Society for Industrial and Applied Mathematics

The 4th Annual Meeting of SIAM Central States Section

University of Oklahoma
October 5 - 7, 2018

Summary

1 SIAM Central States Section

Welcome to the University of Oklahoma and the 4th annual meeting of the SIAM Central States Section.

About SIAM Central States Section

The SIAM Central States Section was formed in 2014 to serve SIAM members in Arkansas, Colorado, Iowa, Kansas, Mississippi, Missouri, Nebraska, and Oklahoma.

Section Purpose

The purpose of this section is to enhance the communication among the section members, promote the collaboration for both basic research and applications of mathematics to industry and science, represent applied and computational mathematics in the entire proposed central region, and support the SIAM mission in the central region of the USA.

Activities

The activities for the SIAM Central Section include annual section meetings, seminars and workshops for advanced topics of common interests of the section members, encouraging new SIAM student chapters and facilitating all the SIAM student chapters in the central region to connect together, promoting collaboration in applied mathematics and its applications to industry and science, and expanding the influence of SIAM in the central states. Participation in SIAM Central States Section activities will be open to all institutions and industries in the region with an interest in applied and computational mathematics.

Leadership

President: *Jiangguo Liu* Colorado State University

Vice President: *Anna Zemlyanova* Kansas State University

Secretary: *Ying Wang* University of Oklahoma

Treasurer: *Stephen Pankavich* Colorado School of Mines

Department of Mathematics, University of Oklahoma

2 Schedule at a glance

All talks are on Saturday (Oct.6) and Sunday (Oct.7)

60 minutes for a plenary talk (all in Physical Sciences Building (PHSC) 201)

20 minutes for a mini-symposium talk in all parallel sessions

Friday, October 5

05:30 pm - 07:00 pm	Welcome Reception (not a dinner)	Physical Sciences Building 209
05:30 pm - 07:00 pm	Registration table opens	Physical Sciences Building 209

Saturday, October 6

08:45 am	Opening remarks by OU officials and announcements by SIAM CSS
09:00 am	Plenary talk by Hong Qian, University of Washington
10:00 am	Photo session and coffee break
10:40 am	Parallel Session I
12:00 pm	Lunch at OU Couch Restaurants
02:00 pm	Plenary talk by Eitan Tadmor, University of Maryland
03:00 pm	Transition to parallel sessions 2
03:10 pm	Parallel Session II
04:30 pm	Coffee break
05:00 pm	Parallel Session III
06:45 pm	Conference dinner at Molly Shi Boren ballroom in the OU Union

Sunday, October 7

09:00 am	Plenary talk by Peter Kuchment, Texas A&M University
10:00 am	Coffee break
10:30 am	Parallel Session IV
11:50 am	Adjourn

The 4th Annual Meeting of SIAM Central States Section

Physical Science Center, The University of Oklahoma

Planery Talks - PHSC 201

Peter Kuchment, Texas A&M University
Hong Qian, University of Washington
Eitan Tadmor, University of Maryland

Mini-Symposia:

	PHSC 114	PHSC 115	PHSC 116	PHSC 117	PHSC 212	PHSC 222	PHSC 313	PHSC 314	PHSC 316	PHSC 317	PHSC 321	PHSC 323
Session I Sat, Oct. 6 10:40am- 12:00pm	**MS15** K.Chen P.Chen S.Acosta	**MS10** B.Hashmi D.Handwerk I.Oprea	**MS05** C.Scoglio T.McAllister S.Eriksson-Bique D.Zosso G.David	**MS02** A.Luo S.Xing Y.Xu C.Guo	**Contrib.** D.Bhatta H.Khudhair J.Hassan	**MS07** E.Gasparovic F.Motta A.Thomas M.K.Chung	**MS06** W.Geng Z.Wang J.Tausch	**MS14** P.Cazeaux Q.Guan X.Tu H.Gao G.Harper		**MS03** H.Mofidi P.Liu W.Liu Z.Wen	**MS01** L.Hoang M.Chen W.Yang X.Yu	**MS08** H.Lee Y.Epshteyn S.Li X.Zhao
Session II Sat, Oct. 6 03:10pm- 04:30pm	**MS15** B.Yuan Y.Yang (MSU) G.Ambart.	**MS09** S.B.,H.C.,T.G. J.Lyu R.Parshad A.Basheer	**MS05** N.Albin G.Speight J.Martin M.Higgins B.Alali	**MS02** Y.Guo Y.Yuan Y.Liu B.Yu J-S.Pei	**Contrib.** U.Farooq Z.Chen C.Zhang	**MS07** K.Xia M.McGuirl N.Giansiracusa D.Guralnik	**MS06** S.Li W.Wang X.Zhang Y.Zhong	**MS14** J.Ku J.Liu S.Luo W.Maimaitiyiming	**MS11** S.Dai J.Murphy T.Kaman	**MS03** Z.Xu J.Chen D.Chen M.Zhang	**MS01** Z.Bradshaw W.Hu H.Qiu K.Yamazaki	**MS08** C.Wang X.Yang X.He
Session III Sat, Oct. 6 05:00pm- 06:20pm	**MS12** J.Mears M.Espanol Y.Godin	**MS09** P.Shipman A.Santhank. W.Fitzgibbon F.Agusto	**MS05** D.Caragea J.Gill P.Horn J.Lind H.Shakeri		**Contrib.** S.Yuan A.Baker Y.Wu	**MS07** J.Segert R.Belton S.Chowdhury J.Bush	**MS06** H.Feng H.Li R.Guo P.Yin	**MS14** A.Miedlar J.Mohebujjaman C.Qiu J.Rossmanith D.Han	**MS11** W.Hu B.Xiao D.Han E.Carlson	**MS04** Y.Yang (MTU) N.Chuenjarern Y.Liu W.Guo Q.Zhuang	**MS01** Y.Dai N.Ju Y.Cao	**MS08** Z.Wang N.Jiang T.Hoang J.Singler
Session IV Sun, Oct. 7 10:30am- 11:50am	**MS12** A.Zemlyanova A.Y.Wu L.Greenleaf	**MS09** B.C-Charpentier M.Beauregard	**MS05** P.Poggi-Corradini H.Hakobyan J.Clemens L.Geyer K.Kottegoda			**MS07** R.Komendarczyk N.Sanderson J.Dover D.Heisterkamp		**MS14** Z.Wang N.Malluwawadu D.Erkmen Z.Yang	**MS11** Y.Pei A.Kolasinski H.Ye Y.Yu			**MS08** J.Zhao Y.Zhang

Plenary Speakers

Peter Kuchment is an University Distinguished Professor in the Mathematics Department of Texas A&M University. He is a Fellow of the AMS, SIAM, Institute of Physics, and AAAS (Amer. Soc. Adv. Sci.), as well as a Senior member of IEEE. His work is focused in the areas of partial differential equations, mathematical physics, spectral theory, medical imaging, material science, and enhancement of K-12 math education. He has authored nearly 200 publications in mathematics and its applications, including three research monographs: Floquet Theory for Partial Differential Equations, Birkhauser 1993, Introduction to Quantum Graphs (joint with G. Berkolaiko), AMS 2013, and The Radon Transform and Medical Imaging, SIAM 2014.

Title: Mathematics of some novel imaging techniques
Abstract: The talk will provide a excursion into the mathematics of hybrid imaging, reconstructions with internal information, and time permitting (unlikely) Compton camera imaging.

Hong Qian received B.A. in astrophysics from Peking University and Ph.D. in molecular biology from Washington University (St. Louis). His research interests turned to theoretical biophysical chemistry and mathematical biology when he was a Post-Doctoral Fellow with the University of Oregon and the California Institute of Technology, where he studied protein folding. He was with the Department of Biomathematics, UCLA School of Medicine, from 1994 to 1997, when he worked on the theory of motor proteins and single-molecule biophysics. He joined the University of Washington (Seattle) in 1997 and is currently the Olga Jung Wan Endowed Professor of Applied Mathematics. He has coauthored two books: Chemical Biophysics: Quantitative Analysis of Cellular Systems (Cambridge University Press, 2008) with D. A. Beard, and in Chinese, Mathematical Kinetic Models: Applications in Biophysics and Biochemistry (Peking Univ. Press, 2017) with H. Ge. His current research interest focuses on stochastic dynamics and its applications to biological systems. He is a fellow of the American Physical Society, and served and serves on the editorial board of journals on biophysical chemistry and quantitative/computational/systems biology.

Title: Mathematicothermodynamics: Stochastic Laws and Emergent Behavior of Population Kinetic Systems
Abstract: There is a growing awareness toward a slow shifting in the foundation of the thermodynamic laws, from several macroscopic, empirical postulates concerning heat as a form of random mechanical motions, to derivable mathematical theorems based on stochastic dynamics of mesoscopic systems. It becomes increasingly clear that a stochastic dynamic description of the Nature is a very effective mathematical representation of the Reality. In this talk, I shall first introduce mathematicothermodynamics as a set of mathematical results in stochastic processes. The result is then applied to complex chemical kinetic systems. Via the limit by merely taking the molecular numbers to be infinite, we are able to derive J. W. Gibbs' macroscopic isothermal equilibrium chemical thermodynamics, as well as generalize it to mesoscopic nonequilibrium systems such as biological cells.

Eitan Tadmor is a Distinguished University Professor at the University of Maryland (UMd) College Park. Earlier he was a Bateman Instructor in CalTech, 1980-1982 and on the faculty of his alma mater, Tel Aviv University. In 1995 Tadmor joined the UCLA Math Department where he was the founding co-director of the NSF Institute for Pure and Applied Math (IPAM), 1999-2001. In 2002 he was recruited to lead the UMd Center for Scientific Computation and Math Modeling (CSCAMM), and served as its first Director, 2002-2016. In 2016-2017 he was a Senior Fellow at the Institute for Theoretical Studies at ETH-Zürich. Tadmor was an ICM invited speaker (Beijing 2002), and delivered plenary addresses in the international conferences on hyperbolic problems (Zurich 1990 and Beijing 1998), the SIAM invited address at the 2014 Joint Math Meeting, and the 2016 Leçons Jacques-Louis Lions at the Université Pierre et Marie Curie. In 2012 he was in the inaugural class of AMS Fellows. In 2015, he was awarded the SIAM-ETH Henrici prize. Tadmor is the Principal Investigator of an NSF Research Network "Kinetic Description of Emerging Challenges in Natural Sciences" (Ki-Net, 2012-2019).

Title: Short-Range Interactions and the Emergence of Higher-Order Patterns
Abstract: A fascinating aspect in collective dynamics is self-organization: ants form colonies, birds flock, mobile networks coordinate a rendezvous and human crowds reach a consensus. We discuss the large-time, large-crowd flocking behavior of different models for collective dynamics driven by alignment. In particular, we address the central question how short-range interactions lead, over time, to the emergence of long-range, higher-order patterns in one- and multi-species dynamics.

3 Parallel Sessions

MS01. Partial Differential Equations in Mathematical Fluid Mechanics

Organizer: Ning Ju, `ning.ju@okstate.edu`, Oklahoma State University
Co-organizer: Jiahong Wu, `jiahong.wu@okstate.edu`, Oklahoma State University

Schedule: PHSC 321 (for all three sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

Developments in Asymptotic Expansions for Solutions of Navier-Stokes Equations
Luan Hoang, Texas Tech University
Abstract: We study the long-time dynamics of the Navier-Stokes equations in the three-dimensional periodic domains with a decaying outer body force. Consider the force has a large-time asymptotic expansion in a very general system of decaying functions. We prove that any Leray-Hopf weak solutions admits an asymptotic expansion of the same kind. This expansion is uniquely determined by the force, and independent of the solutions. Our general theorem not only recovers the previous results obtained for power decaying functions, but also establishes the expansions for the case of log(t), log(log(t)), etc. decaying forces. This is joint work with Dat Cao (Texas tech University).

On classical solutions to the Cauchy problem of the 2D compressible non-resistive MHD equations with vacuum
Mingtao Chen, Oklahoma State University
Abstract: In this paper, we investigate the Cauchy problem of the compressible non-resistive MHD on mr^2 with vacuum as far field density. We prove that the 2D Cauchy problem has a unique local strong solution provided the initial density and magnetic field decay not too slow at infinity. Furthermore, if the initial data satisfies some additional regularity and compatibility conditions, the strong solution becomes a classical one. Additionally, we establish a blowup criterion for the 2D compressible non-resistive MHD depending solely on the density and magnetic fields.

3D incompressible magnetohydrodynamic equations with fractional partial dissipation
Wanrong Yang, North Minzu University
Abstract: In this talk, we will mainly present recent results about the global existence and uniqueness of H^1-solutions to 3D incompressible MHD equations with only directional velocity dissipation and horizontal magnetic diffusion $-(-\Delta_h)^{\frac{5}{4}}b$, where $\Delta_h = p_1^2 + p_2^2$.

New Prodi-Serrin Type Regularity Criteria for the 3D Navier-Stokes Equations
Xinwei Yu, University of Alberta
Abstract: We prove that a Leray-Hopf weak solution for the 3D incompressible Navier-Stokes equations would stay regular if a Prodi-Serrin type integrability condition in Lorentz spaces is satisfied by div$(u/|u|)$, or by the third component u_3, where u is the velocity function. The key to our proofs is a nonlinear Gronwall type inequality. Our method can be easily adapted to ”upgrade” many other Prodi-Serrin type conditions from Lebesgue spaces to Lorentz spaces. This is joint work with Mr. Benjamin Pineau.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Properties of infinite energy solutions to the Navier-Stokes equations
Zachary Bradshaw, University of Arkansas
Abstract: Since their introduction by Lemarie-Rieusset, local Leray solutions to the Navier-Stokes equations have proved useful for analyzing regularity and uniqueness properties of the Navier-Stokes equations. This talk will focus on several recent results concerning the existence, regularity, and properties of local Leray solutions.

Boundary Control of Optimal Mixing in Navier-Stokes Flows
Weiwei Hu, Oklahoma State University
Abstract: We discuss the problem of optimal mixing of an inhomogeneous distribution of a scalar field via an active control of the flow velocity, governed by the Navier-Stokes equations, in a two dimensional open bounded and connected domain. We consider the velocity field steered by a control input that acts tangentially on the boundary of the domain through the Navier slip boundary conditions. This is motivated by the problem of mixing within a cavity or vessel by moving the walls or stirring at the boundaries. Our main objective is to design an optimal Navier slip boundary control that optimizes mixing at a given final time. Non-dissipative scalars, both passive and active, governed by the transport equation will be discussed. In the absence of diffusion, transport and mixing occur due to pure advection. This essentially leads to a nonlinear control problem of a semi-dissipative system. A rigorous proof of the existence of an optimal controller and the first-order necessary conditions for optimality will be presented.

Existence results for Viscoelastic fluids
Hua Qiu, South China Agricultural University
Abstract: In this talk, I will talk about some recent work about the existence results related to the viscoelastic fluids.

Stochastic analysis on PDE in fluid dynamics
Kazuo Yamazaki, University of Rochester
Abstract: In this talk, I will discuss some recent developments of analysis on PDE in fluid dynamics with noise, about which the author has been involved. The discussion will concern the Navier-Stokes equations, magnetohydrodynamics system, the Hall-magnetohydrodynamics system, and possibly the Kardar-Parisi-Zhang equations. The topics should concern around the well-posedness, ergodicity (Markov selection), and possibly rough path theory, regularity structures, and para-controlled distributions.

Session III Sat, Oct. 6, 05:00pm - 06:20pm

Global well-posedness of the magnetohydrodynamics (MHD) equations with fractional diffusion
Yichen Dai, Xiamen University
Abstract: In this talk, we consider the general d-dimensional magnetohydrodynamics (MHD) equations with the fractional dissipation $(-\Delta)^{\alpha}u$ and $(-\Delta)^{\beta}b$. We prove the local existence and uniqueness solutions of the d-D MHD equations and the global existence and uniqueness of weak solutions $(u, b) \in L^2(R^d)$ as a special consequence when $\alpha, \beta = \frac{1}{2} + \frac{d}{4}$.

Solution Regularity of the Primitive Equations
Ning Ju, Oklahoma State University
Abstract: Some recent results on regularity properties for solutions of the Primitive Equations for large scale oceanic flow of viscous fluid will be presented and discussed.

Determining Form for the 2D Rayleigh-Bénard problem
Yu Cao, Indiana University
Abstract: We show that the long-time dynamics (the global attractor) for the 2D Rayleigh-Bénard problem subject to a set of mixed boundary conditions can be embedded in the long-time dynamics of an ordinary differential equation, called a determining form. The phase space for this ODE is a Banach space of trajectories of a finite dimensional projection of velocity. It is shown that steady states of the determining form can be uniquely identified with the trajectories in the global attractor of the Rayleigh-Bénard problem.

