Program and Abstracts





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Society for Industrial and Applied Mathematics (SIAM) College of Sciences and Mathematics, Auburn University Department of Mathematics and Statistics, Auburn University

The 44th SIAM Southeastern Atlantic Section Conference

Auburn University September 18–19, 2021

Organizing Committee

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The 44th SIAM Southeastern Atlantic Section Conference Program

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1 Venue Information, Map, and Conference Schedule

Venue Information

- The conference will take place at the Mell Classroom Building located at 231 Mell Street.
- Free parking is available during the conference at the Library Parking Deck (5 Roosevelt Dr), which is adjacent to Mell Classroom Building.
- The reception and the poster session will be held in Melton Student Center Ballroom A.



Mell Classroom Building Floor Plan



Second floor



Third floor

Fourth floor



Conference Schedule

Saturday, September 18		
7:30AM-8:20AM	Registration	Lobby at Mell Classroom
8:20AM-8:30AM	Welcome Remarks	Mell 2510
8:30AM-9:30AM	Plenary Talk I: James Nagy	Mell 2510
9:30AM-10:00AM	Coffee Break	Lobby at Mell Classroom
	MS1: Reduced Order Modeling in the Age of Data - Part I	Libry 3027
	MS2: Recent Developments in Nonlocal Continuum Modeling - Part I	Libry 3035
	MS3: Recent Advances in Numerical Methods for PDEs - Part I	Libry 3129
	MS4: Modeling and Numerical Methods for Coupled PDE Systems - Part I	Libry 4027
	MS5: PDE, Dynamical Systems and Applications - Part I	Libry 4035
10:00AM-12:00PM Parallel Session 1	MS6: Recent Developments on Partial Differential Equations and Applications - Part I	Libry 4129
	MS7: Recent Developments and Applications in Computational Biology - Part I	Libry 3033
	MS8: Modeling and Data Science in Quantitative Biology: Predictions and Descriptions - Part I	Libry 3041
	MS9: Deep Learning Methods for Data Driven Models - Part I	Libry 3127
	MS10: Theory Meets Practice for Inverse Problems in Imaging Applications - Part I	Libry 4033
	MS11: Recent Progress of Classical and Deep Learning Methods in Inverse Problems and Imaging - Part I	Libry 4127
	MS12: Recent Developments of Numerical Methods for Fluid Flows and Applications - Part I	Libry 4041
	MS16: Recent Advances in Nonlinear Wave Propagation and Interaction - Part I	Libry 3133
	MS19: Recent Advances in Iterative Solvers for Numerical Optimization and Nonlinear Systems - Part I	Mell 3520
	CP: Contributed Presentations - Part I	Mell 4510A
	CP: Contributed Presentations - Part II	Mell 4520
12:00PM-2:00PM	Lunch Break	

Saturday, September 18		
2:00PM-3:00PM	Plenary Talk II: Jianfeng Lu	Mell 2510
3:00PM-3:30PM	Coffee Break	Lobby at Mell Classroom
	MS1: Reduced Order Modeling in the Age of Data - Part II	Libry 3027
	MS2: Recent Developments in Nonlocal Continuum Modeling - Part II	Libry 3035
	MS3: Recent Advances in Numerical Methods for PDEs - Part II	Libry 3129
	MS4: Modeling and Numerical Methods for Coupled PDE Systems - Part II	Libry 4027
3:30PM-5:30PM Parallel Session 2	MS5: PDE, Dynamical Systems and Applications - Part II	Libry 4035
	MS6: Recent Developments on Partial Differential Equations and Applications - Part II	Libry 4129
	MS7: Recent Developments and Applications in Computational Biology - Part II	Libry 3033
	MS8: Modeling and Data Science in Quantitative Biology: Predictions and Descriptions - Part II	Libry 3041
	MS9: Deep Learning Methods for Data Driven Models - Part II	Libry 3127
	MS10: Theory Meets Practice for Inverse Problems in Imaging Applications - Part II	Libry 4033
	MS13: Surrogate Modeling for High-dimensional Problems and Applications - Part I	Mell 3520
	MS14: Numerical Methods and Deep Learning for Nonlinear PDEs - Part I	Libry 4041
	MS15: Mathematical Modeling, Analysis and Applications - Part I	Libry 4127
	MS16: Recent Advances in Nonlinear Wave Propagation and Interaction - Part II	Libry 3133
	CP: Contributed Presentations - Part III	Mell 4510A
	CP: Contributed Presentations - Part IV	Mell 4520
6:00PM-8:00PM	Poster Session and Reception at Melton Student Center	, Ballroom A

