeling barrier properties of intestinal mucus reinforced with IgG and secretory IgA against highly motile bacteria
The gastrointestinal tract is lined with a layer of viscoelastic mucus gel, comprised of an entangled network of mucins together with an abundance of antibodies (Ab) and other macromolecules. Although Ab such as IgG can retard the free diffusion of viruses in mucus to help prevent mucosal infections, whether Ab can immobilize highly motile bacteria in mucus before bacteria swim through mucus layers remains an open question. Here, we developed a mathematical model that takes into account physiologically relevant spatial dimensions and time scales, binding and unbinding rates between Ab and bacteria and between Ab and mucins, the diffusivities of different Ab, and run-tumble aspects of bacterial motility. Our model predicts Ab can accumulate on the surface of individual bacteria at sufficient quantities and speed to exert the necessary avidity to immobilize bacteria in mucus before they penetrate the mucus layer, consistent with experimental observations. Furthermore, modeling predicts that Ab that can weakly associate with mucins was substantially more effective at stopping bacterial penetration than Ab that strictly induce bacterial agglutination. This implies that while sIgA is the most potent Ab isotype at preventing bacterial penetration, IgG represents a practical alternative for mucosal prophylaxis and therapy. Our work improves the mechanistic understanding of Ab-enhanced barrier properties of mucus, and highlights the ability for 'muco-trapping' Ab to protect against a diverse array of pathogens at mucosal

surfaces.

Neda Yaghoobian, Florida State University

Flow over urban-like geometries with complex thermal boundary conditions

Improvements in building energy use, air quality in urban canyons and in general urban microclimates require understanding of the complex interaction between urban morphology, materials, and climate, as well as their interaction with the flow dynamics in urban canyons. Review of the literature indicates that despite a long history of valuable urban microclimate studies, more comprehensive approaches of investigating energy, heat and flow in urban areas are needed. In this research a more comprehensive and realistic simulation of the diurnally varying street canyon flow and associated heat transport is numerically investigated using Large-eddy Simulation (LES). An in-house building energy model with a three-dimensional raster-type geometry provides urban surface heat fluxes as thermal boundary conditions for LES. Compared to analyses that use uniformly distributed thermal forcing on urban surfaces, the present analysis shows that non-uniform thermal forcing can result in complex local air flow patterns. Realistic flow patterns in urban settings are important to be specified, particularly for addressing pollution dispersion issues, pollution control, and energy harvesting in urban areas. The results demonstrate that only local simulations for specific neighborhoods and urban climates can elucidate specific effects of urban mitigation measures, with often surprising outcomes.

Chayu Yang, University of Tennessee at Chattanooga

Impact of awareness programs on cholera dynamics: Two modeling approaches

We propose two differential equation-based models to investigate the impact of awareness programs on cholera dynamics. The first model represents the disease transmission rates as decreasing functions of the number of awareness programs, whereas the second model divides the susceptible individuals into two distinct classes depending on their awareness/unawareness of the risk of infection. We study the essential dynamical properties of each model, using both analytical and numerical approaches. We find that the two models, though closely related, exhibit significantly different dynamical behaviors. Namely, the first model follows regular threshold dynamics while rich dynamical behaviors such as backward bifurcation may arise from the second one. Our results highlight the importance of validating key modeling assumptions in the development and selection of mathematical models toward practical application.

Xiaofeng Yang, University of South Carolina

A novel numerical approach to solve a class of nonlinear thermodynamically consistent Model

The nonlinear thermodynamically consistent model is usually derived from the variational approach of the free energy. Such modeling approach are commonly used in almost all physical passive system that satisfies the laws of thermo-mechanics. One of the main numerical challenges is about the development of the time marching scheme. We introduce a novel, so called Invariant Energy Quadratization approach, that can possess many desired properties. More precisely, the schemes (i) are accurate (second order in time); (ii) are stable (unconditional energy dissipation law holds); and iii) only need to solve a linear, symmetric positive definite system at each time step.