MS02. Numerical Methods and Stability of Nonlinear Dynamical System

Organizer: Bo Yu, yub@uwplatt.edu, University of Wisconsin-Platteville
Co-organizers: Albert Luo, aluo@siue.edu, Southern Illinois University
Yu Guo, gary.rain@gmail.com, Midwestern State University

Schedule: PHSC 117 (for both sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

Stability and bifurcation in Nonlinear dynamical systems
Albert Luo, Southern Illinois University Edwardsville
Abstract: Stability and bifurcation in Nonlinear dynamical systems In this talk, the stability and singularity of equilibriums in nonlinear dynamical systems are discussed in eigenvector space. Based on the eigenspace, covariant and contravariant variables are defined for stability and bifurcation analysis of dynamical systems. The Hopf bifucation and spiral stability are studied through Fourier series rather than circular assumption. Such investigation can help one better understand the stability and bifurcation in nonlinear dynamical systems.

On the quantitative analysis of periodic motions in a time-delayed, softening, Duffing oscillator
Siyuan Xing, Southern Illinois University Edwardsville
Abstract: In this paper, the period-1 and period-2 motions of a time-delayed, softening, Duffing oscillator are determined by a semi-analytical method. Such a semi-analytical method established implicit mappings for periodic motions through discretization of the differential equation of the Duffing oscillator. The stability and the bifurcation conditions of period-1 and period-2 motions in such a Duffing oscillator are predicted through eigenvalue analysis of the mappings of periodic nodes; the bifurcation trees of period-1 to period-2 motions are completed, accordingly. From analytical predictions, numerical simulations of period-1 and period-2 motions in the oscillator are carried out. From Finite Fourier series, the frequency-amplitude analysis for period-1 to period-2 motions are completed. Through this method, the quantitative analysis of periodic motions in such a delayed, nonlinear dynamical system can be achieved.

Semi-analytical solutions of periodic motions in a van der Pol oscillator
Yeyin Xu, Southern Illinois University Edwardsville
Abstract: In this presentation, the periodic solutions of periodic motions of a van der Pol oscillator are achieved from a discrete mapping method. The discrete mapping method produces semi-analytical solutions of periodic motions by discretizing the continuous nonlinear system to form the implicit mappings. Based on these specific mapping structures, the semi-analytical solutions can be obtained very accurately. Based on the discrete mapping method, the stable periodic motion shrinking phenomenon is discovered. The shrinking pattern from stable periodic motion to limit cycle of the van der Pol oscillator is released. The route from independent and symmetric periodic motion adding sequence to chaos in a van

der Pol oscillator are achieved Stability analysis is carried out through eigenvalue analysis. The frequency amplitude characteristics of periodic motions are discussed. Numerical results are calculated in comparison of the analytical results. The phase trajectories of periodic motions are presented and the evolution from unstable periodic motion to stable periodic motion can be clearly observed. The harmonic spectra are shown for a better understanding of the nonlinear properties of the periodic motions of the van der Pol oscillator. The results achieved in this paper have various applications in physics and electronics.

Period-1 and period-2 motions in a periodically forced, damped double pendulum

Chuan Guo, Southern Illinois University Edwardsville

Abstract: In this paper, period-1 and period-2 motions in a periodically forced, damped double pendulum is analytically predicted through a discrete implicit mapping method. The implicit mapping is established via the discretized differential equation. The corresponding stability and bifurcation conditions of the period-1 and period-2 motions are predicted through eigenvalue analysis. Numerical simulation of the period-1 and period-2 motions in the double pendulum is completed from analytical predictions.

Session II Sat, Oct. 6, 03:10pm - 04:50pm

Analytical Bifurcations Trees of a Parametrically Excited Pendulum

Yu Guo, Midwestern State University

Abstract: In this paper, the complete bifurcation trees of a parametrically excited pendulum is investigated using discrete implicit maps obtained through a mid-time scheme. Based on these discrete maps, mapping structures are developed to describe periodic motions in the system. Analytical bifurcation trees of various periodic motions to chaos are obtained through the nonlinear algebraic equations of such implicit maps. Eigenvalue analysis is carried out for stability and bifurcation analysis. Finally, numerical simulation results of various periodic motions are illustrated in verification.

Period Motions and Stability of a Nonlinear Spring Pendulum

Yaoguang Yuan, Southern Illinois University Edwardsville

Abstract: In this paper, bifurcation trees of periodic motions in a periodically forced, nonlinear spring pendulum system are predicted analytically through a semi-analytic method. The stability and bifurcation of the periodic motions are determined through eigenvalue analysis. The frequency- amplitude characteristics of the bifurcation trees of periodic motions are presented. Finally, from the analytical prediction, numerical simulations of periodic motions are completed. The complex periodic motions in the nonlinear spring pendulum are illustrated for a better understanding of motions complexity.

On periodic motions of a two degree of freedom chemical oscillator

Yutong Liu, Southern Illinois University Edwardsville

Abstract: In this paper, a model of oscillating chemical reaction system is given by a 2-D nonlinear dynamical system. Analytical solutions of periodic motions are obtained by analytical method accurately. The corresponding stability and bifurcations of periodic motions are calculated through the eigenvalue analysis of equilibrium points. Numerical solutions of periodic motions are calculated by transforming the 2-D nonlinear dynamical system into a nonlinear dynamical system of coefficients in the Fourier series. From this study, some insight of oscillatory behavior in a specific chemical reaction system can be gained.

Investigation of vertical galloping and periodic motions using the method of implicit mapping

Bo Yu, University of Wisconsin Platteville

Abstract: Current methods for analyzing periodic motion of a structure with a noncircular cross section use a one-degree-of-freedom galloping model. This model requires approximating the vertical force coefficient as a polynomial using a power series expansion. This approximation has limitations, including limited accuracy and restriction to period-I motion. The current approximation derives the first two coefficients of the power series analytically and uses curve-fit experimental data to determine the rest of the coefficients. In this presentation, a technique is proposed to use implicit discrete mapping to analytically predict the periodic motions of the system. These maps are obtained by transferring the differential equation used to describe the one-degree-of-freedom galloping model into discrete counterparts. Using these mapping structures, bifurcation trees of periodic motions are predicted and corresponding stability and bifurcation analysis are carried out utilizing eigenvalue analysis. Numerical results of periodic motions are generated to verify the theoretical analytical prediction. Employing this implicit discrete mapping technique will improve on the accuracy of current methods used to analyze periodic motions.

A Brief Introduction to "Mem-Models" in Engineering Mechanics Applications

Jin-Song Pei, University of Oklahoma

Abstract: A significant event happened for electrical engineering in 2008, when researchers at HP Labs announced that they had found "the missing memristor", a fourth basic circuit element that was postulated nearly four decades earlier by Dr. Leon Chua who also developed the theory of memristive systems. One consequence of this announcement has been revitalized research in all areas of brain-imitating computer technologies, primarily because memristors mimic synapses. Moreover, the theory involving memristor devices and memristive systems was extended to include memcapacitors and meminductors, thereby introducing an entire class of "mem-models". This model class is the foundation of the present study. By applying well-known mechanical-electrical system analogies, the mathematics of mem-models may be transferred to the setting of engineering mechanics, resulting in mechanical counterparts of memristors, memcapacitors, etc. We identify some recent examples of "mem-dashpots" and "mem-springs". In addition to a "zero-crossing" condition, we highlight the role played by discontinuities in the model and/or the excitation, the combination of which enables mem-models to produce numerous hysteresis patterns. We also consider some new properties and modeling techniques that call for further improvement so that these new types of mechanical models can become more usable for analyzing real-world data.

MS03. Recent Advances in Modeling, Numerics, and Analysis of Electrodiffusion Phenomena

Organizer: Mingji Zhang, mingji.zhang@nmt.edu, New Mexico Institute of Mining and Technology
Co-organizer: Duan Chen, Duan.Chen@uncc.edu, Uiversity of North Carolina Charlotte

Schedule: PHSC 317 (for both sessions)

Session I Sat, Oct. 6. 10:40am - 12:00pm

Effects of permanent charges and ion sizes on ionic fluxes
Hamidreza Mofidi, University of Kansas
Abstract: In this talk, we will report our ongoing project concerning combined effects of (small) permanent charges and ionic sizes on ionic fluxes via the Poisson-Nernst-Planck models with a hard-sphere component for ion channel problems. For the three-constant-piece permanent charge with one nonzero region, we are able to derive the expansion of the fluxes in the small nonzero permanent charge and ionic diameter, up to quadratic order terms. Based on the leading order terms, we determine several critical potentials in terms of the other key physical parameters that identify boundaries of different effects on fluxes rom the interaction between the permanent charge and ionic sizes. Other effects on fluxes due to high order terms will be reported too.

Non-Isothermal Electrokinetics: Energetic Variational Approach
Pei Liu, Penn State University
Abstract: Fluid dynamics accompanies with the entropy production thus increases the local temperature, which plays an important role in charged systems such as the ion channel in biological environment and electrodiffusion in capacitors/batteries. In this article, we propose a general framework to derive the transport equations with heat flow through the Energetic Variational Approach. According to the first law of thermodynamics, the total energy is conserved and we can use the Least Action Principle to derive the conservative forces. From the second law of thermodynamics, the entropy increases and the dissipative forces can be computed through the Maximum Dissipation Principle. Combining these two laws, we then conclude with the force balance equations and a temperature equation. To emphasis, our method provide a self consistent procedure to obtain the dynamical equations satisfying proper energy laws and it not only works for the charge systems but also for general systems.

Permanent charge effects on ionic flows
Weishi Liu, University of Kansas
Abstract: In this talk, we will report our analytical and numerical studies of permanent charge effects on ionic fluxes via Poisson-Nernst-Planck type models. A flux ratio associated to each ion species was identified through analysis that quantifies a key effect of permanent charges in the sense that > 1 (resp. < 1) corresponds to an enhancing (resp. a reducing) effect of the permanent charge on the flux.

Boundary layer effects on ionic flows via classical Poisson-Nernst-Planck models
Zhenshu Wen, Huaqiao University
Abstract: We study a quasi-one-dimensional steady-state Poisson-Nernst-Planck model for ionic flows of multiple charged ion species through a membrane channel. Of particular interest is to study boundary layer effects on ionic flows in terms of individual fluxes. More precisely, we study the flow properties of interest without assuming electro-neutrality boundary. Two cases are carefully analyzed, case one involves two ion species, one negatively charged and one positively charged, while case two involves two positively charged ion species and one negatively charged ion species. In both cases, new phenomena are observed and much more rich dynamics of ionic flows are obtained.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Model of Visco-elastic Incompressible Fluid Flow and its Application
Zhiliang Xu, University of Notre Dame
Abstract: Energetic Variational Approach is used to derive a novel thermodynamically consistent three-phase model of a mixture of Newtonian and visco-elastic flu-

ids. The model which automatically satisfies the energy dissipation law and is Galilean invariant, consists of coupled Navier-Stokes and Cahn-Hilliard equations. Modified General Navier Boundary Condition with fluid elasticity taken into account is also introduced for using the model to study moving contact line problems. The model can be applied for studying various biological or biophysical problems such as blood clotting.

Boundary layer effects on ionic flows via Poisson-Nernst-Planck models with local hard-sphere potentials

Jianing Chen, New Mexico Tech

Abstract: We study a quasi-one-dimensional steady-state Poisson-Nernst-Planck model with a local hard-sphere potential for ionic flows of two oppositely charged ion species through a membrane channel. Of particular interest is to study qualitative properties of ionic flows in terms of individual fluxes without assuming electro-neutrality boundary conditions (indicating the existence of boundary layers). Compared with our previous results with electro-neutrality boundary conditions, new phenomena are observed, which further indicates the rich and complicated dynamics of the flow properties of interest in the study of ion channel problem.

Fractional Poisson-Nernst-Planck Model for Ion Channels

Duan Chen, University of North Carolina at Charlotte

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

Channel geometry and permanent charge effects on ionic flows via Poisson-Nernst-Planck models

Mingji Zhang, New Mexico Tech

Abstract: We study effects of permanent charges on ionic flows through ion channels via a quasi-one-dimensional classical Poisson-Nernst-Planck (PNP) model. The geometry of the three-dimensional channel is presented in this model to a certain extent, which is crucial for the study in this paper. Two ion species, one positively charged and one negatively charged, are considered with a simple profile of permanent charges. The classical PNP model can be viewed as a boundary value problem (BVP) of a singularly perturbed system. The singular orbit of the BVP depends on Q_0 in a regular way. Assuming $|Q_0|$ is small, a regular perturbation analysis is carried out for the singular orbit. Our analysis indicates that effects of permanent charges depend on a rich interplay between boundary conditions and the channel geometry. Furthermore, interesting common features are revealed: for $Q_0 = 0$, only an average quantity of the channel geometry plays a role; however, for $Q_0 \neq 0$, details of the channel geometry matter, in particular, to optimize effects of a permanent charge, the channel should have a short and narrow neck within which the permanent charge is confined. The latter is consistent with structures of typical ion channels.

MS04. Recent Developments of High-order Discontinuous Galerkin Methods

Organizer: Yang Yang, `yyang7@mtu.edu`, Michigan Technological University

Schedule: PHSC 317

Session III Sat, Oct. 6, 05:00pm - 06:40pm

High-order bound-preserving discontinuous Galerkin methods for compressible miscible displacements in porous media on triangular

Yang Yang, Michigan Technological University

Abstract: In this talk, we develop high-order bound-preserving (BP) discontinuous Galerkin (DG) methods for the coupled system of compressible miscible displacements on triangular meshes. We consider the problem with multi-component fluid mixture and the (volumetric) concentration of the j-th component, c_j, should be between 0 and 1. There are three main difficulties. Firstly, c_j does not satisfy a maximum-principle. The main idea is to apply the positivity-preserving techniques to all c_j's and enforce $\Sigma c_j = 1$ simultaneously. By doing so, we have to treat the time derivative of the pressure dp/dt as a source in the concentration equation and choose suitable fluxes in the pressure and concentration equations. Secondly, the construction of high-order BP schemes on triangular meshes. We use interior penalty DG methods for the concentration equations, and the first-order numerical fluxes are not easy to construct. Therefore, we will construct second-order BP schemes and then combine the second-

and high-order fluxes to obtain a new one. Finally, c_j's are not the conservative variables, as a result, the classical slope limiter cannot be applied. Moreover, for fluid mixture with more than two components, we cannot simply set the upper bound of each c_j to be 1. Therefore, a suitable limiter for multi-component fluid will be introduced. Numerical experiments will be given to demonstrate the high-order accuracy and good performance of the numerical technique.

Fourier analysis of local discontinuous Galerkin methods on overlapping meshes
Nattaporn Chuenjarern, Michigan Technological University
Abstract: The local discontinuous Galerkin (LDG) method is a popular one for solving parabolic equations such as the heat equation by introducing the auxiliary variable q to represent the derivative of the primary variable u, and solve them on the same mesh. A new LDG method was introduced to solve u and q on different meshes to improve the computational cost. In this talk, we will use the new method and Fourier analysis to analyze the error estimate of one dimension parabolic equations on overlapping meshes. We also demonstrate the relationship of the ratio of the overlapping mesh and the super convergence points to obtain the super convergence. Numerical experiments will be given to demonstrate the analysis.

An implicit sparse grid discontinuous Galerkin method for high dimensional reaction-diffusion equations
Yuan Liu, Mississippi State University
Abstract: In this talk, we will introduce a class of implicit sparse grid discontinuous Galerkin(DG) method with the aim of breaking the curse of dimensionality. The key ingredient of the spatial discretization is a set of multiwavelet basis functions on nested grids. Krylov implicit integration factor method is used for temporal discretization in order to relax the CFL constraints. Numerical examples in 2D and 3D cases are provided to show the performance of our proposed method.

An alternative formulation of discontinous Galerkin schemes for solving Hamilton-Jacobi equations
Wei Guo, Texas Tech University
Abstract: In this talk, we will introduce an alternative formulation of discontinuous Galerkin (DG) schemes for approximating the viscosity solutions to nonlinear Hamilton-Jacobi (HJ) equations. The main difficulty in designing DG schemes lies in the inherent non-divergence form of HJ equations. One effective approach is to explore the elegant relationship between HJ equations and hyperbolic conservation laws: the standard DG scheme is applied to solve a conservation law system satisfied by the derivatives of the solution of the HJ equation. In this work, we consider an alternative approach to directly solving the HJ equations, motivated by a class of successful direct DG schemes by Cheng et al. [J. Comput. Phys., v223 (2009); J. Comput. Phys., 268(2014)].The proposed scheme is derived based on the idea from the central-upwind scheme by Kurganov et al. [SIAM J. Sci. Comput., v23 (2001)]. In particular, we make use of precise information of the *local speeds of propagation* at discontinuous element interface with the goal of adding adequate numerical viscosity and hence naturally capturing the viscosity solutions. A collection of numerical experiments is presented to demonstrate the performance of the method for solving general HJ equations with linear, nonlinear, smooth, non-smooth, convex, or non-convex Hamiltonians.