Sunday, September 19		
8:00AM-9:00AM	Plenary Talk III: Oscar Bruno	Mell 2510
9:00AM-10:00AM	Plenary Talk IV: Juan M. Restrepo	Mell 2510
10:00AM-10:30AM	Coffee Break	Lobby at Mell Classroom
	MS1: Reduced Order Modeling in the Age of Data - Part III	Libry 3027
	MS2: Recent Developments in Nonlocal Continuum Modeling - Part III	Libry 3035
	MS3: Recent Advances in Numerical Methods for PDEs - Part III	Libry 3129
10:30AM-12:30PM	MS4: Modeling and Numerical Methods for Coupled PDE Systems - Part III	Libry 4027
I araller Session 5	MS5: PDE, Dynamical Systems and Applications - Part III	Libry 4035
	MS6: Recent Developments on Partial Differential Equations and Applications - Part III	Libry 4129
	MS11: Recent Progress of Classical and Deep Learning Methods in Inverse Problems and Imaging - Part II	Libry 3127
	MS12: Recent Developments of Numerical Methods for Fluid Flows and Applications - Part II	Libry 3041
	MS13: Surrogate Modeling for High-dimensional Problems and Applications - Part II	Mell 3520
	MS14: Numerical Methods and Deep Learning for Nonlinear PDEs - Part II	Libry 4041
	MS15: Mathematical Modeling, Analysis and Applications - Part II	Libry 4127
	MS16: Recent Advances in Nonlinear Wave Propagation and Interaction - Part III	Libry 3133
	MS17: Modeling and Numerical Methods for Image Problems	Libry 3033
	MS18: Advances in Memory Efficient Numerical Algorithms for Kinetic Problems	Libry 4033
	MS19: Recent Advances in Iterative Solvers for Numerical Optimization and Nonlinear Systems - Part II	Mell 4520

2 Plenary Talks

MATLAB Tools for Large-Scale Linear Inverse Problems

SPEAKER: James Nagy, Department of Mathematics, Emory University

SCHEDULED: Saturday, September 18, 8:30AM-9:30AM at Mell Classroom 2510

DETAILS: Plenary Talk I

Abstract: Inverse problems arise in a variety of applications: image processing, finance, mathematical biology, and more. Mathematical models for these applications may involve integral equations, partial differential equations, and dynamical systems, and solution schemes are formulated by applying algorithms that incorporate regularization techniques and/or statistical approaches. In most cases these solutions schemes involve the need to solve a large-scale ill-conditioned linear system that is corrupted by noise and other errors. In this talk we describe and demonstrate capabilities of a new MAT-LAB software package that consists of state-of-the-art iterative methods for solving such systems, which includes approaches that can automatically estimate regularization parameters, stopping iterations, etc., making them very simple to use. Thus, the package allows users to easily incorporate into their own applications (or simply experiment with) different iterative methods and regularization strategies with very little programming effort. On the other hand, sophisticated users can also easily access various options to tune the algorithms for certain applications. Moreover, the package includes several test problems and examples to illustrate how the iterative methods can be used on a variety of large-scale inverse problems.

The talk will begin with a brief introduction to inverse problems, discuss considerations that are needed to compute an approximate solution, and describe some details about new efficient hybrid Krylov subspace methods that are implemented in our package. These methods can guide users in automatically choosing regularization parameters, and can be used to enforce various regularization schemes, such as sparsity. We will use imaging examples that arise in medicine and astronomy to illustrate the performance of the methods.

This is joint work with Silvia Gazzola (University of Bath) and Per Christian Hansen (Technical University of Denmark).

Solving Eigenvalue Problems in High Dimension

Speaker:	Jianfeng Lu, Department of Mathematics, Duke University
Scheduled:	Saturday, September 18, 2:00 PM–3:00 PM at Mell Classroom 2510
DETAILS:	Plenary Talk II

ABSTRACT: The leading eigenvalue problem of a differential operator arises in many scientific and engineering applications, such as quantum many-body problems. Conventional algorithms become impractical due to the huge computational and memory complexity from the curse of dimensionality. In this talk, we will discuss some recent works on new algorithms for eigenvalue problems in high dimension based on randomized and coordinate-wise methods and also machine learning approaches. (joint work with Jiequn Han, Yingzhou Li, Zhe Wang and Mo Zhou).

"Interpolated Factored Green Function" Method for Accelerated Solution of Scattering Problems