Guannan Zhang, Oak Ridge National Laboratory

A multilevel reduced-basis method for parameterized partial differential equations

An important approximation scheme for alleviating the overall computational complexity of solving parameterized PDEs is known as multilevel methods, which have been successfully used in the Monte Carlo and collocation setting. In this effort, we propose to improve the multilevel methods with the use of reduced-basis (RB) techniques for constructing the spatial-temporal model hierarchy of PDEs. Instead of approximating the solution manifold of the PDE, the key ingredient is to build approximate manifolds of first-order differences of PDE solutions on consecutive levels. To this end, we utilize a hierarchical finite element (FE) framework to formulate an easy-to-solve variational FE system for the first-order differences. Moreover, by deriving a posteriori error estimates for the RB solutions, we also intend to develop a greedy-type adaptive strategy in order to construct a good set of snapshots. The main advantage of our approach lies in the fact that the manifold of the first-order differences becomes progressively linear as the physical level increases. Thus, much fewer expensive snapshots are required to achieve a prescribed accuracy, resulting in significant reduction of the offline computational cost of greedy algorithms. Furthermore, our approach combines the advantages of both multilevel Monte Carlo and multilevel collocation methods, in the sense that it can generate snapshots anywhere in the parameter domain but also features fast convergence.

Guannan Zhang, Oak Ridge National Laboratory
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.

Yanzhi Zhang, Missouri University of Science and Technology
A fast algorithm for solving the space-time fractional diffusion equation
In this talk, we discuss a fast algorithm for efficient and accurate solution of the space-time fractional diffusion equations defined in a rectangular domain. Due to the non-locality, numerical discretization of the spectral fractional Laplacian results in a large dense matrix. This causes considerable challenges not only for storing the matrix but also for computing matrix-vector products in practice. We propose an algorithm to avoid storing the large matrix from discretizing the nonlocal operator and significantly reduce the computational costs. We then use the Laplace transform method for time integration of the semi-discretized system and a weighted trapezoidal method to numerically compute the convolutions needed in the resulting scheme. Various experiments are presented to demonstrate the efficiency and accuracy of our method.

Jia Zhao, University of North Carolina at Chapel Hill
On Energy-stable Schemes for Complex-fluid Hydrodynamic Equations
Complex fluids are fluids whose micro-structure have impact on the fluid macroscopic properties, which include complex fluid mixtures of different types. In this talk, I will first present a system-

atic development of a general hydrodynamic model for complex fluid system using the generalized Onsager relation. Then, a semi-discrete scheme to solve this general model, which satisfies the discrete energy dissipation law, will be presented. Specific tricks on linearizing and decoupling the schemes will be presented for particular reduced models. In the end, several 3D simulations will be shown to illustrate the effectiveness of our schemes.

Wenju Zhao, Florida State University
Auxiliary Equation Approach Numerical Methods for the time dependent stochastic Navier-Stokes equations with additive noise
In this research, we provide a regularized method for the stochastic Navier-Stokes equations with additive noise. The trace of the noise can be finite or infinite with an appropriate regularization parameter. The stability and convergence of the path-wise modified Navier-Stokes equations are proved with numerical examples. Comparisons between the influences of regularized and non-regularized noises are also given.

Yanxiang Zhao, George Washington University
Crawling and turning in a minimal reaction-diffusion cell motility model
We study a minimal model of a crawling eukaryotic cell with a chemical polarity controlled by a reaction-diffusion mechanism describing Rho GTPase dynamics. The size, shape, and speed of the cell emerge from the combination of the chemical polarity, which controls the locations where actin polymerization occurs, and the physical properties of the cell, including its membrane tension. We find in our model both highly persistent trajectories, in which the cell crawls in a straight line, and turning trajectories, where the cell transitions from crawling in a line to crawling in a circle. We discuss the controlling variables for this turning instability and argue that turning arises from a coupling between the reaction-diffusion mechanism and the shape of the cell. This emphasizes the surprising features that can arise from simple links between cell mechanics and biochemistry. Our results suggest that similar instabilities may be present in a broad class of biochemical descriptions of cell polarity.