Solving Interface Problems of the Helmholtz Equation
Qiao Zhuang, Virginia Tech
Abstract: This presentation reports our explorations of solving interface problems of Helmholtz equation by the immersed finite elements with an interface independent mesh. Two immersed finite element (IFE) methods are investigated: the partial penalized IFE (PPIFE) and discontinuous Galerkin IFE (DGIFE) methods. Optimal convergence rates are observed for these IFE methods once the mesh size is smaller than an optimal mesh size which is mainly dictated by the wave number. Our explorations also suggest that higher degree IFE methods are more efficient than their lower degree counterparts because of their large optimal mesh size and higher convergence rates.

MS05. Interactions among Analysis, Optimization and Network Science

Organizer: Pietro Poggi-Corradini, `pietro@math.ksu.edu`, Kansas State University
Co-organizer: Nathan Albin, `albin@math.ksu.edu`, Kansas State University

Schedule: PHSC 116 (for all four sessions)

Session I Sat, Oct. 6, 10:40am - 12:20pm

SIS Epidemics in Temporal Networks: a Multilayer Approach
Caterina Scoglio, Kansas State University
Abstract: To improve the accuracy of network-based SIS models we introduce and study a multi-layer representation of a time-dependent network. In particular, we assume that individuals have their long-term (permanent) contacts that are always present, identifying in this way the first network layer. A second network layer also exists, where the same set of nodes can be connected by occasional links created with a given probability. While links of the first layer always exist, a link of the second layer is

only activated with some probability and under the condition that the two nodes, connected by this link, are simultaneously participating to the temporary link. We develop a model for the SIS epidemic on this time-dependent network, analyze equilibrium and stability of the corresponding mean-field equations, and shed some light on the role of the temporal layer on the spreading process.

Period collapse in Ehrhart quasi-polynomials
Tyrrell McAllister, University of Wyoming
Abstract: The problem of counting integer lattice points in rational polytopes arises in many contexts, including the geometry of toric varieties and the representation theory of semisimple Lie algebras. If a polytope $P \subset \mathbb{R}^n$ has rational vertices, then a seminal result of E. Ehrhart says that the number of lattice points in the kth dilate of P (where k is a positive integer) is a quasi-polynomial function of k — that is, a "polynomial" in which the coefficients are themselves periodic functions of k. "Period collapse" occurs when these coefficients have smaller periods than naively expected. This phenomenon has connections to the deformation theory of the corresponding toric varieties. We present tools for constructing polytopes in which the periods of the coefficients take on prescribed values. The cyclic polytopes of McMullen's upper bound theorem will make a surprise appearance.

How to prove a Poincare inequality?
Sylvester Eriksson-Bique, University of California Los Angeles
Abstract: I will discuss some of my recent work and collaborations on conditions guaranteeing and characterizing Poincare inequalities, and some ways these can be used in particular applications. For example, I will discuss the existence of a Semmes family of curves given a 1-Poincare inequality, and an idea of iteration that can be used to prove and improve Poincare inequalities. Time permitting some applications and consequences will be mentioned.

Studying the shape of data: From geometric probability to data science
Dominique Zosso, Montana State University
Abstract: In this talk I will first provide a lay-man's random walk from geometric measure theory to integral geometry of convex bodies, loosely based on Gian-Carlo Rota's 1997 AMS colloquium lecture. An important result is the following: the volume of a convex body A thickened (dilated) by r is a polynomial in r (Steiner formula). Its coefficients are called Minkowski functionals, mixed volumes, or Quermassintegrals (for different normalizations); they can be identified with properties such as volume, perimeter, mean width, etc. of the initial body, and fully characterize A from a geometric probability point of view.I will then sketch how we now would like to use well-established extensions of the above to the convex ring (finite unions of convex bodies) as a starting point for further inquiry into studying the shape of data: Consider a data set in the form of a point cloud in some potentially high-dimensional feature space, where individual points are samples from a nice underlying structure that we are trying to uncover (think: samples from a donut in 3-space—gotta have this donut). We can generate a finite union of convex bodies parametrized by that data set by associating a ball of radius R+r with each data point. By estimating the volume (with multiplicities) of this ball-cloud, for different thickenings r, we can determine the Quermassintegrals through polynomial fitting (at scale R).We anticipate that such a tool will be useful in generic data science as well as in some concrete low-dimensional "shape-from-samples" problems, such as the shape description of biofilms or the characterization of percolation.

Metric spaces as limits of graphs and the Analyst's Traveling Salesman Theorem
Guy C. David, Ball State University
Abstract: We describe a class of highly non-Euclidean metric spaces, constructed by Cheeger and Kleiner, that have interesting analytic properties and are built as inverse limits of finite simplicial graphs. We then report on recent joint work of the speaker and Raanan Schul, which proves a version of Peter Jones's "Analyst's Traveling Salesman Theorem" in these spaces. This characterizes subsets of rectifiable curves as those which are quantitatively flat in a certain sense, which must be correctly interpreted in these non-Euclidean spaces.

Session II Sat, Oct. 6, 03:10pm - 04:50pm

Spanning Tree Modulus
Nathan Albin, Kansas State University
Abstract: Spanning tree modulus on a graph is related to a number of interesting problems. For example, through the concept of blocking duality, spanning tree modulus is strongly connected to the modulus of a transverse family of objects, the feasible partitions. The solution to either of these problems immediately yields the solution to the other. On the other hand, when viewed through a probabilistic framework, spanning tree modulus is dual to two interrelated problems involving random spanning trees: the fairest edge usage problem and the minimum expected overlap problem. The former asks for a probability distribution on spanning trees that spreads the edge usage probabilities as evenly as possible, while the latter asks for a distribution with the property that the expected overlap of two independent, identically distributed random spanning trees is as small as possible. Finally, through a process known as deflation of homogeneous subgraphs, spanning tree modulus is connected to two combinatorial problems:

the densest subgraph problem and the minimum feasible partition problem. This talk will introduce all of these problems and show how all are connected through the spanning tree modulus.

Maximal Directional Derivatives and Universal Differentiability Sets

Gareth Speight, University of Cincinnati

Abstract: Rademacher's theorem asserts that every Lipschitz function from $\mathbb{R}^n$ to $\mathbb{R}^m$ is differentiable except on a set of measure zero. Depending on the dimensions of the spaces involved, this theorem may or may not be sharp. If $n > 1$ then there exists a measure zero set in $\mathbb{R}^n$ containing a point of differentiability for every Lipschitz function from $\mathbb{R}^n$ to $\mathbb{R}$. Such sets are called universal differentiability sets. We investigate universal differentiability sets in Euclidean spaces and Carnot groups. Carnot groups are spaces with much of the Euclidean structure (translations, dilations, Haar measure and a path distance) but where the shortest distance between points may not be along a straight line.

Oscillation estimates of eigenfunctions via the combinatorics of noncrossing partitions

Jeremy Martin, University of Kansas

Abstract: We study oscillations in the eigenfunctions for a fractional Schrödinger operator on the real line. An argument in the spirit of Courant's nodal domain theorem applies to an associated local problem in the upper half plane and provides a bound on the number of nodal domains for the extensions of the eigenfunctions. Using the combinatorial properties of noncrossing partitions, we turn the nodal domain bound into an estimate for the number of sign changes in the eigenfunctions. We discuss applications in the periodic setting and the Steklov problem on planar domains. This is joint work with Vera Mikyoung Hur (University of Illinois) and Mat Johnson (University of Kansas). Since I am the one combinatorialist on the team, my talk will focus more on the combinatorial techniques used than the underlying PDE problems.

New methods for incorporating network cyclic structures to improve community detection

Michael Higgins, Kansas State University

Abstract: A distinguishing property of communities in networks is that cycles are more prevalent within communities than across communities. Hence, the detection of these communities may be aided through the use of measures of the local "richness" of cyclic structures. We investigate the use of two methods for quantifying this richness—loop modulus (LM) and renewal non-backtracking random walks (RNBRW)—to improve the performance of existing community detection algorithms. LM solves a quadratic program to find an optimal allocation of edge usage across cycles to minimize cycle overlap, thereby giving a rigorous way to quantify the importance of edges. RNBRW, introduced for the first time in this paper, quantifies edge importance as the likelihood of an edge completing a cycle in a non-backtracking random walk. We argue that RNBRW provides an efficient and scalable alternative to LM. We give simulation results that suggest pre-weighting edges by the proposed methods can improve the performance of popular community detection algorithms substantially. Our methods are especially efficient for the challenging case of detecting communities in sparse graphs.

Spectral methods for peridynamic models

Bacim Alali, Kansas State University

Abstract: Linear peridynamic-type operators, with symmetric integrable kernels, can be expressed in terms of compact self-adjoint operators, which makes them suitable to study using spectral methods. A spectral numerical method is developed for solving scalar peridynamic equations with periodic boundary conditions. A Fourier Continuation method can be used to extend the spectral method to study other boundary conditions. An investigation of sources of discontinuities and their evolution in peridynamic models is provided.

Session III Sat, Oct. 6, 05:00pm - 06:40pm

Android Malware Detection Using Graph-based Label Propagation Approaches

Doina Caragea, Kansas State University

Abstract: Android devices and apps are becoming increasingly popular. At the same time, malware apps are becoming more prevalent, and current app vetting technologies are lagging behind the threats. Recent research has focused on automated malware detection approaches that combine machine learning techniques with static and dynamic code analysis. However, for Android malware detection, precise ground truth is a rare commodity. As security knowledge evolves, what may be considered ground truth at one moment in time may change, and apps once considered benign turn out to be malicious. The inevitable noise in data labels poses a challenge to creating effective machine learning models. Our work is focused on approaches for learning classifiers for Android malware detection in a manner that is methodologically sound with regard to the uncertain and ever-changing ground truth in the problem space. More specifically, we study graph-based label propagation approaches, where the nodes represent apps, and the links between nodes denote the similarity between apps. The similarity is determined based on metrics that make use of features extracted using static analysis. Given a graph that contains a small number of labeled apps and a large number of unlabeled apps, the goal is to propagate the labels from the labeled apps to the unlabeled apps, while accounting for

potential noise in the original labels. Several label propagation approaches are studied and compared to identify those approaches that can best handle the noisy ground truth and produce accurate classifications.

Finite Perimeter Sets in Metric Measure Spaces and Minimality

James Gill, Saint Louis University

Abstract: We discuss sets of finite perimeter in arbitrary metric measure spaces with doubling condition and Poincare inequality. We are specifically interested in tangent spaces in the blow-up. This is joint research with Sylvester Eriksson-Bique, Panu Lahti, and Nageswari Shanmugalingam.

Gradient and Harnack type inequalities for PageRank

Paul Horn, University of Denver

Abstract: PageRank, as introduced by Brin and Page, and more generally 'personalized PageRank,' has been of fundamental importance in network search. A key parameter in PageRank is the 'jumping constant' which allows (among other things) one to tailor the sensitivity of PageRank to local cuts. In this talk, we describe new gradient estimates (akin to the Li-Yau inequality for solutions to the heat equation) and Harnack type inequalities for graphs satisfying certain curvature conditions. These allow us to compare the 'importance' of different nodes, and how PageRank regularizes as the jumping constant goes to zero. This is based on joint work with Lauren Nelsen.

Effect of random time changes on Loewner hulls

Joan Lind, University of Tennessee

Abstract: Loewner hulls are determined by their real-valued driving functions, via the Loewner differential equation. We study the geometric effect on the Loewner hulls when the driving function is composed with a random time change, such as the inverse of an α-stable subordinator. In contrast to Schramm-Loewner evolution (SLE), we show that for a large class of random time changes, the time-changed Brownian motion process does not generate a simple curve. Further we develop criteria which can be applied in many situations to determine whether the Loewner hull generated by a time-changed driving function is simple or non-simple. To aid our analysis of an example with a time-changed deterministic driving function, we prove a deterministic result that a driving function that moves faster than at^r for $r \in (0, 1/2)$ generates a hull that leaves the real line tangentially.

Optimizing Extremal Eigenvalues in Multiplex Networks

Heman Shakeri, Kansas State University

Abstract: We can learn much about graphs by calculating the extremal eigenvalues of the Laplacian matrix. These values are closely connected to the node and link connectivity, isoperimetric properties, max-cut and rate of mixing in Markov chains. In this talk, we discuss how to design interlayer links in multiplex networks to push these extremal eigenvalues further and improve the overall performance. Therefore, we find the best interlayer weight distributions that with a given budget; first, minimize the smallest nonzero eigenvalue known as the algebraic connectivity; second, maximize the largest eigenvalue known as the Laplacian spectral radius; and finally, minimize the spectral gap of the Laplacian.

Session IV Sun, Oct. 7, 10:30am - 12:10pm

Discrete approximation of continuous modulus using grids

Pietro Poggi-Corradini, Kansas State University

Abstract: p-Modulus of curve families is a common tool in complex analysis and more generally geometric function theory in metric spaces with controlled geometry such as higher-dimensional Euclidean spaces. A parallel theory of p-Modulus has been developed on graphs, hence a natural question arises: can continuous modulus be approximated by discrete modulus? We show that connecting modulus on topological quadrilateral in the complex plane can be approximated by discrete connecting modulus when using very general Skopenkov-Werness-type quadrangular grids.The proof makes use of the theory of Fulkerson duality developed by the author, N. Albin et al. We will also describe several remaining open questions.

Quasisymmetric embeddings of Sierpinski spaces into the plane

Hrant Hakobyan, Kansas State University

Abstract: We will provide some necessary and some sufficient conditions for the existence of quasisymmetric (QS) embeddings of planar domains and Sierpinski carpets into the plane. For some classes of constructions this gives a complete characterization of the Sierpinski carpets which QS embed into the plane. The main tool is a version of transboundary modulus of families of curves due to Schramm.

A greedy approach to modulus

Jason Clemens, Wichita State University

Abstract: Given a family of objects on a network, the modulus problem can be formulated as a convex optimization problem. It has been shown that the dual problem can be viewed as another modulus problem on a related family of objects. This talk will introduce a greedy algorithm developed to solve these modulus problems, as long as a minimum object can be found.

p-modulus and p-resistor networks

Lukas Geyer, Montana State University

Abstract: I will discuss the concepts of p-resistor networks and effective p-resistance and its connection to p-modulus and p-extremal length. These concepts were introduced by Jarek Kwapisz in his investigation of the conformal dimension of Sierpinski carpets. It turns out that effective p-resistance is comparable to p-extremal length, but easier to handle computationally. The notion of p-resistor networks also naturally lead to notions of convex and topological duality, which are useful both computationally and theoretically.

Spanning tree modulus for secure broadcast games
Kapila Kottegoda, Kansas State University
Abstract: The p-modulus is a general framework for quantifying the richness of a family of objects on a graph. When applied to the family of spanning trees, p-modulus has an interesting probabilistic interpretation. In particular, the 2-modulus problem in this case has been shown to be equivalent to the problem of finding a probability distribution on spanning trees that utilizes the edges of the graph as evenly as possible. For this reason, there is a strong connection between 2-modulus of the family of spanning trees and the edge-disjointness of this family. We use this fact to produce a game-theoretic interpretation of modulus and apply modulus to the problem of minimizing the number of broadcast messages intercepted by an eavesdropper listening on an unknown link.

MS06. Recent Development in Numerical PDEs and Applications

Organizer: Peimeng Yin, `pemyin@iastate.edu`, Iowa State University
Co-organizers: Songting Luo, `luos@iastate.edu`, Iowa State University
Hailiang Liu, `hliu@iastate.edu`, Iowa State University

Schedule: PHSC 313 (for all three sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

On preconditioning the treecode-accelerated boundary integral (TABI) Poisson-Boltzmann solver
Weihua Geng, Southern Methodist University
Abstract: We recently developed a treecode-accelerated boundary integral (TABI) solver for solving Poisson-Boltzmann (PB) equation. The solver has combined advantages in accuracy, efficiency, memory, and parallelization as it applies a well-posed boundary integral formulation to circumvent many numerical difficulties associated with the PB equation and uses an $O(N * \log(N))$ treecode to accelerate the GMRES iterative solver. However, as observed in our previous work, occasionally when the triangular mesh generator produces low quality triangles, the number of GMRES iterations required to solve the discretized boundary integral equations $Ax = b$ could be large. To address this issue, we design a preconditioning scheme using preconditioner matrix M such that $M^{(}-1)A$ has much improved condition while $M^{(}-1)z$ can be rapidly computed for any vector z. The numerical results show that this new preconditioning scheme improves the TABI solver with significantly reduced iteration numbers and better accuracy, particularly for protein sets on which TABI solver previously converges slowly.