SPEAKER: Oscar Bruno, Department of Computing and Mathematical Sciences, Caltech

SCHEDULED: Sunday, September 19, 8:00AM-9:00AM at Mell Classroom 2510

DETAILS: Plenary Talk III

ABSTRACT: We present a novel "Interpolated Factored Green Function" method (IFGF) for the accelerated evaluation of the integral operators in scattering theory and other areas. Like existing acceleration methods in these fields, the IFGF algorithm evaluates the action of Green function-based integral operators at a cost of $O(N \log N)$ operations for an N-point surface mesh. Importantly, the proposed method does not utilize previously-employed acceleration elements such as the Fast Fourier transform (FFT), special-function expansions, high-dimensional linear-algebra factorizations, translation operators, equivalent sources, or parabolic scaling. Instead, the IFGF strategy, which leads to an extremely simple algorithm, capitalizes on slow variations inherent in a certain Green-function "analytic factor", which is analytic up to and including infinity, and which therefore allows for accelerated evaluation of fields produced by groups of sources on the basis of a recursive application of classical interpolation methods. In particular, the IFGF method runs on a small memory footprint, and, as it does not utilize the Fast Fourier Transforms (FFT), it is better suited than other methods for efficient parallelization in distributed-memory computer systems. Related integral equation techniques and associated device-optimization problems will be mentioned, including a novel time-domain scattering solver that accurately and effectively solves time-domain problems of arbitrary duration via Fourier transformation in time. (IFGF work in collaboration with graduate student Christoph Bauinger. Device-optimization work in collaboration with former postdoc Constantine Sideris and former students Emmanuel Garza and Agustin Fernandez-Lado. Time-domain work, in collaboration with former graduate student Thomas Anderson.)

"How Warm is it Getting?" and other Uncertainty Tales

SPEAKER: Juan M. Restrepo, Computer Science and Mathematics Division, Oak Ridge National Laboratory

SCHEDULED: Sunday, September 19, 9:00AM-10:00AM at Mell Classroom 2510

DETAILS: Plenary Talk IV

ABSTRACT: In the statistics community "Big Data" science is meant to suggest the combining of inferential and computational thinking. We also speak of big data in the geosciences. However, the problems we pursue are often extreme in the number of degrees of freedom, and in many instances, non-stationary in their statistics. This usually means that we are working with sparse observational data sets, even if the number of observations is large. The Bayesian framework is a natural inferential data assimilation strategy in geosciences, to some extent because the degrees of freedom in the problem vastly outnumber observations but more critically, because the models we use to represent nature have considerable predictive power.

> Looking toward the future, two trends appear: we expect improvements in computational efficiency and finer resolutions in models, as well as improved field measurements. This will force us to contend with physics and statistics across scales and thus to think of ways to couple multiphysics and computational resolution, as well as to develop efficient methods for adaptive statistics and statistical marginalization. How this coupling is exploited to improve estimates that combine model outcomes and data will be described in tracking hurricanes and improving the prediction of the time and place of coastal flooding due to ocean swells. Estimating the trend of Earth's temperature from sparse multi-scale data will be used as an example of adaptivity in time series analysis. The other trend, driven by the success of AI in other realms, is that empirical fidelity of poorly understood processes should play an increasingly important role in climate and weather forecasting. The presentation will conclude with a personal view on where research opportunities arise, within these two thrusts, for collaborations between quantitative and domain scientists.

3 List of Mini-symposia and Contributed Talks

MS1: Reduced Order Modeling in the Age of Data (Part I)

ORGANIZERS:	Traian Iliescu, Virginia Tech
	Alessandro Veneziani, Emory University
	Omer San, Oklahoma State University

TALKS & SPEAKERS:

- 1. Data-Driven variational multiscale reduced order models Changhong Mou, *Virginia Tech*
- Scheduled at:

Parallel Session 1 Saturday, September 18, 10:00–12:30 Room: Libry 3027

- 2. Stochastic closure model via parametric inference Fei Lu, Johns Hopkins University
- 3. Dynamics informed data-driven closures for chaotic systems Honghu Liu, *Virginia Tech*
- 4. Ill-effects of model inconsistency in reduced order models of incompressible flows
 - Leo Rebholz, Clemson University
- 5. Interpolatory tensorial reduced-order models for parametric dynamical systems Maxim Olshanskii, University of Houston

MS1: Reduced Order Modeling in the Age of Data (Part II)

Organizers:	Traia	n Iliescu, Virginia Tech
	Aless	andro Veneziani, Emory University
	Omer	: San, Oklahoma State University
Talks & Speaki	ERS:	1. A hybrid variational multiscale and machine learning approach for nonlinear model order reduction Shady E Ahmed, Oklahoma State University
Scheduled at:	:	2. Modified neural ordinary differential equations for stable
Parallel Session	n 2	learning of chaotic dynamics
Saturday,		Romit Maulik, Argonne National Laboratory
September 18,		3. Physics-guided machine learning for projection-based
3:30-5:30		reduced-order modeling
Room: Libry 3	3027	Suraj Pawar, Oklahoma State University
		4. Data-driven realistic wind data generation for safe opera- tion of Small Unmanned Air Vehicles in urban environment

Rohit Vuppala, Oklahoma State University

MS1: Reduced Order Modeling in the Age of Data (Part III)

Organizers: T	raian Iliescu, Virginia Tech
A	lessandro Veneziani, Emory University
O	mer San, Oklahoma State University
Talks & Speakers	 Some applications of Model Reduction in Cardiovascular Mathematics Alessandro Veneziani, Emory University
Scheduled at:	2. An efficient reduced order modeling method for Lagrangian
Parallel Session 3	data assimilation of turbulent flows
Sunday,	Nan Chen, University of Wisconsin-Madison
September 19,	3. Modeling land ice with deep operator networks
10:30 –12:30	Mauro Perego, <i>Sandia National Laboratory</i>
Room: Libry 302	7 4. Adaptive surrogate modeling for variational inference with normalizing flow Daniele Schiavazzi, University of Notre Dame