Positivity preserving, conservative, and free energy dissipating finite difference methods for multi-dimensional Poisson–Nernst
Zhongming Wang, Florida International University
Abstract: We develop simple but effective finite difference methods for solving the multi-dimensional Poisson–Nernst–Planck (PNP) equations with multiple ionic species. A novel central-differencing discretization based on harmonic-mean approximations is proposed for the Nernst–Planck (NP) equations. The forward and backward Euler discretizations in time are employed to derive an explicit scheme and a linearized semi-implicit scheme, respectively. Numerical analysis proves that the numerical schemes respect three desired properties that are possessed by analytical solutions: I) ionic mass conservation, II) positivity of ionic concentrations, and III) free-energy dissipation. The semi-implicit scheme is further shown to preserve positivity unconditionally, whereas a constraint on a mesh ratio is required for the explicit scheme to ensure positivity. The positivity preservation is established based on advantages brought by the harmonic-mean approximations, In addition, theoretical and computational investigations are performed to study condition numbers of the semi-implicit discretization of the NP equations, further revealing advantages of the scheme in computational efficiency and stability. Our estimates on the upper bound of condition numbers indicate that the developed discretization based on harmonic-mean approximations can effectively solve a known issue — a large condition number is often accompanied by the use of Slotboom variables. Numerical tests verify that the numerical solution respects desired properties, and is second-order accurate in space and first-order accurate in time. An application of the numerical scheme to an electrochemical charging system demonstrates its effectiveness in solving realistic problems. This is a joint work with D. Jie and S. Zhou.

A shape optimization approach for Stefan problems
Johannes Tausch, Southern Methodist University
Abstract: The Stefan problem is reformulated as a shape optimization problem for the position of the phase transition as a function of time. The functional to be minimized

is the mismatch of the Dirichlet to Neumann map and the Stefan condition. The only stationary point of the functional is the minimum which is also the solution of the Stefan problem. A gradient based optimization method is derived from shape calculus. The state and adjoint equation of the heat equation are solved using integral equation techniques which avoids a discretization in the domain. A Nyström quadrature method is analyzed and numerical results are presented.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Computation of a shrinking interface problem

Shuwang Li, Illinois Institute of Technology

Abstract: In this talk, we present an adaptive rescaling method for computing a shrinking interface in a Hele-Shaw cell with a time increasing gap width $b(t)$. We focus our study on a one-phase interior Hele-Shaw problem where a blob of fluid, surrounded by air, dynamically responds to the changing gap width. To explore the full nonlinear interface dynamics, we develop a spectrally accurate boundary integral method in which a new time and space rescaling is implemented. In the rescaled frame, the motion of the interface is slowed down, while the area/volume enclosed by the interface remains unchanged. This method, for the first time, enables us to adaptively remove the severe numerical stiffness imposed by the rapidly shrinking interface (especially at late times) and accurately compute the dynamics to far longer times than could previously be accomplished. Numerical tests demonstrate that the method is stable, efficient and accurate.

A high order well-balanced particle-in-cell method for shallow water equations

Wei Wang, Florida International University

Abstract: A hybrid Eulerian–Lagrangian particle–in–cell (PIC) type numerical method is developed for the solution of advection dominated flow problems. For smooth flows the method presented is of formal high–order accuracy in space. The method is applied to solve the non–linear shallow water equations resulting in a new, and novel, shock capturing shallow water solver. The approach is able to simulate complex shallow water flows which can contain an arbitrary number of discontinuities. Both trivial and non–trivial bottom topography is considered and it is shown that the new scheme is inherently well–balanced exactly satisfying the C–property. The scheme is verified against several 1D benchmark shallow water problems.

A residual-based a posteriori error estimation for immersed finite element method

Xu Zhang, Mississippi State University

Abstract: Interface problems arise in many applications in science and engineering. Partial differential equations (PDEs) are often used to model interface problems. Solutions to these PDE interface problems often involves kinks, singularities, discontinuities, and other non-smooth behaviors. The immersed finite element method (IFEM) is a class of numerical methods for solving PDE interface problems with unfitted meshes. In this talk, we introduce a residual-based a posteriori error estimation for IFEM. We show that the error estimator is globally reliable and locally efficient, with the reliability and efficiency constants independent of the interface location. This error estimator can provide accurate assessment of the numerical approximation and can also be used as a guidance for adaptive mesh refinement for IFEM. Numerical results are provided to demonstrate the features of the adaptive IFEM.

A fast algorithm for radiative transport

Yimin Zhong, University of California Irvine

Abstract: We propose in this work a fast numerical algorithm for solving the equation of radiative transfer (ERT) in isotropic media. The algorithm has two steps. In the first step, we derive an integral equation for the angularly averaged ERT solution by taking advantage of the isotropy of the scattering kernel, and solve the integral equation with a fast multipole method (FMM). In the second step, we solve a scattering-free transport equation to recover the original ERT solution. Numerical simulations are presented to demonstrate the performance of the algorithm for both homogeneous and inhomogeneous media.

Session III Sat, Oct. 6, 05:00pm - 06:20pm

An augmented matched interface and boundary (MIB) method for solving elliptic interface problem

Hongsong Feng, University of Alabama

Abstract: A second order accurate augmented matched interface and boundary (MIB) is introduced for solving two-dimensional (2D) elliptic interface problems with piecewise constant coefficients. The augmented MIB seamlessly combines several key ingredients of the standard MIB, augmented immersed interface method (IIM), and explicit jump IIM, to produce a new fast interface algorithm. Fictitious values generated by MIB method provide a simple procedure to reconstruct Cartesian derivative jumps as auxiliary variables and couple them with the jump-corrected Taylor series expansions, which allow us to restore the order of the central difference across the interface to two. Moreover, by using the Schur complement to disassociate the algebraic computation of auxiliary variables and function values, the discrete Laplacian can be efficiently inverted by using the fast Fourier transform (FFT). Our numerical experiments shows that the iteration number in solving the auxiliary system weakly depends on the mesh size. As a consequence, the total computational cost of the augmented MIB is about $O(n^2)$

for a Cartesian grid with dimension $n \times n$ in 2D. Therefore, the augmented MIB outperforms the classical MIB in all cases by significantly reducing the CPU time, while keeping the same second order of accuracy in dealing with complicated interfaces. Moreover, our experiments indicate that the AMIB scheme can produce a second order of accuracy in approximating the solution gradients.

A fourth order accurate bound-preserving compact finite difference scheme for scalar convection diffusion equations
Hao Li, Purdue University
Abstract: We demonstrate that the classical fourth order accurate compact finite difference scheme satisfies a natural weak monotonicity property for solving scalar convection-diffusion equations. Based on such a property, we design a simple limiter to enforce the bound-preserving or positivity-preserving property of numerical solutions without losing conservation or high order accuracy. Higher order schemes including 6th and 8th order schemes satisfying the weak monotonicity can also be constructed. We show that the bound-preserving property is still valid when a total-variation-bounded (TVB) limiter is used to reduce oscillations. All these results can be easily extended to higher dimensions and passive convection such as incompressible flows. More general boundary conditions such as the inflow-outflow boundary condition will also be discussed. This is a joint work with Prof. Shusen Xie at Ocean University of China and Prof. Xiangxiong Zhang at Purdue University.

The Application of Immersed Finite Element Methods on Elasticity Interface Problems
Ruchi Guo, Virginia Tech
Abstract: In this talk, we present a group of immersed finite element (IFE) spaces for solving planar elasticity equation involving interface. The shape functions in these IFE spaces are constructed through some specific approximate jump conditions such that the unisolvence of the bilinear and rotated Q1 IFE shape functions are always guaranteed regardless of the Lame parameters and the interface location. A group of nice properties for these IFE shape functions are established. The optimal approximation capabilities of these IFE spaces are analyzed thorough the multiple point Taylor expansion technique. The IFE spaces can be used in the partially penalized IFE (PPIFE) method to solve the elasticity interface problems with the optimal convergence rate.

A mixed discontinuous Galerkin method without interior penalty for time-dependent fourth order problems
Peimeng Yin, Iowa State University
Abstract: A novel discontinuous Galerkin (DG) method is developed to solve time-dependent bi-harmonic type equations involving fourth derivatives in one and multiple space dimensions. We present the spatial DG discretization based on a mixed formulation and central interface numerical fluxes so that the resulting semi-discrete schemes are L^2 stable even without interior penalty. For time discretization, we use Crank-Nicolson so that the resulting scheme is unconditionally stable and second order in time. We present the optimal L^2 error estimate of $O(h^{k+1})$ for polynomials of degree k for semi-discrete DG schemes, and the L^2 error of $O(h^{k+1} + (\Delta t)^2)$ for fully discrete DG schemes. Extensions to more general fourth order partial differential equations and cases with non-homogeneous boundary conditions are provided. Numerical results are presented to verify the stability and accuracy of the schemes. Finally, an application to the one-dimensional Swift-Hohenberg equation endowed with a decay free energy is presented.

MS07. Applied and Computational Topology

Organizer: Henry Adams, `henry.adams@colostate.edu`, Colorado State University
Co-organizers: Mehmet Aktas, `maktas@uco.edu`, University of Central Oklahoma
Wenwen Li, `wli11@ou.edu`, University of Oklahoma
Murad Ozaydin , `mozaydin@math.ou.edu`, University of Oklahoma

Schedule: PHSC 222 (for all four sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

Persistence-based summaries of metric graphs
Ellen Gasparovic, Union College
Abstract: This talk will focus on topological summary information that one can capture from metric wedge sums, gluings, and graphs. We will give a complete characterization of the persistence diagrams in dimension 1 for metric graphs under a particular intrinsic setting. We will look at two persistence-based distances that one may define for metric graphs and discuss progress toward establishing their discriminative capacities. We will show that the Vietoris-Rips (resp., Cech) complex of a wedge sum, equipped with a natural metric, is homotopy equivalent to the wedge sum of the Vietoris-Rips (resp., Cech) complexes. We also provide generalizations for when two metric spaces are glued together along a common isometric subset. As a result, we can describe the persistent homology, in all homological dimensions, of the Vietoris-Rips complexes of a wide class of metric graphs. This talk covers joint work with Michal Adamazsek, Henry Adams, Maria Gommel, Emilie Purvine, Radmila Sazdanovic, Bei Wang, Yusu Wang, and Lori Ziegelmeier.

Automated Learning of Topological Features: Predicting Protein Stability

Francis Motta, Florida Atlantic University
Abstract: Considerable effort has been spent developing tools that are designed to strengthen the applicability of computational statistics and machine learning to persistent homology. For example, several methods that transform persistence diagrams into vectors, which aim to map the algebraic content of a persistence diagram to feature vectors to be subsequently used with machine learning paradigms, have been proposed. Often these transformations require choices, which may be regarded as model hyperparameters to be tuned to a given problem or determined by prior subject-matter expertise. We show how to use the Cover-tree Differencing via Entropy Reduction algorithm (CDER)—a general tool for performing supervised learning on labeled point clouds—to automatically learn discriminating and parsimonious sets of coordinates to vectorize persistence diagrams. We apply this technique to the problem of predicting synthetic protein stability and discuss its potential to reveal new biological insights via interpretation of the learned coordinates. This material is based upon work supported by the Defense Advanced Research Projects Agency (DARPA) and the Air Force Research Laboratory under Contract No. FA8750-17-C-0054 (and related contracts by SD2 Publication Consortium Members).

Multirank: a combinatorial multiparameter persistent homology invariant
Ashleigh Thomas, Duke University
Abstract: This talk introduces a novel multiparameter persistence invariant – the multitrank function – that captures geometric information about how homology classes move through a filtration, including how classes persist, merge, and branch. Multiranks of persistence modules are ranks of homomorphisms between finite direct sums of homology groups. In the case where the source and target direct sums have one summand each, multirank is the usual rank function. Multirank extends the behavior of the rank function to multiparameter persistence in that it 1) directly measures how many homology classes persist across subposets that are "wider" than intervals and 2) determines the degree and multiplicity at which all births and deaths occur. A computationally friendly version of multirank, called m-rank, restricts the number of source and target direct summands to at most m; it determines all births and deaths when m is sufficiently large.

Persistent homology on dynamically changing functional brain network
Moo K. Chung, University of Wisconsin-Madison
Abstract: Advances in functional magnetic resonance imaging (fMRI) techniques enabled us to measure spontaneous fluctuations of neural signals in the brain. Many previous studies on resting-state fMRI have mainly focused on the topological characterization of static graph theory features that will not fluctuate over time. In this talk, we present a simple but very effective data-driven approach to assess the dynamic pattern of resting state functional connectivity using persistent homology.Persistent homology has been successfully applied to various static brain networks by building graph filtrations by sequentially thresholding edge weights. For dynamic networks, we propose to build graph filtrations over time and edge weights at the same time. Stable connectivity pattern that behaves like the backbone of networks through fluctuating functional connectivity are also identified. The recently proposed exact combinatorial inference procedure for static network was adapted for statistically quantifying dynamic brain networks. This talk is based on arXiv:1509.04771.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Topological modeling of biomolecular data
Kelin Xia, Nanyang Technological University
Abstract: The understanding of biomolecular structure, flexibility, function, and dynamics is one of the most challenging tasks in biological sciences. In this talk, I will introduce molecular topological fingerprints (MTFs), which are derived from the persistent homology analysis and provide a unique representation of the biomolecular structure. Further, I will talk about a special multidimensional persistent homology and its application in protein folding analysis. The simulation of the unfolding process is done by using steered molecular dynamics. An excellent consistence between my persistent homology prediction and folding energy is found. More importantly, topological quantities from this unique topological representation can be used as features in machine learning models and have been proved to be highly efficient, particularly in drug design. Finally, I will discuss a weighted persistent homology model which can incorporate the weight information of simplicial complexes into the filtration process.

A Topological Approach to Spatio-temporal Pattern Formation
Melissa McGuirl, Brown University
Abstract: Spatio-temporal pattern formation appears in a range of natural applications, from Rayleigh–Bénard convection to vegetation patches. Many dynamical system models have been created and analyzed to better understand the evolution of these patterns. In this talk we apply methods from topological data analysis to analyze an agent-based model for pattern formation on zebrafish and the Rossler system for the study of spiral wave patterns. In particular, we will use topological properties of the spatio-temporal patterns for both classification and stability analyses.

Classifying fingerprints with persistent homology

Noah Giansiracusa, Swarthmore College
Abstract: Classifying fingerprints (dividing them into loops, whorls, arches, etc.) is a natural problem to apply topological methods to since these classes are independent of choice of coordinates. I'll discuss joint work with Chul Moon where we apply persistent homology and perform machine learning feature selection in several different ways and compare the results.

Learning non-positively curved cubical complexes
Dan Guralnik, University of Pennsylvania
Abstract: I will show how Sageev-Roller duality of finite CAT(0) cubical complexes (AKA "cubings") may be exploited for learning and maintaining a dynamically evolving, modality-agnostic internal representation of an agent's interactions with its environment. The emphasis of this representation method is on computational efficiency, to be achieved by distributing the tasks of representation and control among multiple binary agents, each deciding whether to act or not to act, at any given time, according to a private prediction extracted from an internal representation which takes the form of the dual poc set of a cubing. I will present some results on learning such representations, relate them to the homotopy type of the system's configuration/state space, together with simulations of such agents "at work". This is a joint work with Daniel Koditschek.

Session III Sat, Oct. 6, 05:00pm - 06:20pm

On Kernels and Cokernels in Persistent Homology
Jan Segert, University of Missouri
Abstract: In a recent paper (arXiv:1701.02055 [math.AT]) we introduced an alternative categorical framework for persistent homology, and studied barcode decompositions in the alternate framework. In this talk I will consider kernels and cokernels of a morphism in the alternate categorical framework, explained with simple concrete examples.

Learning Simplicial Complexes from Persistence Diagrams
Robin Belton, Montana State University
Abstract: Topological Data Analysis (TDA) studies the "shape" of data. A common topological descriptor is the persistence diagram, which encodes topological features in a topological space at different scales. Turner, Mukherjee, and Boyer showed that one can reconstruct a simplicial complex embedded in $\mathbb{R}^3$ using persistence diagrams generated from all height filtrations (an uncountably infinite number of directions). In this talk, we present an algorithm to reconstruct plane graphs, $K = (V, E)$ in $\mathbb{R}^2$, i.e., a planar graph with vertices in general position and a straight line embedding, from a quadratic number of height filtrations and their respective persistence diagrams. If time allows, we will also discuss current work on how one can use collections of persistence diagrams generated from height filtrations for shape alignment.