MS2: Recent Developments in Nonlocal Continuum Modeling (Part I)

Organizers: Jame	es Scott, University of Pittsburgh
Pabl	o Seleson, Oak Ridge National Laboratory
Talks & Speakers:	1. Nonlocal brittle fracture modeling with applied traction forces Robert Lipton, Louisiana State University
SCHEDULED AT:	 Regularity estimates for nonlocal space-time master equa-
Parallel Session 1	tions Pablo Paul Stinga, Iowa State University
September 18,	3. Relaxation phenomena in the localized limit of nonlocal en-
10:00–12:00	ergies motivated by bond-based peridynamics
Room: Libry 3035	James Scott, University of Pittsburgh
	4. One-side fractional diffusion equations and their finite ele- ment approximations Mitchell Sutton, University of Tennessee

MS2: Recent Developments in Nonlocal Continuum Modeling (Part II)

Organizers: Jam Pab	es Scott, University of Pittsburgh lo Seleson, Oak Ridge National Laboratory
Talks & Speakers:	1. Overall equilibrium in the coupling of peridynamics and classical continuum mechanics William Oates, Florida State University
Scheduled at:	2. A symmetric force-based method for the atomistic-to-
Parallel Session 2	continuum coupling
Saturday	Elaine Gorom, University of North Carolina at Challotte
September 18, 3:30–5:30 Room: Libry 3035	3. Overall equilibrium in the coupling of peridynamics and classical continuum mechanics Pablo Seleson, Oak Ridge National Laboratory
L	4. A Petrov-Galerkin method for nonlocal convection- dominated diffusion problems Xiaochuan Tian, University of California San Diego

MS2: Recent Developments in Nonlocal Continuum Modeling (Part III)

ORGANIZERS:	James Scott, University of Pittsburgh
	Pablo Seleson, Oak Ridge National Laboratory

Speakers:	1. A fast numerical method for a state-based PD model
	Hong Wang, University of South Carolina

2. Convergence studies in meshfree peridynamic wave and crack propagation

Marco Pasetto, Oak Ridge National Laboratory

- 3. An RBF quadrature rule approach for solving nonlocal continuum models Isaac Lyngaas, Oak Ridge National Laboratory
- 4. The evolution of the peridynamics co-authorship network Biraj Dahal, Georgia Institute of Technology

SCHEDULED AT: Parallel Session 3 Sunday, September 19, 10:30 -12:30

Room: Libry 3035

Talks &

MS3: Recent Advances in Numerical Methods for PDEs (Part I)

ORGANIZERS: S.S. Ravindran, University of Alabama in Huntsville

Talks & Speakers:	 High-order multirate time integration for multi-physics sys- tems Dan Reynolds, Southern Methodist University
Scheduled at:	2. Improving accuracy and stability of existing time integra-
Parallel Session 1	tors with nonintrusive post-processing
Saturday,	Victor DeCaria, Oak Ridge National Laboratory
September 18,	3. Numerical solution of supersonic Euler and Magnetohydro-
10:00-12:30	dynamic flow past cones
Room: Libry 3129	Ian Holloway, Wright State University
	4. A low Mach number model and associated numerical algo- rithm for simulating complex multiphase flows with mass transfer in a cryogenic fuel tank Mark Sussman, <i>Florida State University</i>
	5. Low rank CP tensor decomposition for model order reduc- tion Carmeliza Navasca, University of Alabama at Birmingham

MS3: Recent Advances in Numerical Methods for PDEs (Part II)

ORGANIZERS: S.S. Ravindran, University of Alabama in Huntsville

Talks & Speakers:	1. New finite difference methods on irregular grids for solving Maxwell's equations Yingjie Liu, <i>Georgia Tech</i>
Scheduled at:	2. Scalable time-stepping for nonlinear PDEs through Krylov
Parallel Session 2	subspace spectral methods
Saturday.	James Lambers, The University of Southern Mississippi
September 18,	3. Robust architectures, initialization, and training for deep
03:30-05:30	neural networks via the adaptive basis inter-pretation
Room: Libry 3129	Mamikon Gulian, Sandia National Laboratory
	4. Fractional deep deural network and inverse problems
	Deepanshu Verma, Emory University

MS3: Recent Advances in Numerical Methods for PDEs (Part III)

ORGANIZERS: S.S. Ravindran, University of Alabama in Huntsville

Talks & Speakers:	 Adaptive two-grid finite element algorithms for linear and nonlinear problems Yi Zhang, University of North Carolina at Greensboro
Scheduled at:	2. A decoupled, linear, and unconditionally energy stable fi-
Parallel Session 3	nite element method for a two-phase ferrohydrodynamics model Xiaoming He, Missouri University of Science and Technology
Sunday, September 19,	
10:30-13:00	3. Sparse discretization of optimal control problems with
Room: Libry 3129	PDEs Evelyn Herberg, <i>George Mason University</i>
	4. Meshfree methods for problems with variable-order Lapla- cian

Yanzhi Zhang, Missouri University of Science and Technology

5. A fast algorithm for parameter-dependent and random PDEs

Xiaobing Feng, University of Tennessee at Knoxville

MS4: Modeling and Numerical Methods for Coupled PDE Systems (Part I)

problem with boundary correction Michael Neilan, University of Pittsburgh

ORGANIZERS:	Xiaoming He, Missouri University of Science and Technology
	Xiaofeng Yang, University of South Carolina

TALKS & SPEAKERS: 1. A divergence-free finite element method for the Stokes

Scheduled at: Parallel Session 1

Saturday,

September 18, 10:00–12:00

Room: Libry 4027

- 2. Cell-average based neural network method for hyperbolic and parabolic partial differential equations Jue Yan, *Iowa State University*
- 3. Hybridization and postprocessing in finite element exterior calculus Ari Stern, Washington University in St. Louis
- 4. Structure-preserving discontinuous Galerkin methods for Hamiltonian PDEs: energy conservation and multisymplecticity

Zheng Sun, The University of Alabama

MS4: Modeling and Numerical Methods for Coupled PDE Systems (Part II)

Organizers: Xiac Xiac	oming He, Missouri University of Science and Technology ofeng Yang, University of South Carolina
Talks & Speakers:	1. Boundary control for fluid mixing: analysis and computa- tion Weiwei Hu, University of Georgia
Scheduled at:	2. Optimal control of volume-preserving mean curvature flow
Parallel Session 2	Shawn Walker, Louisiana State University
Saturday, September 18, 3:30–5:30	3. Variational discretization for optimal control with BV func- tions based on the mixed formulation Evelyn Herberg, <i>George Mason University</i>
Room: Libry 4027	4. , Variational data assimilation for parabolic interface prob- lems Xuejian Li, Missouri University of Science and Technology

MS4: Modeling and Numerical Methods for Coupled PDE Systems (Part III)

Organizers:	Xiaoming He, Missouri University of Science and Technology
	Xiaofeng Yang, University of South Carolina

Talks & Speakers:	1. Finite element/holomorphic operator-value function approach for nonlinear eigenvalue problems Jiguang Sun, Michigan Technological University
Scheduled at:	2. Locking-free 2-field finite element solvers for poroelasticity
Parallel Session 3	Jiangguo Liu, Colorado State University
Sunday, September 19, 10:30–12:30 Boom: Libry 4027	 3. A simple flux-recovery on quadtree meshes Shuhao Cao, Washington University in St. Louis 4. A nonconforming hybridized model for the 2D vector Lapla-
1000m. Libry 4027	cian Mary Barker, Washington University in St. Louis

MS5: PDE, Dynamical Systems and Applications (Part I)

Organizers:	Selin	n Sukhtaiev, Auburn University
	Magg	gie Han, Auburn University
	Wenz	xian Shen, Auburn University
Talks & Speak	KERS:	1. Multi-strain Epidemic Model Rachidi Salako, Ohio State University/University of Nevada at Las Vegas
		2. Embedded eigenvalues for the Neumann-Poincare operator
Scheduled at	r:	Stephen Shipman, Louisiana State University
Parallel Sessio	on 1	3. The essential spectrum of breathing pulses in a femtosecond
Saturday,		laser
September 18	,	John Zweck, University of Texas at Dallas
10:00-12:30		
Boom Libry	4035	4. Traveling wave solutions for two species competitive chemo-
Toolii. Libry	1000	taxis systems
		Tahir Issa, San Jose State University

5. Isentropic approximation Ronghua Pan, Georgia Tech

MS5: PDE, Dynamical Systems and Applications (Part II)

Organizers:	Selim Sukhtaiev, Auburn University
	Maggie Han, Auburn University
	Wenxian Shen, Auburn University

TALKS & SPEAKERS:

1. Small breathers of nonlinear Klein-Gordon equations via exponentially small homoclinic splitting Chongchun Zeng, *Georgia Tech*

SCHEDULED AT:2. TBD
Zhiwu Lin, Georgia TechParallel Session 23. Spectral decomposition and decay to grossly determined
solutions for a simplified BGK model
Alim Sukhtaiev, Miami UniversityRoom: Libry 40354. Modeling density dependent dispersal and habitat fragmen-
tation via reaction diffusion equations
Jerome Goddard, Auburn University at Montgomery

Mag. Wen	gie Han, Auburn University xian Shen, Auburn University
Talks & Speakers:	 Delayed model for the transmission and control of COVID- 19 — the role of Fangcang shelter hospital in Wuhan Guihong Fan, Columbus State University
SCHEDULED AT: Parallel Session 3 Sunday, September 19, 10:30–1:00 Room: Libry 4035	 Nonlocal dispersal equations with almost periodic dependence Maria Amarakristi Onyido, Auburn University Long transient dynamics in stochastic systems Zhongwei Shen, University of Alberta Global stability analysis of some classes of predator-prey models Wenzhang Huang, University of Alabama at Hunstville Traveling wave solutions for multi-species predator-prey systems
	Shangbing Ai, University of Alabama at Hunstville