The importance of forgetting: Limiting memory improves recovery of topological characteristics from neural data
Samir Chowdhury, The Ohio State University
Abstract: Place cells in the hippocampus are known for their importance in spatial learning. Previously, Curto and Itskov showed that knowledge of which groups of place cells cofire in a rodent hippocampus is sufficient to recover the topology of the rodent's physical environment. The topological method here comprises the following steps: represent the place cells as vertices of an abstract simplicial complex, insert higher simplices corresponding to cells that fire together, and then compute the homology of the resulting complex. This follows the classical Hebbian "fire together, wire together" learning model. Prior studies have used models where only synaptic potentiation ("wire together") events are considered. However, depotentiation ("unwiring" or "forgetting") is a key complementary event that has recently been proposed as an important component of spatial learning. We explore this possibility by first simulating a model of rodent place cell activity that incorporates depotentiation according to a memory parameter, and then computing the accuracy with which the place cell representations can tell apart different environments as a function of memory. We obtain the surprising conclusion that some amount of forgetting is beneficial for the learning process—likely by erasing "errors" that occur when learning place cell representations.

Vietoris-Rips thickenings of the circle and centrally-symmetric orbitopes
Johnathan Bush, Colorado State University
Abstract: Given a metric space X and scale parameter $r > 0$, the Vietoris-Rips simplicial complex $VR(X;r)$ has as its simplices all finite subsets of X of diameter less than r. A result of Jean-Claude Hausmann states that the homotopy type of X often may be recovered from $VR(X;r)$ for sufficiently small r. However, much less is known about the topological behavior of these complexes for large values of r, despite the fact that they arise naturally in applications of persistent homology. One result along these lines, due to Adams and Adamaszek, provides the homotopy type of the Vietoris-Rips complex of the circle for all r. On the other hand, a simplicial complex $VR(X;r)$ does not preserve metric information about X, and this deficiency motivates the consideration of a separate but related construction, called the Vietoris-Rips metric thickening. We will discuss the homotopy type of the Vietoris-Rips thickening of the circle for a range of scale parameters. Our primary tools will be an embedding of

the Vietoris-Rips thickening into Euclidean space via a symmetric moment curve, together with the facial structure of the Barvinok-Novik orbitope.

Session IV Sun, Oct. 7, 10:30am - 11:50am

On homology reconstruction of geodesic subspaces
Rafal Komendarczyk, Tulane University
Abstract: In this work in progress, we develop a persistence based algorithm for the homology/homotopy groups reconstruction of the unknown underlying geodesic subspace of R^n from a point cloud. In the case of a metric graph, we can output a subspace which is an arbitrarily good approximation of the underlying graph.

Enhancing witness complexes modeling chaotic dynamical systems
Nicole Sanderson, University of Colorado Boulder
Abstract: Topological data analysts often model point cloud data with a simplicial complex and compute the persistent homology as a topological signature. When point cloud data comes from a dynamical system, the object we seek to model topologically is inherently not stagnant. Properties of the dynamics can inform us about the underlying topology of the attractor of the dynamical system that may be obscured by the geometry of the point cloud. Encoding the local dynamics as unit tangent vector approximations at each data point and penalizing the distance between points in the reconstructed state space traveling in dissimilar directions, we can both cheapen the construction of filtrations of witness complexes and enhance the topological signature of the attractor as reported by the persistent homology. We demonstrate this through a set of new topological statistics on the persistent homology of delay reconstructions of chaotic dynamical systems.

Restricted Configuration Spaces of a Metric Graph
James Dover, Cameron University
Abstract: We consider the space of configurations of n ordered points on a finite, connected metric graph with a vector-valued restraint parameter r dictating the minimum distance permitted between each pair of points. This restricted configuration space arises naturally in topological robotics when the n points represent robots of varying sizes. In this talk, we discuss the homeomorphism and homotopy types of this space, which are indexed by the faces of a hyperplane arrangement in the space of parameters r.

Thin position motivated weight regularization for deep neural networks
Doug Heisterkamp, Oklahoma State University
Abstract: This talk presents an initial investigation of a topologically motivated weight regularization for deep neural networks. The topological approach uses the algorithms of topologically intrinsic lexicographic ordering (TILO), pinch ratio clustering (PRC), and thin tree position (TTP) which are inspired by thin position for knots and 3-dimensional manifolds. Artificial neural networks conduct computations distributed over the nodes of the network and this computation is typically opaque (hard to interpret). Current weight regularization is typically applied uniformly over the weights of the network. The approach of this talk is to use topological information to create a relative importance scores for weights and nodes that are then used for non-uniform regularization. The long term goal of this approach is to bias the distributed computation into functional submodules which are interpretable and reusable.

MS08. Recent Advances of Numerical Methods in Fluid Mechanics with Applications

Organizer: Jia Zhao, `jia.zhao@usu.edu`, Utah State University
Co-organizer: Daozhi Han, `handaoz@mst.edu`, Missouri University of Science and Technology

Schedule: PHSC 323 (for all four sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

Partitioning algorithms for the system of a fluid and a poroelastic structure
Hyesuk Lee, Clemson University
Abstract: Computational algorithms for the generalized Stokes-Biot coupled system are proposed for the interaction of a free fluid with a poroelastic structure. The talk is focused on decoupling schemes that allow the non-Newtonian fluid and the poroelastic structure computed independently using a common stress force along the interface. This approach is based on a nonlinear operator equation, where the operator measures violation of some interface conditions. Numerical algorithms based on a Newton-type updating technique are discussed and numerical results are provided to validate the accuracy and efficiency of the proposed algorithms.

Well-Balanced Positivity Preserving Central-Upwind Scheme with a Novel Wet/Dry Reconstruction on Triangular Grids for the Saint-
Yekaterina Epshteyn, The University of Utah
Abstract: In this talk we will introduce and discuss second-order central-upwind scheme for the Saint-Venant system of shallow water equations on triangular grids. The Saint-Venant system is widely used in many scientific and engineering applications related to modeling of water flows in rivers, lakes and coastal areas. The development of robust and accurate numerical methods for the simulation of shallow water equations is important and challenging problem. In our talk we will show that

the designed central-upwind scheme preserves ”lake at rest” steady states, guarantees the positivity of the computed fluid depth and delivers accurate reconstruction of “dry”/“almost dry states” (waves arriving or leaving the shore). Moreover, it can be applied to models with discontinuous bottom topography and irregular channel widths. We will demonstrate these features of the proposed scheme, as well as its high resolution and robustness in a number of numerical examples.

Modeling and computation of an elastic tumor-host interface

Shuwang Li, Illinois Institute of Technology

Abstract: We consider the nonlinear dynamics of an avascular tumor at the tissue scale using a two-fluid flow Stokes model, where the viscosity of the tumor and host micro-environment may be different. In an effort to understand the role the interface stiffness plays on tumor evolution, here we model the tumor-host interface as an elastic membrane governed by the Helfrich bending energy. Using an energy variation approach, we derive a modified Laplace-Young condition for the stress jump across the interface in the Stokes equation. We then perform a linear morphological stability analysis of the tumors, and investigate the role of nonlinearity using boundary-integral simulations in two dimensions. Simulation results are consistent with linear theory for nearly circular tumors. As perturbations develop and grow, preliminary nonlinear results show that the tumors tend to develop invasive fingers and a branched- like structure, if the tumor is more viscous than its environment.

A Second Order Fully-discrete Linear Energy Stable Numerical Scheme of a Binary Compressible Viscous Fluid Model

*Xueping Zhao,*University of South Carolina

Abstract: We derive a thermodynamically consistent hydrodynamic phase field model of binary compressible fluid flow mixtures using the generalized Onsager Principle, warranting not only the variational structure, but also the mass, linear momentum conservation, and the energy dissipation law in an isothermal case. To solve this mathematical model, we present a linear, second order fully discrete numerical scheme on a staggered grid. We prove the unique solvability of the linear scheme rigorously. Finally, we present several numerical examples, including phase separation due to the spinodal decomposition of two polymeric fluids and the gas-liquid mixture, to show the convergence property, stability, and efficiency of the new scheme.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Optimal rate convergence analysis for Cahn-Hilliard equation coupled with fluid flow

Cheng Wang, University of Massachusetts Dartmouth

Abstract: A few fully discrete numerical schemes for the Cahn-Hilliard-Hele-Shaw and Cahnn-Hilliard-stokes equations, a modified Cahn-Hilliard model coupled with with the the Darcy or Stokes flow law, are analyzed in details. The unique solvability comes from the variational calculation, while and unconditional energy stability comes from the energy estimate. In turn, a uniform in time H^1 bound for the numerical solution becomes available. Moreover, with the help of discrete Gagliardo-Nirenberg type inequality, derived in terms of discrete Fourier analysis, we are able to obtain the $L^2(0,T;H^3)$ stability of the numerical solution. Subsequently, we perform a discrete $L^\infty(0,T;H^1)$ and $L^2(0,T;H^3)$ error estimate, instead of the $L^\infty(0,T;L^2)$ and $L^2(0,T;H^2)$ one, which represents the typical analysis. Such an approach allows us to treat the nonlinear convection term in a positive way, since one essential nonlinear inner product turns out to be non-negative. Some numerical simulation results are also presented in the talk.

Stabilized-IEQ and Stabilized SAV method for gradient flow models with strong anisotropy

Xiaofeng Yang, University of South Carolina

Abstract: We consider numerical approximations for gradient flow models with strong anisotropy by taking the anisotropic Cahn-Hilliard/Allen-Cahn equations with their applications to the faceted pyramids on nano scale crystal surfaces and the dendritic crystal growth problems, as special examples. The main challenge of constructing numerical schemes with unconditional energy stabilities for these type of models is how to design proper temporal discretizations for the nonlinear terms with the strong anisotropy. We combine the recently developed IEQ/SAV approach with the linear stabilization approach, where some linear stabilization terms are added. These terms are shown to be crucial to remove the oscillations caused by the anisotropic coefficients, numerically. The novelty of the proposed schemes is that all nonlinear terms can be treated semi-explicitly, and one only needs to solve some coupled/decoupled, but linear equations at each time step. We further prove the unconditional energy stabilities rigorously, and present various 2D and 3D numerical simulations to demonstrate the stability and accuracy.

A dual-porosity-Stokes model and finite element method for coupling dual-porosity flow and free flow

Xiaoming He, Missouri University of Science and Technology

Abstract: We propose and numerically solve a new model considering confined flow in dual-porosity media coupled with free flow in embedded macro-fractures and conduits. Such situation arises, for example, for fluid flows in hydraulic fractured tight/shale oil/gas reservoirs. The flow in dual-porosity media, which consists of

both matrix and micro-fractures, is described by a dual-porosity model. And the flow in the macro-fractures and conduits is governed by the Stokes equation. Then the two models are coupled through four physically valid interface conditions on the interface between dual-porosity media and macro-fractures/conduits, which play a key role in a physically faithful simulation with high accuracy. All the four interface conditions are constructed based on fundamental properties of the traditional dual-porosity model and the well-known Stokes-Darcy model. The weak formulation is derived for the proposed model and the well-posedness of the model is analyzed. A finite element semi-discretization in space is presented based on the weak formulation and four different schemes are then utilized for the full discretization. The convergence of the full discretization with backward Euler scheme is analyzed. Four numerical experiments are presented to validate the proposed model and demonstrate the features of both the model and numerical method, such as the optimal convergence rate of the numerical solution, the detail flow characteristics around macro-fractures and conduits, and the applicability to the real world problems.

Session III Sat, Oct. 6, 05:00pm - 06:20pm

Efficient algorithms for simulating ensembles of parameterized flow problems

Zhu Wang, University of South Carolina

Abstract: Many computational fluid dynamics applications require multiple simulations of a flow under different input conditions. In this talk, we consider such settings for which one needs to perform a sequence of simulations based on the Navier-Stokes equations, each having different initial condition data, boundary condition data, forcing functions, and/or coefficients such as the viscosity. For such settings, we propose ensemble methods to accelerate the solutions. The main idea is to manipulate the time-stepping scheme so that all the problems could share a common coefficient matrix, then, instead of solving a sequence of linear systems with one right-hand-side vector, the method needs to solve one linear system with multiple right-hand-sides. The computational efficiency is then improved by using block iterative algorithms. Rigorous analyses are given proving the conditional stability and establishing error estimates for the proposed algorithms. Numerical experiments are presented to illustrate the analyses.

Eddy viscosity models for turbulence not at statistical equilibrium

Nan Jiang, Missouri University of Science and Technology

Abstract: Standard eddy viscosity models, while robust, cannot represent backscatter and have severe difficulties with complex turbulence not at statistical equilibrium. In this talk, we give a new derivation of eddy viscosity models from an equation for the evolution of variance in a turbulent flow. The new derivation also shows how to correct eddy viscosity models. We prove that the corrected models preserve important features of the true Reynolds stresses and give algorithms for their discretization including a minimally invasive modular step to adapt an eddy viscosity code to the extended models.

Conservative Explicit Local Time-Stepping Schemes for the Shallow Water Equations

Thi-Thao-Phuong Hoang, Auburn University

Abstract: In this talk, we present explicit local time-stepping schemes of second and third order accuracy for the shallow water equations. The system is discretized in space by a C-grid staggering method, namely the TRiSK scheme adopted in MPAS-Ocean, a global ocean model with the capability of resolving multiple resolutions within a single simulation. The time integration is designed based on the strong stability preserving Runge-Kutta methods but with different time step sizes in different regions of the domain restricted by respective local CFL conditions. The proposed local time-stepping schemes preserve all important properties in the discrete sense, such as exact conservation of the mass and potential vorticity and conservation of the total energy within time-truncation errors. Extensive numerical tests are presented to illustrate the performance of the proposed algorithms.

Incremental POD mode algorithm for fluids with a computable error bound

John Singler, Missouri University of Science and Technology

Abstract: We discuss an incremental algorithm for proper orthogonal decomposition (POD) computations. Specifically, we develop an incremental matrix SVD algorithm with respect to a weighted inner product for POD computations of data arising from Galerkin-type simulation methods for time dependent PDEs. The algorithm initializes and efficiently updates the POD eigenvalues and modes during the time stepping in a PDE solver without storing the simulation data. Also, the algorithm returns an easily computed error bound. We demonstrate the effectiveness of the algorithm using finite element computations for fluid flows.

Session IV Sun, Oct. 7, 10:30am - 12:10pm

Fully Discrete Second-order Linear Schemes for Hydrodynamic Phase Field Models of Binary Viscous Fluid Flows with Variable Density

Jia Zhao, Utah State University

Abstract: In this talk, we present spatial-temporally second-order, energy stable numerical schemes for two classes of hydrodynamic phase field models of binary viscous fluid mixtures of different densities and viscosities. One is quasi-incompressible while the other is incompressible. We introduce a novel invariant energy qudratization (IEQ) technique to arrive at fully discrete linear schemes, where in each time step only a linear system needs to be solved. These schemes are then proved to be unconditionally energy stable rigorously so that a large time step is plausible. Both spatial and temporal mesh refinements are conducted to illustrate the second- order accuracy of the schemes. Several Numerical examples and conducted, and predictions by the two fluid-mixture models are compared and discussed. As a conclusion, we believe the quasi-incompressible model is more reliable than the incompressible one.

An HDG Method for Tangential Boundary Control of Stokes Equations

Yangwen Zhang, University of Delaware

Abstract: We propose a hybridizable discontinuous Galerkin(HDG) method to approximate the solution of a tangential Dirichlet boundary control problem governed by Stokes equation. Dirichlet boundary control problems are naturally studied in the L2-setting, and therefore well-known to be challenging due to its non variational form and low regularity, even for simpler elliptic PDEs. Although there are many works in the literature on Dirichlet boundary control problems for fluids flow, the authors are not aware of any existing theoretical or numerical analysis for Dirichlet boundary control of Stokes or Navier-Stokes equation in such setting. To avoid the extreme low regularity of solutions for Stokes Dirichlet boundary control, this work gives a first attempt to the analysis of tangential boundary control of fluid flows with controls in L2. The contribution of this paper is twofold. First, we obtain well-posedness and regularity results for the tangential Dirichlet control problem. Second, under certain assumptions on the domain and the target state, we obtain optimal a priori error estimates for the control in 2D for the HDG method. We present numerical experiments to demonstrate the performance of the HDG method.

MS09. Modeling and Analysis in Ecology and Epidemiology

Organizer: Matthew Beauregard, `beauregama@sfasu.edu`, Stephen F. Austin State University

Schedule: PHSC 115 (for all three sessions)

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Analysis of Modified Trojan Y-Chromosome Model for Eradicating Nonnative Fish

Sarah Boon, Stephen F Austin State University
Harley Conaway, Stephen F Austin State University
Thomas Griffin, Stephen F Austin State University

Abstract: The Trojan Y-Chromosome (TYC) strategy is a proposed method to eradicate an invasive species. The strategy consists of introducing sex-reversed males containing two Y chromosomes into a habitat to skew the sex ratio of subsequent generations toward an increasing number of males. A new mathematical model that incorporates both a strong Allee effect and intraspecies competition between supermales and wild-type males for females mates is provided. The efficacy of the strategy is examined through the mathematical model. The influence of the frequency and amplitude of introduction on the strategy effectiveness will also be discussed. This is joint talk with Sarah Boon, Harley Conaway, and Thomas Griffin

A comparison of the TYC Strategy to pure harvesting

Jingjing Lyu, Clarkson University

Abstract: The Trojan Y Chromosome Strategy (TYC) is a promising method for biological control of invasive species that works on manipulating the sex ratio of an invasive population towards all males. In the current manuscript we compare the classical TYC strategy to a pure harvesting strategy, as well as explore hybrid methods that combine the pure strategy with harvesting methods.The dynamical analysis leads to results on stability, global boundedness and bifurcations of the model. Next, via optimal control methods we draw several conclusions about the different methods. Our results have key implications for preserving native species under invasion by non-natives. In particular they we affirm that a pure harvesting strategy or a hybrid method works better than the classical TYC method.

The effect of additional food on introduced predators for biological control

Rana Parshad, Iowa State University

Abstract: Biological control, the use of predators and pathogens to control target pests, is a promising alternative to chemical control. It is hypothesized that the predators efficacy can be boosted by providing it with an additional food source. In the current literature it is proved that if the additional food is of sufficient constant quantity and quality then pest eradication is possible in finite time. We show to the contrary that pest eradication is not possible in finite time, and will occur only in infinite time to which end we derive decay rates. However for a density dependent quantity of additional food, we show pest eradication in finite time is indeed possible. We also consider the case of both predator and prey evolution taking place, and its effect on the dynamics of the system. Our results have many consequences for designing effective biological control strategies.

The "destabilizing" effect of cannibalism in a spatially explicit three-species age structured predator-

prey model
Aladeen Al Basheer, The University of Georgia

Abstract: Cannibalism, which is the act of killing and consumption of conspecifics, has been considered primarily in the predator, despite strong ecological evidence that it exists among prey. In the current manuscript, we investigate both the ODE and spatially explicit forms of a Holling–Tanner model, with ratio dependent functional response, and show that cannibalism in the predator provides a stabilizing influence as expected. However, when cannibalism in the prey is considered, we show that it cannot stabilize the unstable interior equilibrium in the ODE case, in certain parameter regime, but can destabilize the stable interior equilibrium, leading to a stable limit cycle or "life boat" mechanism, for prey. We also show that prey cannibalism can lead to pattern forming Turing dynamics, which is an impossibility without it.

Session III Sat, Oct. 6, 05:00pm - 06:20pm

Landscape heterogeneity
Patrick Shipman, Colorado State University

Abstract: Landscape heterogeneity and long-distance transportation connections can be factors in the spread of an infectious disease or an invasive species. We analyze mathematical models including these factors for the spread of the invasive cheatgrass and for the spread of white-nose syndrome in bat populations.

Flapping Flight of Ecologically Important Tiny Insects
Arvind Santhanakrishnan, Oklahoma State University

Abstract: Miniature flying insects with body lengths less than 1 mm, such as thrips and some parasitoid wasps, serve important ecological roles that include: transmitting pollen during feeding, invasive pests of agriculturally important plants, and biological vectors of microbial plant pathogens. However, the aerodynamics of flapping flight of these insects has been relatively unexplored. Understanding single-organism level aerodynamics is needed prior to the development of mathematical models of their collective dispersal. The flapping wing kinematics in thrips is characterized by wing-wing interaction (clap and fling), such that the wings clap at the end of the upstroke and fling apart at the beginning of the downstroke. These insects also show unique adaptations in their wing design, consisting of a thin solid membrane with long bristles at the fringes. Given the challenges of acquiring real-time recordings of freely flying insects at length scales of under a millimeter while resolving fast wing beats on the order of 100 Hz, we use experiments on dynamically scaled physical models and 2D numerical simulations for investigation. In this talk, I will discuss the importance of bristled wing morphology and wing-wing interaction in the aerodynamics of tiny insect flight.

The Spatio-Temporal Spread of a Vector Host Disease over a Large Domain
William Fitzgibbon, University of Houston

Abstract: We are concerned with a class of models describing the spatio-temporal spread of vector host disease over a large domain. Previous work has considered the case where the host and vector population inhabit the same domain or the case of vectors inhabiting subdomains of a larger domain inhabited by the host. Here we shall consider the case of the host occupying subdomains of a larger domain. The work contained herein is further differentiated from previous work by virtue of the fact we define the vector habitat as all of $\mathbb{R}^2$. Of particular interest is the spread of the disease over a large geographic disease free region by virtue of the introduction of infected hosts into a relatively small subregion. Our work is motivated by Blue Tongue Disease. Blue Tongue disease is a non-contagious viral disease transmitted via bites of the midges of the genus culicoides to a variety of both domestic and wild ruminants including cattle, deer, goats, dromedaries, and antelopes.

Optimal Control Strategies for Dengue Transmission in Pakistan
Folashade Agusto, University of Kansas

Abstract: This paper presents a deterministic model for dengue virus transmission. The model was parameterized using data from the 2017 dengue outbreak in Pakistan. We estimated the basic reproduction number ($\mathcal{R}_0$) without any interventions for the 2017 dengue outbreak in Peshawar district of Pakistan as $\mathcal{R}_0 \approx 2.64$, the distribution of the reproduction number lies in the range $\mathcal{R}_0 \in [1.21, 5.24]$ (with a mean $\mathcal{R}_0 \approx 2.64$). Optimal control theory was then applied to investigate the optimal strategy for curtailing the spread of the disease using two time-dependent control variables determined from sensitivity analysis. These control variables are insecticide use and vaccination. The results show that the two controls avert the same number of infections in the district regardless of the weights on the costs this is due to the reciprocal relationship between the cost of insecticide use and vaccination. A strong reciprocal relationship exists between the use of insecticide and vaccination; as the cost of insecticide increases the use of vaccination increases. The use of insecticide on the other hand slightly increases when vaccination level decreases due to increase in cost.

Session IV Sun, Oct. 7, 10:30am - 11:50am

Tree Harvesting In Age-structured Forests Subject To Beetle Infestations
Benito Chen-Charpentier, University of Texas at Arlington

Abstract: In this presentation we investigate a mathematical model for age-structured forest-beetle interac-

tions. In the first part of this study, we consider different scenarios of the forest infestation by the beetle and observe that the quantitative age profile of the forest is significantly dependent on whether the beetle population is in an endemic or epidemic state. In the second part we include harvesting of the forest trees and analyze two different harvesting strategies: clear cutting trees older than a certain age, and using a cut rate proportional to the number of trees older than a certain age. Numerical simulations are implemented to determine the optimal cutting age for both harvesting strategies. The numerical simulations reveal that, independent of the beetle population's steady state (that is, no beetles, endemic or epidemic state) clear cutting all trees older than a given age provides a higher harvesting benefit. Our numerical simulations further indicate that in order to obtain a fixed harvesting yield, a forest under an beetle epidemic state have to be cut at a younger age than if the forest were at an endemic beetle state or a no beetle state.

Numerical Realizations of Nonlinear Population Models with Self and Cross Diffusion
Matthew Beauregard, Stephen F. Austin State University
Abstract: Self- and cross-diffusion are important and often neglected nonlinear spatial derivative terms that are included into population models in ecology. Self-diffusion models overcrowding effects, while cross-diffusion incorporates the response of one species in light of the concentration of another. The underlying diffusion matrix is no longer positive definite which complicates the theoretical analysis and development of numerical approximations. In this talk, we explore a convergent nonlinear operator splitting routine and then compare this to a newly developed positivity-preserving numerical approximation.

MS10. Complex Patterns

Organizer: Patrick Shipman, shipman@math.colostate.edu, Colorado State University

Schedule: PHSC 115

Session I Sat, Oct. 6, 10:40am - 12:00pm

Pattern Structures in Vapor-to-Particle Reactions
Bahaudin Hashmi, Texas State University
Abstract: When ammonia and hydrogen chloride react in a tube, an oscillatory reaction front of the vapor ammonium chloride is formed that nucleates to the formation of solid ammonium chloride. After corroborating experimental data with our threshold function, additional simulations were conducted with parametric variations that demonstrated pattern structures observed in other similar reactions. We will also demonstrate how the topological positioning of the reactants affects the resulting pattern of the solid ammonium chloride.

Effects of anisotropy in pattern forming systems
Derek Handwerk, Colorado State University
Abstract: The isotropic complex Ginzburg-Landau (CGL) equation has been derived as an amplitude equation for Poiseuille flows and reaction-diffusion equations. The Kuramoto-Sivashinky (KS) equation can be extracted via a multiple-scales expansion from the CGL as a phase equation. Both of these equations have been well studied and exhibit wide ranging dynamics including spatio-temporal chaos. The anisotropic versions of these equations, ACGL and AKS, have arisen in the study of electroconvection of nematic liquid crystals, surface nanopatterning by ion-beam erosion, chemical waves in catalytic surface reactions, epitaxial growth, and solidification from a melt. The effects of the added anisotropy will be discussed.

Spatiotemporal Complex Patterns in Anisotropic Systems
Iuliana Oprea, Colorado State University
Abstract: Unlike low dimensional systems, where different scenarios for the transition to chaos have been established, in spatially extended systems the transition from regular stationary patterns to complex spatiotemporal regimes is only partially understood. In this presentation we identify and characterize the instability mechanisms generating the spatiotemporal complex patterns, such as spatiotemporal intermittency and chaos, in the numerical simulations of a system of four globally coupled complex Ginzburg Landau equations. Applications to the electroconvection of nematic liquid crystals are also presented.

MS11. Partial Differential Equations: Analysis, Modeling, and Applications

Organizer: John Singler, singlerj@mst.edu, Missouri University of Science and Technology
Co-organizer: Weiwei Hu, weiwei.hu@okstate.edu, Oklahoma State University

Schedule: PHSC 316 (for all three sessions)

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Degenerate FCH Functional and Defects in Amphiphilic Structures
Shibin Dai, The University of Alabama
Abstract: We introduce a modified functionalized Cahn-Hilliard (FCH) functional to model the free energy of amphiphilic mixtures. We prove that the modified FCH functional admits geometrically localized minimizers, which correspond to lipid bilayers, filamentous pores, or micelles. In addition, we identify the leading order profile of the bilayers under the assumption that the geometri-

cally localized minimizers have bounded variations along the tangential directions. We will also describe how to handle defects caused by the presence of nanoparticles or molecules.

Stability of solitary waves for the 1d NLS with a delta potential

Jason Murphy, Missouri University of Science and Technology

Abstract: In this talk we will discuss recent joint work with S. Masaki (Osaka University) and J. Segata (Tohoku University) on the problem of asymptotic stability of small solitary wave solutions to the one-dimensional nonlinear Schr odinger equation with a delta potential.

Recent Performance Optimizations of Front Tracking Based Simulation Package

Tulin Kaman, University of Arkansas

Abstract: Performance studies are conducted to identify the optimization potential in the computational fluid dynamics (CFD) code used for efficient numerical simulations of compressible turbulent mixing problems on high performance computing systems. For these studies, one of the most powerful supercomputers, Blue Waters, is used. A case study on the use of CrayPat Profiler Toolkit for performance analysis and the recent enhancements to front tracking based CFD code are presented.

Session III Sat, Oct. 6, 05:00pm - 06:20pm

On the long–time behavior of a perturbed conservative system with degeneracy

Wenqing Hu, Missouri University of Science and Technology

Abstract: We consider in this work a model conservative system subject to dissipation and Gaussian–type stochastic perturbations. The original conservative system possesses a continuous set of steady states, and is thus degenerate. We characterize the long–time limit of our model system as the perturbation parameter tends to zero. The degeneracy in our model system carries features found in some partial differential equations related, for example, to turbulence problems.

Partially dissipative 2D Boussinesq equations with Navier type boundary conditions

Bei Xiao, Oklahoma State University

Abstract: This talk will focus on the system of the 2D Boussinesq equations with only kinematic dissipation in bounded domains with the Navier type boundary conditions. Firstly, because the Navier boundary conditions generate boundary terms and require compatibility conditions compared to the whole space and the periodic domains, we will provide a direct and transparent approach that explicitly reveals the impacts of the Navier boundary conditions. Then, we will present a proof of the global existence and uniqueness of the aforementioned system under minimal regularity assumptions on the initial data. The proof resorts to the existence and regularity results on the associated Stokes problem with Navier boundary conditions and Yudovich techniques with the introduction of a lower regularity counterpart of the temperature.

Boundary layers for primitive equations in a cube

Daozhi Han, Missouri University of Science and Technology

Abstract: It is well-known that the inviscid primitive equations (IPE) are ill-posed for any local boundary conditions. We propose a set of nonlocal boundary conditions for the IPE in a cube by investigating the boundary layers associated with the viscous primitive equations. We establish the convergence in energy norms.

An Analysis of Parameter Sensitivity in Continuous Data Assimilation of Turbulent Flow

Elizabeth Carlson, University of Nebraska-Lincoln

Abstract: One of the challenges of the accurate simulation of turbulent flows is that initial data is often incomplete. Data assimilation circumvents this issue by continually incorporating the observed data into the model. Recently a new approach to data assimilation known as the Azouani-Olson-Titi (AOT) algorithm introduced a feedback control term to the 2D incompressible Navier-Stokes equations in order to incorporate sparse measurements. It was proven that the solution to the AOT algorithm for continuous data assimilation converges exponentially to the true solution of 2D incompressible Navier-Stokes equations with respect to the given initial data. In this talk we examine the parameter sensitivity of viscosity. Specifically, we analyze how perturbations of viscosity affect the convergence of the AOT algorithm to the 2D incompressible Navier-Stokes equations. Analytical and computational results will be presented.

Session IV Sun, Oct. 7, 10:30am - 11:50am

On the velocity-vorticity-Voigt formulation of the 3D Navier-Stokes equations

Yuan Pei, Western Washington University

Abstract: In this talk, we propose a new regularization of the 3D Navier-Stokes equations, which we call the 3D velocity-vorticity-Voigt (VVV) model, with a Voigt regularization term added to momentum equation in velocity-vorticity form, but with no regularizing term in the vorticity equation. We prove global well-posedness and regularity of this model along with an energy identity. We also show convergence of the model's velocity and vorticity to their counterparts in the 3D Navier-Stokes equations as the Voigt modeling parameter tends to zero. Further, we provide a criterion for finite-time blow-up of the 3D Navier-Stokes equations based on this inviscid regu-

larization. This is joint work with Adam Larios and Leo Rebholz.

A surface moving mesh method based on the equidistribution and alignment

Avary Kolasinski, University of Kansas

Abstract: We will propose an approach for mesh adaptation on surfaces that, to our best knowledge, is the only surface moving mesh method that can be directly applied to a general surface. We will formulate a surface functional based on equidistribution and alignment conditions and employ an MMPDE to find its minimizer. We will then discuss various theoretical properties, which enable us to prove mesh nonsingularity. Finally, we will present numerical results in two and three-dimensions.

The self-similar very singular solution for nonlinear diffusion equations with gradient absorption

Hailong Ye, Shenzhen University

Abstract: In this talk, I will present the uniqueness of self-similar very singular solutions with compact support for the following diffusion equation with gradient absorption $\frac{\partial u}{\partial t} = \text{div}\left(|\nabla u^m|^{p-2}\nabla u^m\right) - |\nabla u|^q$, $x \in \mathbb{R}^N$, $t > 0$, where $m > 0$, $p > 1$, $m(p-1) > 1$ and $q > 1$.

Effects of Permanent Charge and Boundary Condition on Ionic Flow via a Quasi-1D Poisson-Nernst-Planck Model

Yufei Yu, University of Kansas

Abstract: Ionic channels – large proteins on cell membrane – are a major way for ions to transport through cell membrane that carries electric signals for cells to communicate with each other. The permanent charge of an ion channel is the crucial structure for ionic flow properties of the channel. The effects of permanent charges interacting with boundary conditions have been studied analytically via the Quasi-1D Poisson-Nernst-Planck (PNP) model for small permanent charge and for large permanent charge. In this talk, we will present results of numerical investigation to bridge between the two extrema. As expected, our numerical results verify the analytical predictions for small and large permanent charges. On the other hand, non-trivial behavior emerges as one varies the permanent charge from small to large, in particular, bifurcations are revealed, showing the rich phenomena of permanent charge effects by the power of combining the analytical and numerical studies. An adaptive moving mesh finite element method has been applied which is critical due to the presence of Debye layers at the interface between the permanent charge regions and uncharged regions of ion channels.