MS5: PDE, Dynamical Systems and Applications (Part III)

Selim Sukhtaiev, Auburn University

ORGANIZERS:

MS6: Recent developments on Partial Differential Equations and Applications (Part I)

Organizers: Loc Dinh	Nguyen, University of North Carolina at Charlotte n-Liem Nguyen, Kansas State University
Talks & Speakers:	1. Optimal rates of convergence in periodic homogenization of linear elliptic equations in non-divergence form Hung Tran, University of Wisconsin-Madison
SCHEDULED AT: Parallel Session 1 Saturday	2. Infinite series asymptotic expansions for solutions of dissi- pative nonlinear differential equations Luan Hoang, Texas Tech University
September 18, 10:00–12:00 Room: Libry 4129	3. Orthogonality sampling methods for inverse scattering problems Dinh-Liem Nguyen, Kansas State University
	4. A system of first order H-J equations related to an optimal debt management problem

Khai Nguyen, North Carolina State University

MS6: Recent developments on Partial Differential Equations and Applications (Part II)

Organizers: Loc Dinh	Nguyen, University of North Carolina at Charlotte -Liem Nguyen, Kansas State University
Talks & Speakers:	1. Convergence of an inverse iterative scheme for the Hessian eigenvalue Nam Le, Indiana University Bloomington
Scheduled at:	2. Imaging scatterers from acoustic near-field measurements
Parallel Session 2	Thi-Phong Nguyen, Purdue University
Saturday, September 18,	3. Sampling methods for bi-anisotropic Maxwell's equations Thu Le, Kansas State University
3:30–5:30 Room: Libry 4129	4. Numerical viscosity solutions to Hamilton-Jacobi equatio via a Carleman estimate and the convexification method Loc Nguyen, University of North Carolina at Charlotte

MS6: Recent developments on Partial Differential Equations and Applications (Part III)

Organizers: Loc Dini	Nguyen, University of North Carolina at Charlotte n-Liem Nguyen, Kansas State University
Talks & Speakers:	1. Convexification-based globally convergent numerical method for a 1D coefficient inverse problem with experi- mental data
Scheduled at:	I huy Le, University of North Carolina at Charlotte
Parallel Session 3 Sunday, September 19,	2. On well-posedness and regularity estimates of solutions to a class of degenerate parabolic equations Tuoc Phan, University of Tennessee-Knoxville
10:30–12:30 Room: Libry 4129	3. Inverse Born series method for a periodic inverse scattering problem Trung Truong, Kansas State University
	4. Convexification for a 3D inverse scattering problem with moving point sources

Khoa Vo, Florida A&M University

MS7: Recent Developments and Applications in Computational Biology (Part I)

Organizers: Sha	n Zhao, University of Alabama		
Xint	feng Liu, University of South Carolina		
Talks & Speakers:	 Synchronization properties of scale-free networks of pitu- itary cells Richard Bertram, Florida State University 		
SCHEDULED AT:	2. MicroRNAs govern bistable cell differentiation and lineage		
Parallel Session 1	segregation via noncanonical feedback		
Saturday.	Tian Hong, University of Tennessee		
September 18,	3. Mathematical modeling, computation and experimental in-		
10:00–12:00	vestigation of dynamical heterogeneity in breast cancer		
Room: Libry 3033	Xinfeng Liu, University of South Carolina		
	4. Modeling and simulating the transmission dynamics of COVID-19		

Jin Wang, University of Tennessee at Chattanooga

MS7: Recent Developments and Applications in Computational Biology (Part II)

Organizers:	Shan Zhao, University of Alabama
	Xinfeng Liu, University of South Carolina

Talks & Speakers:	t. Micro-macro coupling of fluid dynamics in complex fluids
	Paula Vasquez, University of South Carolina

	2. A hybrid model for simulating sprouting angiogenesis in
Scheduled at:	biofabrication Yi Sun, University of South Carolina
Parallel Session 2	
Saturday, September 18, 3:30–5:30	3. A regularization approach for biomolecular electrostatics involving singular charge sources and diffuse interfaces Shan Zhao, University of Alabama
Room: Libry 3033	4. Determination of protein-membrane interface using surface
	phase field with random potential
	Yongcheng Zhou, Colorado State University

MS8: Modeling and Data Science in Quantitative Biology: Predictions and Descriptions (Part I)

ORGANIZERS: Bhargav Karamched, Florida State University

Talks & Speakers:	1. Delay-induced uncertainty in a paradigmatic glucose- insulin model Bhargav Karamched, <i>Florida State University</i>
Scheduled at:	2. Management strategies using optimal control for disease
Parallel Session 1 Saturday.	outbreaks George Lytle, University of Montevallo
September 18, 10:00–12:00	3. Data-driven approaches for predicting and reconstructing cardiac electrical dynamics
Room: Libry 3041	Elizabeth Cherry, Georgia Institute of Technology
	4. Fast-slow analysis of a stochastic mechanism for electrical bursting Mehran Fazli, <i>Florida State University</i>

MS8: Modeling and Data Science in Quantitative Biology: Predictions and Descriptions (Part II)

ORGANIZERS: Bhargav Karamched, Florida State University

Talks & Speakers:	1. Cyclic network structure and multistationarity in biochem- ical networks Casian Pantea, West Virginia University
Scheduled at:	2. Modeling and data analysis for filament organization in cells
Parallel Session 2	Veronica Ciocanel, Duke University
Saturday, September 18,	3. Gene expression level classification using conditional ran- dom fields
3:30–5:30	Xiyuan Liu, Louisiana Tech University
Room: Libry 3041	4. The epidemiological implications of jails for COVID-19 Kellen Myers, <i>Tusculum University</i>

MS9: Deep Learning Methods for Data Driven Models (Part I)

Organizers: Zhu	Wang, University of South Carolina
Lili	Ju, University of South Carolina
Talks & Speakers:	1. Alternating the population and control neural networks to solve high-dimensional Stochastic mean-field games Wuchen Li, University of South Carolina
Scheduled at:	2. Neural parametric Fokker-Planck equations
Parallel Session 1	Shu Liu, <i>Georgia Tech</i>
Saturday,	3. Equivariant neural network in computer vision and scien-
September 18,	tific computing
10:00–12:00	Wei Zhu, University of Massachusetts Amherst
Room: Libry 3127	4. Solving and learning phase-field models using the modified physics informed neural networks Jia Zhao, Utah State University

MS9: Deep Learning Methods for Data Driven Models (Part II)

Organizers: Zhu Lili	Wang, University of South Carolina Ju, University of South Carolina
Talks & Speakers:	1. Reproducing Activation Functions for Deep Learning Chunmei Wang, University of Florida
	2. Solving PDEs on unknown manifolds with machine learning
Scheduled at:	Senwei Liang, Purdue University
Parallel Session 2	3. A nonlocal gradient for high-dimensional black-box opti-
Saturday,	mization in scientific machine learning
September 18,	Guannan Zhang, Oak Ridge National Laboratory
3:00-5:30	4. Improved perlineer level act learning for high dimensional
Room: Libry 3127	function approximation
	Anthony Gruber, Florida State University

MS10: Theory Meets Practice for Inverse Problems in Imaging Applications (Part I)

ORGANIZERS:	Anuj Abhishek, University of North Carolina at Charlotte Caufiquar Khan, University of North Carolina at Charlotte
Talks & Speakef	s: 1. A new nonlinear sparse optimization framework for two- photon photoacoustic computed tomography Souvik Roy, University of Texas at Arlinton
Scheduled at: Parallel Session	2. TBD Shyla Kupis, Clemson University
Saturday, September 18, 10:00–12:00	3. On accelerating iterative gradient type methods for solving Electrical Impedance Tomography problem Sanwar Ahmad, Colorado State University
Room: Libry 40	33 4. Adaptive estimation of function from exponential radon transform data Sakshi Arya, <i>Pennsylvania State University</i>

MS10: Theory Meets Practice for Inverse Problems in Imaging Applications (Part II)

•	Organizers: Anuj Tauf	Abhishek, University of North Carolina at Charlotte Aquar Khan, University of North Carolina at Charlotte
,	Talks & Speakers:	1. Streak artefacts in X-ray tomography Yiran Wang, <i>Emory University</i>
	Scheduled at:	2. From static to dynamic inverse problems: new edge- preserving methods for image reconstruction
Ì	Parallel Session 2	Mirjeta Pasha, Arizona State University
	Saturday, September 18, 3:30–5:00	3. An optimal Bayesian estimator for a stochastic problem of diffuse optical tomography Anuj Abhishek, UNC Charlotte

Room: Libry 4033

MS11: Recent Progress of Classical and Deep Learning Methods in Inverse Problems and Imaging (Part I)

Organizers: Xia	ojing Ye, Georgia State University
Yar	19 Yang, Michigan State University
Talks & Speakers:	1. Structure probing neural network deflation Chunmei Wang, University of Florida
Scheduled at:	2. Optimal transport for parameter identification of chaotic dynamics via invariant measures
Parallel Session 1	Yunan Yang, New York University
Saturday,	3. Deep learning theory for solving PDEs: approximation, op-
September 18,	timization, and generalization
10:00–12:00	Haizhao Yang, Purdue University
Room: Libry 4127	4. Model predictions in epidemiology by using stable param- eter estimation and real data Alexandra Smirnova, <i>Georgia State University</i>