MS12. Novel Mathematical Methods with Applications to Continuum Mechanics

Organizer: Anna Zemlyanova,, azem@ksu.edu, Kansas State University
Co-organizer: Thomas DeLillo, delillo@math.wichita.edu, Wichita State University

Schedule: PHSC 114 (for both sessions)

Session III Sat, Oct. 6, 05:00pm - 06:20pm

Potential flow in a multiply connected circle domain using series methods

Justin Mears, Wichita State University

Abstract: We study series solutions to potential flow over an assembly of disks in the complex plane. Boundary value problems are solved for both streaming flow uniform at infinity and flow with circulation using Laurent series. The circles are the images of multi-element airfoils under conformal mapping and the circulations around the disks can be found so that the combined flow satisfies the Kutta condition at the preimages of the trailing edges. Some comparisons with other methods for computing the flow, such as reflection methods, will be given.

Discrete-to-Continuum Modeling of Weakly Interacting Incommensurate Chains

Malena Espanol, The University of Akron

Abstract: In this talk, we present a formal discrete-to-continuum procedure to derive a continuum variational model for two chains of atoms with slightly incommensurate lattices. The chains represent a cross-section of a three-dimensional system consisting of a graphene sheet suspended over a substrate. The continuum model recovers both qualitatively and quantitatively the behavior observed in the corresponding discrete model. We show that numerical solutions for both models demonstrate the presence of large commensurate regions separated by localized incommensurate domain walls. Joint work with Dmitry Golovaty and Patrick Wilber.

Dispersion of waves in periodic media

Yuri Godin, University of North Carolina at Charlotte

Abstract: We consider propagation of acoustic waves in a three-dimensional medium containing a periodic lattice of spherical inclusions. Propagation of waves is described by the Helmholtz equation with transmission boundary conditions on inclusions' interfaces. We assume that the dimensionless wave frequency is small that allows us to view the governing equation as a perturbation of the Laplace equation. The approach is based on the employment of periodic harmonic functions. Solution of the problem is sought in the form of a power series in terms of the magnitude of the wave vector of the Bloch wave. We provide a uniform explicit asymptotic expansion of

the dispersion relation, analyze it, and rigorously estimate the remainder.

Session IV Sun, Oct. 7, 10:30am - 11:50am

Surface elasticity in Steigmann-Ogden form in contact problems
Anna Zemlyanova, Kansas State University
Abstract: A problem of a frictionless or adhesive contact of a rigid stamp with an elastic semi-plane is treated analytically with the help of complex analysis techniques. The surface of the semi-plane is subjected to surface elasticity in the form proposed by Steigmann and Ogden. The boundary conditions on the banks of the semi-plane connect the stresses and the derivatives of the displacements. The mechanical problem is reduced to systems of singular integro-differential equations which are further reduced to the systems of equations with logarithmic singularities. The existence and uniqueness of the solution for almost all the values of the parameters is proved. Additionally, it is shown that introduction of the surface mechanics into the contact problems leads to the size-dependent equations. A numerical scheme of the solution of the systems of singular integro-differential equations is suggested, and the numerical results are presented for different values of the mechanical and the geometric parameters.

Rapidly Rotating Stars
Yilun (Allen) Wu, University of Oklahoma
Abstract: A rotating star may be modeled as a fluid under self gravity and with a given total mass and prescribed angular velocity. Mathematically this leads to the Euler-Poisson system. In this talk, we present an existence theorem for such stars that are rapidly rotating, depending continuously on the speed of rotation. No previous results using continuation methods allowed rapid rotation. The key tool for the result is global continuation theory via topological degree, combined with a delicate limiting process. The solutions form a connected set K in an appropriate function space. As the speed of rotation increases, we prove that either the supports of the stars in K become unbounded or the density somewhere within the stars becomes unbounded. We permit any equation of state of the form $p = \rho^\gamma$; $6/5 < \gamma < 2$, so long as $\gamma \neq 4/3$. This result is joint work with Walter Strauss.

Modeling and data inversion applied to a girder
Lynn Greenleaf, Stephen F. Austin State University
Abstract: Dynamic models of elastic structures are used to capture the behavior of a system under study. In this work, a concrete girder is loaded with different forces and the resulting displacements are measured. Given a priori engineering requirements, an underlying model with spatially dependent elastic properties is derived based on energy considerations. Least squares estimation techniques to calibrate a family of models with experimental data are considered. A probabilistic inversion approach focusing on the ability of models to capture the information contained in the data is discussed.

MS13. No scheduled talk

MS14. Recent Advances in Numerical PDEs

Organizer: Xiaoming He, `hex@mst.edu`, Missouri University of Science and Technology
Co-organizer: Erik Van Vleck, `erikvv@ku.edu`, University of Kansas

Schedule: PHSC 314 (for all four sessions)

Session I Sat, Oct. 6, 10:40am - 12:20pm

Modeling moire-driven mechanical relaxation in incommensurate multilayer structures
Paul Cazeaux, University of Kansas
Abstract: We discuss novel mathematical models for the analysis and computational prediction of mechanical relaxation of two-dimensional layered atomic crystals in the presence of large-scale moiré patterns. The concept of configuration space or hull, previously introduced for the study of transport properties in aperiodic materials by Bellissard et al., is shown to allow for a unified description of continuum as well as atomistic models of elastic relaxation for a wide range of materials in the truly incommensurate (aperiodic) regime.In the case of twisted bilayers with identical materials, we will present some preliminary analysis and numerical results in the asymptotic regime of small twist angle (inducing a large-scale moiré pattern) and small interlayer Van der Waals forces, in particular the well-known case of graphene/graphene but also MoS2/MoS2.

Weak Galerkin finite element method for Poisson's equation on polytopal meshes with small edges or faces
Qingguang Guan, Missouri University of Science and Technology
Abstract: The weak Galerkin finite element method for second order elliptic problems employing polygonal or polyhedral meshes with small edges or faces was analyzed. With new shape regular assumptions, optimal convergence rate for H^1 and L_2 error estimates were obtained. Also element based and edge based error estimates were proved.

BDDC domain decomposition for Stokes equation
Xuemin Tu, University of Kansas
Abstract: A Balancing domain decomposition by constraints (BDDC) algorithm is studied for solutions of large sparse linear algebraic systems arising from the discretization of incompressible Stokes. The condition num-

ber for the preconditioned system is estimated and numerical results are provided to confirm the results.

A linearized energy preserving finite element method for the dynamical incompressible magnetohydrodynamics equations

Huadong Gao, University of South Carolina

Abstract: We present and analyze a linearized finite element method (FEM) for the dynamical incompressible magnetohydrodynamics (MHD) equations. The finite element approximation is based on mixed conforming elements, where Taylor–Hood type elements are used for the Navier–Stokes equations and Nedelec edge elements are used for the magnetic equation. The divergence free conditions are weakly satisfied at the discrete level. Due to the use of Nedelec edge element, the proposed method is particularly suitable for problems defined on non-smooth and multi-connected domains. For the temporal discretization, we use a linearized scheme which only needs to solve a linear system at each time step. Moreover, the linearized mixed FEM is energy preserving. We establish an optimal error estimate under a very low assumption on the exact solutions and domain geometries.Numerical results which includes a benchmark lid-driven cavity problem are provided to show its effectiveness and verify the theoretical analysis.

Bernardi-Raugel Elements Renovated for Linear Elasticity

Graham Harper, Colorado State University

Abstract: The Bernardi-Raugel finite elements were originally developed for Stokes problems. Now they can be renovated for solving linear elasticity problems. This can be done on simplicial, quadrilateral, and hexahedral meshes. This yields locking-free solvers for linear elasticity. We will show error estimates for the elements and present numerical results for several benchmark problems.This is a joint work with Drs. James Liu, Simon Tavener (Colorado State), Ruishu Wang, Ran Zhang (Jilin University, China).

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Flux based finite element methods

JaEun Ku, Oklahoma State University

Abstract: In this talk, we present a new finite element method based on flux variables. In many applications, the flux variables are often the quantity of interest. To approximate the flux variable accurately and efficiently, one transforms the second-order equations into a system of first-order and approximates both the primary and flux variables simultaneously. While this indeed produces accurate approximations for the flux variables, the resulting algebraic system is large and expensive to solve. We present a new method approximating the flux variables only without approximations of the primary variable. If necessary, the primary variable can be recovered from the flux approximation with the same order of accuracy.

Machine Learning and Transport Simulators for Groundwater Anomaly Detection

Jiangguo (James) Liu, Colorado State University

Abstract: This talk presents some preliminary work on development of models, algorithms, and code modules for groundwater anomaly detection. Specifically, dissolved oxygen along with four other surrogates are used for identifying anomaly, support vector machine is utilized for model training, and real data from Colorado Water Watch is used for testing the models. Numerical simulators for Darcy and transport equations are also used for testing the code. This talk is based on a joint work with Jianli Gu (DuPont Pioneer R&D), Huishu Li (ColoState), and Ken Carlson (ColoState).

Asymptotic Methods for Time-Dependent Schrodinger Equation

Songting Luo, Iowa State University

Abstract: We will present an asymptotic method for numerically solving the time-dependent Schrodinger equation with perfectly matched layers. The method is based on a short-time propagator of the wavefunction. The short-time propagator is given in a form of integral that combines Huygen's principle and WKB approximation. In the integral, the phase and amplitude can be obtained through eikonal and transport equations, respectively. The integral can be evaluated efficiently by fast Fourier transform. Numerical experiments will be presented.

Positive and free energy satisfying schemes for diffusion with interaction potentials

Wumaier Maimaitiyiming, Iowa State University

Abstract: We design and analyze a second order accurate free energy satisfying finite volume method for solving diffusion equations with interaction potentials. Both semi-discrete and fully discrete schemes are shown to conserve total mass, preserve non-negativity for the solution, and satisfy the free energy dissipation law at the discrete level. These properties guarantee that the numerical solution is a probability density and the schemes obtained are energy stable. In particular, the fully-discrete scheme is shown to satisfy the three properties without a strict restriction on time steps, in both one and two-dimensional cases with nonuniform meshes. In addition, the scheme is easy to implement, and efficient in computing numerical solutions over long time. This is a joint work with professor Hailiang Liu.

Session III Sat, Oct. 6, 05:00pm - 06:40pm

A posteriori error estimates for hp-adaptive approximations of non-selfadjoint PDE eigenvalue problems

Agnieszka Miedlar, University of Kansas
Abstract: In this talk we present new residual a posteriori eigenvalue/eigenvector error estimates based on Kato's square root theorem, applied to diagonalizable non-selfadjoint differential operators of convection-diffusion-reaction type with real spectrum. Under certain condition, the existence of the square root operator provides a Bauer-Fike type estimate. We present an hp-adaptive finite element algorithm with residual a posteriori hp-finite element error estimates which are of higher order in the residual norm and, together with the Bauer-Fike theorem, guarantee the first order convergence of the eigenvalues. We illustrate our statements with several numerical examples. This is a joint work with S. Giani, L. Grubii and J. S. Ovall.

Physically-Constrained Data-Driven Reduced Order Modeling of Fluid Flows

Muhammad Mohebujjaman, Virginia Tech
Abstract: In this talk, we present two approaches for enforcing better conservation properties for reduced order models (ROMs) of fluid flows. In the first approach, to construct the centering trajectory, we use the Stokes extension instead of the standard snapshot average. We show that the Stokes extension yields significantly more accurate results. In the second approach, we enforce physical constraints in the data-driven modeling of the ROM closure term. The constrained data-driven ROM is significantly more accurate than its unconstrained counterpart.

An efficient ensemble algorithm for numerical approximation of stochastic Stokes-Darcy equations

Changxin Qiu, Missouri University of Science and Technology
Abstract: Many engineering and geological applications require effective simulations of the coupling of groundwater flows (in porous media) and surface flows. Accurate simulations are usually not feasible due to the fact it is physically impossible to know the exact parameter values, e.g., the hydraulic conductivity tensor, at every point in the domain as the realistic domains are of large scale and natural randomness occur at small scales. This presentation discusses an efficient ensemble algorithm for fast computation of multiple realizations of the stochastic Stokes-Darcy model with a random hydraulic conductivity tensor. The algorithm results in a common coefficient matrix for all realizations at each time step making solving the linear systems much less expensive while maintaining comparable accuracy to traditional methods that compute each realization separately. Moreover, it decouples the Stokes-Darcy system into two smaller sub-physics problems, which reduces the size of the linear systems and allows parallel computation of the two sub-physics problems. Numerical examples are presented to support the theoretical results and illustrate the application of the algorithm.

Locally-implicit schemes with realizability limiters for moment-closure approximations of kinetic equations

James Rossmanith, Iowa State University
Abstract: In many applications, the dynamics of gas and plasma can be accurately modeled using kinetic Boltzmann equations. These equations are integro-differential systems posed in a high-dimensional phase space, which is typically comprised of the spatial coordinates and the velocity coordinates. If the system is sufficiently collisional the kinetic equations may be replaced by a fluid approximation that is posed in physical space (i.e., a lower dimensional space than the full phase space). The precise form of the fluid approximation depends on the choice of the moment-closure. In general, finding a suitable robust moment-closure is still an open scientific problem.In this work we consider a specific moment-closure called the Quadrature-based Method of Moments (QMOM). The distribution function is approximated by Dirac deltas with variable weights and abscissas. The resulting fluid approximations have differing properties depending on the detailed construction of the Dirac deltas. We then develop a high-order, locally-implicit, discontinuous Galerkin scheme to numerically solve resulting fluid equations. We also develop limiters that guarantee that the inversion problem between moments of the distribution function and the weights and abscissas of the Dirac deltas is well-posed. This work is joint with Christine Wiersma (Iowa State) and Erica Johnson (Bexar County).

PIFE-PIC: A 3-D Parallel Immersed-Finite-Element Particle-in-Cell Method for Plasma Simulations

Daoru Han, Missouri University of Science and Technology
Abstract: We present a recently developed simulation framework, IFE-PIC, a 3-D Parallel Immersed Finite Element (IFE) Particle-in-Cell (PIC) code for particle simulations of plasmas. This code is based on a recently developed non-homogeneous electrostatic IFE-PIC algorithm for particle simulations of plasma-material interactions, which is designed to handle complex interface boundary conditions associated with irregular geometries while maintaining the computational speed of the Cartesian-mesh-based PIC. 3-D domain decomposition is used in both field-solve and particle-push to distribute the computation among multiple processors. A verification case of orbital-motion limited (OML) sheath of a dielectric sphere immersed in a stationary plasma is carried out to demonstrate the capability of the code. Applications of PIFE-PIC to lunar surface plasma interactions are also going to be presented.

Session IV Sun, Oct. 7, 10:30am - 11:50am

A Two-field Finite Element Solver for Linear Poroelasticity on Quadrilateral Meshes

Zhuoran Wang, Colorado State University

Abstract: This talk presents a finite element solver for linear poroelasticity on quadrilateral meshes based on the two-field model (solid displacement and fluid pressure). This solver combines the Bernardi-Raugel elements for the displacement in elasticity and the weak Galerkin elements for the pressure in Darcy flow through the implicit Euler discretization. The solver is penalty-free and has fewer unknowns compared to other existing methods. Numerical experiments on two widely tested benchmarks will be presented to show the solver is free of nonphysical pressure oscillations. This is a joint work with Graham Harper, Dr. James Liu, and Dr. Simon Tavener.

Weak Galerkin Finite Element Methods for the Time-dependent Biharmonic Equation

Nolisa Malluwawadu, Colorado State University

Abstract: This talk presents a novel weak Galerkin finite elements method for solving the time-dependent biharmonic equation. The biharmonic operator is discretized on general convex polygonal meshes. Degree-k polynomial basis functions are used to approximate the scalar unknown in element interiors and on inter-element boundaries and also its normal derivative on inter-element boundaries. The discrete weak Laplacians of these basis functions are established as degree-k polynomials as well, which are used to approximate the classical Laplacian in the variational form. For temporal discretization, we utilize Backward Euler method or Crank-Nicolson method. Numerical experiments are presented to corroborate the theoretical analysis.

A Defect-Deferred Correction Method for Fluid-Fluid Interaction

Dilek Erkmen, Michigan Tech University

Abstract: A method is proposed to improve two aspects of numerical simulations for a model of two fluids coupled across a at interface. This problem is motivated by atmosphere-ocean interaction. A deferred correction approach lifts the numerical order of accuracy formally from first order (very common in applications) to second order, in terms of the time interval of communication between the fluid code components. This is accomplished in a two-step predictor-corrector type method. In the second step, a further defect correction is included as well. The "defect" represents artificial diffusion used in the fluid solvers, which is often included to control numerical noise or to model subscale mixing processes. The addition of the defect correction adds only marginally to the expense, but in exchange may provide a significant reduction of overdiffusive effects.The defect and deferred correction approaches are combined into a so-called defect-deferred correction (DDC) method. A full DDC algorithm is studied using finite elements in space, including an analysis of the stability and convergence. The method is unconditionally stable, optimally convergent and also enforces a formal reduction in artificial diffusion effects. A computational example using a known (manufactured) solution illustrates the theoretical predictions. We observe a computational benefit in this example even for coarse time steps and over a wide range of artificial viscosity values. Some discussion is provided regarding the possibility to generalize the approach for appli-cation codes. Briefly, legacy atmosphere and ocean codes may be used as-is over a coupling time interval for a predictor computation. The corrector step would then potentially be implemented as a straight-forward modification of the predictor step that leverages the existing code structure.

Optimal control of stochastic flow using the adaptive dynamically low-dimensional approximation method

Zhipeng Yang, Beijing Computational Science Research Center

Abstract: We explore the dynamically bi-orthogonal method (DyBO) for solving the stochastic optimal control problem for incompressible Newtonian channel flow past a circular cylinder. We assume the inlet flow and the rotation speed of the cylinder have stochastic perturbations. To achieve objectives of control, we adjust the rotation speed of the cylinder. Based on the effective gradient-based optimization algorithm to solve the optimality systems, the computational cost of the classical Monte Carlo method (MC) is unaffordable. The polynomial chaos expansions method (PCE) is a wise choice to reduce the cost, but it still requires high computational cost as the number of expansion terms increase quickly if we want more accurate solutions. The DyBO method could get a high-accuracy with lower computational cost based on the Karhunen-Loeve expansion (KLE) that gives the sparsest representation of the stochastic solutions. To perform the DyBO method for the incompressible Navier Stokes equations (NSE) with open boundary conditions, we combine DyBO method with the pressure Poisson equation formulation. Numerical tests are performed to validate our methodology.

MS15. Inverse Problems in Tomography and Wave Propagation

Organizer: Yang Yang, `yangy5@msu.edu`, Michigan State University

Schedule: PHSC 114 (for both sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

Stability of Stationary Inverse Transport Equation in Diffusion Scaling

Ke Chen, University of Wisconsin-Madison

Abstract: We consider the inverse problem of reconstructing the optical parameters for stationary radiative transfer equation (RTE) from velocity-averaged measurement. The RTE often contains multiple scales characterized by the magnitude of a dimensionless parameter—the Knudsen number (Kn). In the diffusive scaling (Kn ¡¡ 1), the stationary RTE is well approximated by an elliptic equation in the forward setting. However, the inverse problem for the elliptic equation is acknowledged to be severely ill-posed as compared to the well-posedness of inverse transport equation, which raises the question of how uniqueness being lost as Kn goes to 0. We tackle this problem by examining the stability of inverse problem with varying Kn. We show that, the discrepancy in two measurements is amplified in the reconstructed parameters at the order of Kn^p (p=1 or 2), and as a result lead to ill-posedness in the zero limit of Kn. Our results apply to both continuous and discrete settings. Some numerical tests are performed in the end to validate these theoretical findings.

Breaking the curse of dimensionality: sparse quadrature for high-dimensional Bayesian inverse problems

Peng Chen, The University of Texas at Austin

Abstract: It is one of the central topics to evaluate statistics, such as mean and variance of a given quantity of interest, with respect to the posterior distribution of a (high-dimensional) parameter in the context of Bayesian inverse problems. In this talk, we present a sparse quadrature method for this problem and demonstrate that under certain assumptions on the prior distribution and the forward map, the convergence rate of the sparse quadrature error is independent of the parameter dimensions and can be much higher than that of Monte Carlo average approximation error.

Some advances in photoacoustic tomography - attenuation and media properties

Sebastian Acosta, Texas Children's Hospital

Abstract: Concerning mathematical analysis of photoacoustic tomography, we will talk about some advances in accounting for attenuation effects and the simultaneous recovery of some acoustic properties of the media.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Ultrasound-switchable fluorescence imaging in deep tissues

Baohong Yuan, University of Texas at Arlington

Abstract: Tissue imaging via fluorescence has been widely used for many years. It stands out due to high sensitivity, high specificity, low cost, use of non-ionizing radiation, capability of multiplex imaging and providing tissue structural, functional and molecular information. However, it suffers from limitations: poor spatial resolution (i.e., fluorescence diffuse optical tomography) or small penetration depth (i.e., fluorescence microscopy) due to the strong tissue light scattering. Thus, high-resolution fluorescence imaging in deep tissue has been sought after for many years. Recently, we developed a new imaging technique—ultrasound-switchable fluorescence (USF) which has been demonstrated to overcome the limitations. We successfully imaged centimeter-large mammary tumors in live mice with much higher spatial resolution than conventional 2D planar fluorescence imaging or 3D fluorescence diffuse optical tomography and demonstrated the capability of USF for high-resolution in vivo imaging. We also compared USF images with micro-CT to further validate the technology. In this talk, I will introduce USF and demonstrate recently acquired images from in vitro and in vivo deep tissues.

Fluorescence Ultrasound-Modulated Optical Tomography in the Diffusive Regime

Yang Yang, Michigan State University

Abstract: Fluorescence optical tomography (FOT) is an imaging technology that localizes fluorescent targets in tissues. FOT is unstable and of poor resolution in highly scattering media, where the propagation of multiply-scattered light is governed by the smoothing diffusion equation. We study a hybrid imaging modality called fluorescent ultrasound-modulated optical tomography (fUMOT), which combines FOT with acoustic modulation to produce high-resolution images of optical properties in the diffusive regime. The principle of fUMOT is to perform multiple measurements of photon currents at the boundary as the optical properties undergo a series of perturbations by acoustic radiation, in which way internal information of the optical field is obtained. We set up a mathematical model for fUMOT, prove well-posedness for certain choices of parameters, and present reconstruction algorithms and numerical experiments for the well-posed cases.

Inversion of the star transform

Gaik Ambartsoumian, University of Texas at Arlington

Abstract: The star transform maps a function of two variables to a two-dimensional family of its integrals along unions of n rays emanating from a common vertex. Such transforms have been studied in relation to imaging modalities using single-scattered particles. The talk will present new exact inversion formulas for this transform and discuss the novel approach for deriving these formulas. The efficiency of these results will be demonstrated by numerical examples.

Contributed Talks

Schedule: PHSC 212 (for all three sessions)

Session I Sat, Oct. 6, 10:40am - 12:00pm

Effect of vertical variations in diffusivity and resistivity due to convection in a porous medium

Dambaru Bhatta, University of Texas Rio Grande Valley

Abstract: We consider a hydro-thermal convective flow in a horizontal porous medium. The governing system consists of the continuity equation for conservation of mass, the heat equation for conservation of energy, and the conservation of momentum equation which is governed by Darcy's law. We investigate the effect of linear variations in diffusivity and resistivity in the vertical direction for two dimensional case. Applying weakly nonlinear approach, we derive the linear and first-order systems. Then these systems are solved numerically for quantities such as temperature and vertical velocity. Numerical results for those quantities are presented.

Numerical study of pattern formation in the fractional Gray–Scott model

Hatim Khudhair, Missouri university of Science and Technology

Abstract: In this talk, we numerically study pattern formation of the spatial-fractional Gray-Scott equation to understand the nonlocal effects of the fractional Laplacian. The linear stability analysis is provided to predict the conditions of the Turing pattern. To investigate the nonlinear effects, we discretize the fractional Gray-Scott equation by the Fourier pseudo-spectral method in space and the 4th order Runge-Kutta method in time. Then we numerically study the effects of the fractional exponent on the spatiotemporal patterns formation and pattern selection in Gray-Scott system. The pattern formations in the standard and fractional Gray-Scott models are compared to provide more insights of the nonlocal effects.

Stability of solutions in reproducing kernel Hilbert spaces on a semi-infinite domain with applications to the telegraph equation

Jabar Hassan, Missouri University of Science and Technology

Abstract: In this talk, stability of solutions in certain type of reproducing kernel Hilbert space methods will be introduced to the non-homogeneous telegraph equation on a semi-infinite domain. These spaces are convenient for numerical approximation because the kernels are piecewise polynomial functions. In this presentation, numerical results are also implemented to demonstrate the efficiency and accuracy of the method.

Session II Sat, Oct. 6, 03:10pm - 04:30pm

Rate Transient Analysis of Arbitrarily Oriented Hydraulic Fractures

Umer Farooq, University of Tulsa

Abstract: Objective: An analytical solution in three-dimensional Cartesian space, generated for pressure constrained production from an arbitrarily inclined well in an anisotropic reservoir, is extended to the case of arbitrarily oriented, fully penetrating, vertical fractures. Thus, we produce a forward discrete fracture model for application to well performance in unconventional reservoirs.

Methods: A solution is generated from 3D heat equation using the Newman product method. The solution is then extended to add a fully penetrating fracture orthogonal to the well. The model uses convolution in Laplace domain to capture constant bottomhole pressure constrained production. Analytic Laplace inversion is performed to yield a result in time with exponential decay terms.

Conclusions: This analytical solution to the Diffusivity Equation under constant pressure constraint gives a new mathematical structure for analyzing rate decline in unconventional wells.The created analytic model grants a reservoir engineer the ability to analyze the case of rate transient production from fractured horizontal well while accounting for the permeability anisotropy. This lays the ground work for analytically modeling the most general and widely studied case of having a number of fracture stages in a horizontal well.

Max-min Fairness Hierarchical Dissection of Networks

Zizhen Chen, Southern Methodist University

Abstract: Given a graph of relations between entities a max-min fairness hierarchical dissection is shown to reveal a fundamental contraction of the entities into a relatively small number of components with their own relational network structure. Our network flow/cut duality based model determines both these components and which component pairs remain adjacent in the contracted graph. The structure follows from the series of max-min determined cuts that create the component partition.The reduced graph, known as a "minor" of the original graph of relations, exhibits a topology of relations between the components. We use novel two and three-dimensional visualizations to show how the graph minor, termed a "backbone", is generated and also to illustrate the iterative refinement of backbones over levels. In summary, this process, determined by a simple all pairs network traffic flow linear programming formulated model, allows the large domain of relations between all pairs of entities to be reduced to a subset of significant relations between highly connected component communities of the original graph. We consider the impact of these results for congestion studies of transportation networks and community detection investigation of social networks.

Unconditionally energy stable linear schemes for a multi-component two-phase diffuse interface model with Peng-Robinson equation
Chenfei Zhang, University of South Carolina
Abstract: Numerical solution of the diffuse interface model with Peng-Robinson equation of state can be applied to describe real states of hydrocarbon fluids in petroleum industry. How to develop appropriate temporal discretizations to overcome the strong nonlinearity of the source term and preserve energy dissipation law of the discretized system is a major challenge. We develop efficient first and second order time stepping schemes for this model based on the "Invariant Energy Quadratization" approach and stabilized method. Both schemes lead to linear systems which are symmetric and positive definite at each time step, and their unconditional energy stabilities are rigorously proved. Numerical experiments in 2D and 3D are presented to demonstrate accuracy and stability of the proposed schemes.

Session III Sat, Oct. 6, 05:00pm - 06:40pm

An ensemble based projection method with sparse grad div stabilization for solving the Navier-Stokes equations
Shuai Yuan, University of South Carolina at Columbia
Abstract: We developed a first order projection method for ensemble-based simulations of the NSE in which not only the initial data and body force function, but also the viscosity coefficient, may vary from one ensemble member to another. Numerical experiments are provided that illustrate the accuracy and efficiency of the computing by using this method.

Mathematics of the Significant Tornado Parameter
Aaron Baker, Stephen F. Austin State Univeristy
Abstract: The significant tornado parameter (STP) is one of many models recently created by the National Storm Prediction Center (SPC) to predict the possibility of severe weather. This parameter looks at the winds, potential energy, and rotation in the atmosphere and performs calculations based on its predicted state. As more research on tornadoes has become available, this relatively new model has become more refined. The purpose of this project was to learn how physics and math work in meteorology, specifically in severe weather systems. Derivation of each component of the STP is a basic multivariable calculus function using basic concepts of thermodynamics.

Accurate numerical methods on the variable-order fractional Laplacian
Yixuan Wu, Missouri University of Science and Technology
Abstract: In the last decades, fractional partial differential equations have been widely applied in sciences and engineering. In particular, recently it has been found that some complex phenomena, e.g., viscoelastic mechanics in geosciences, are governed by the fractional PDEs with variable-order fractional Laplacian. In this talk, we will present an accurate finite difference methods to solve the variable-order fractional Laplacian. Numerical accuracy in discretizing the operator and in solving the fractional Poisson problems will be discussed. This is a joint work with Ying Li (Missouri S&T) and Yanzhi Zhang (Missouri S&T).

Posters

Schedule: Sat, Oct. 6, 5:00pm - 6:20pm at PHSC 209

Mathematical models linking within-host and between-host HIV Dynamics
Carlos Villanueva, University of Oklahoma
Abstract: Lack of HIV vaccines have made therapy essential to the reduction of HIV transmission and control of epidemics. For the implementation of control strategies, it is critical to understand between-host transmission dynamics involving proper risk of infection, which depends on the within-host HIV dynamics of source-host. In this study we develop mathematical models linking within-host and between-host HIV Dynamics. In particular, we incorporate antibody response into within-host viral dynamic models to estimate the probability of infection from an infected individual to an uninfected individual. Our models predict that this probability is largely dependent upon the source-host's disease status, including viral load and antibody level. Using the probability of infection resulting from within-host models, we then develop models to describe the dynamics of between-host transmission, which is consistent with HIV prevalence data from South Africa. With these models, we evaluate how within-host disease status of infected individuals influences the between-hosts spread of HIV within communities.

A Mechanistic Model of Plant-Symbiont Interactions
Rebekah Wagner, University of Kansas
Abstract: The influence of microbial symbionts on the phenotype of their plant host is not well understood despite their known importance. Microbial symbionts, such as mycorrhizal fungi and rhizobia bacteria, reside within plant roots and exchange resources with their plant host. These relationships can be classified as mutualistic or non-mutualistic depending on environmental conditions and life history characteristics of plants and symbionts. Mycorrhizal fungal mutualists supply their host with phosphorus in exchange for allotted carbon produced through photosynthesis by the host plant. Rhizobia bacteria also deliver fixed nitrogen in exchange for allotted carbon. The resource complimentary of these relationships

can facilitate increased host growth and can generate synergisms. A mechanistic model of plant-symbiont interactions was developed and shows when a pool resource is available to the host plant (i.e. soil fertility), the relative abundance of each symbiont decreases. The cost of preferentially allocated carbon to the symbionts decreases when the resource pool of phosphorus or nitrogen is available. Productivity of the host plant increases as a measure of total plant biomass increases over time before reaching the saturating equilibrium when interacting with either symbiont.

Performance Studies for the Numerical Simulations of Rayleigh-Taylor Instability

Alaina Edwards, University of Arkansas

Abstract: The Rayleigh-Taylor instability is a fluid instability which occurs in turbulent mixing problems such as oceanography and supernovae. Usually, it involves the interaction between two fluids of differing densities. As the two fluids mix, the interaction forms bubbles and spikes on the interface. We use Front Tracking and Large Eddy Simulations with subgrid-scale models for the numerical simulations. With the help of the Blue Waters supercomputing system, we focus on performance studies and improvements of the numerical simulations for the Rayleigh-Taylor instability. Utilizing both the Cray and GNU programming environments, we have performed scaling studies and used performance tools to explore profiling and optimization techniques.

Development of a COMSOL microdialysis model, towards creation of microdialysis on a chip with improved geometries and recovery

Patrick Pysz, University of Arkansas

Abstract: Microdialysis (μD) is diffusion-limited sampling method used in basic and clinical research. Research needs for collecting low, non steady-state concentration (pg/mL) and large (>10 kDa) signaling proteins (cytokines) are hampered by significant limitations with the technique. Low protein diffusivity leads to low values for the device calibration even under controlled benchtop conditions. Microdialysis device designs have not improved upon the cylindrical geometry currently available commercially for over 35 years. COMSOL Multiphysics finite element method (FEM) software was used to iteratively model and refine microfluidic-based (μF) μD device designs with the primary focus on optimizing innovative channel geometry for improved calibration metrics. The current μF μD design uses a simple asymmetric linear-looped (LL) geometry optimized to use 68% of the total cross-sectional area and an equal 10 mm length in comparison to a commercial CMA 20 μD device. The simulated LL μF μD achieves a 35.7% relative increase in RR vs. experimental data at a 1.0 μL/min inlet flow rate using a model 10 kDa dextran as the analyte. LL μF μD devices are currently being fabricated, characterized, and compared to simulation data. This mathematical modeling work is a critical first step towards uniquely innovative and improved microdialysis devices.

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