MS11: Recent Progress of Classical and Deep Learning Methods in Inverse Problems and Imaging (Part II)

Organizers: Xiac Yang	ojing Ye, Georgia State University g Yang, Michigan State University
Talks & Speakers:	1. Neural primal dual methods for mean field games Wuchen Li, University of South Carolina
Scheduled at:	2. Quantitative PAT with simplified P_N approximation Yimin Zhong, <i>Duke University</i>
Parallel Session 3 Sunday, September 19, 10:30–12:30 Room: Libry 3127	 Machine learning for inverse problems in sonar imaging Christina Frederick, New Jersey Institute of Technology Geometry inspired DNNs on manifold-structured data Rongjie Lai, Rensselaer Polytechnic Institute

MS12: Recent Developments of Numerical Methods for Fluid Flows and Applications (Part I) $\,$

ORGANIZERS: Thi-Thao-Phuong Hoang, Auburn University

Talks & Speakers:	1. A weighted least-squares finite element method for Biot's consolidation problem Hyesuk Lee, <i>Clemson University</i>
Scheduled at:	2. Efficient methods for non-Newtonian fluids Sara Pollock, University of Florida
Parallel Session 1	
Saturday, September 18, 10:00–12:00	3. An artificial compressibility CNLF method for the Stokes- Darcy model and application in ensemble simulations Ying Li, University of Florida
Room: Libry 4041	4. High-order multirate explicit time-stepping schemes for the baroclinic-barotropic split dynamics in primitive equations Rihui Lan, University of South Carolina

MS12: Recent Developments of Numerical Methods for Fluid Flows and Applications (Part II)

ORGANIZERS: Thi-Thao-Phuong Hoang, Auburn University

Talks & Speakers:	1. Stabilized integrating factor Runge-Kutta method and un- conditional preservation of maximum bound principle Lili Ju, University of South Carolina
Scheduled at:	 Exponential integrators for meteorological equations Vu Thai Luan, Mississippi State University Pressure robust scheme for incompressible flow Lin Mu, University of Georgia Geometric multigrid for massively parallel, adaptive, large scale Stokes flow problem
Parallel Session 3	
Sunday, September 19, 10:30–12:30 Room: Libry 3041	
	Timo Heister, Clemson University

MS13: Surrogate modeling for high-dimensional problems and applications (Part I)

Organizers: Ho	ang Tran, Oak Ridge National Laboratory
Arr	menak Petrosyan, Georgia Tech
Talks & Speakers:	1. Robust Identification of differential equations from noisy data Sung Ha Kang, <i>Georgia Tech</i>
Scheduled at:	2. Plateau phenomenon in gadient descent training of ReLU
Parallel Session 1	networks: explanation, quantification, and avoidance
Saturday,	Yeonjong Shin, Brown University
September 18,	3. Optimal transport methods in nonlinear dimensionality re-
3:30–5:30	duction
Room: Mell 3520	Keaton Hamm, University of Texas at Arlington
L	4. A bandit-learning approach to multifidelity approximation Yiming Xu, University of Utah

MS13: Surrogate modeling for high-dimensional problems and applications (Part II)

Organizers: Hoa	ang Tran, Oak Ridge National Laboratory
Arm	nenak Petrosyan, Georgia Tech
Talks & Speakers:	1. Gaussian process and Bayesian optimization – Bridging the gap between theory and practice in materials science Anh Tran, Sandia National Laboratory
Scheduled at:	2. TBD
Parallel Session 3	Oleksander Vlasiuk, Vanderbilt University
Sunday,	3. Non-convex analysis of matching and embedding of image
September 19,	keypoints
10:30–12:30	Vahan Huroyan, University of Arizona
Room: Mell 3520	4. Learning high-dimensional Hilbert-valued functions with deep neural networks from limited data Nick Dexter, Simon Fraiser University

MS14: Numerical Methods and Deep Learning for Nonlinear PDEs (Part I)

Organizers: Chu Sara	anmei Wang, University of Florida a Pollock, University of Florida
Talks & Speakers:	1. On the equations of electroporoelasticity A.J. Meir, Southern Methodist University
Scheduled at:	 Solving high-dimensional PDEs using weak adversarial networks Xiaojing Ye, Georgia State University Learning nonlocal constitutive PDE models with vector- cloud neural networks Jiequn Han, Flatiron Institute
Parallel Session 1	
Saturday, September 18, 3:30–5:30	
Room: Libry 4041	4. Deep network approximation via function composition Shijun Zhang, National University of Singapore

MS14: Numerical Methods and Deep Learning for Nonlinear PDEs (Part II)

Organizers: Ch Sar	unmei Wang, University of Florida a Pollock, University of Florida
Talks & Speakers:	1. Transition path theory with low complexity models Yuehaw Khoo, University of Chicago
	2. Large eddy simulation reduced order models
Scheduled at:	Traian Iliescu, Virginia Tech
Parallel Session 3	3. A C_0 Interior Penalty Method for the Phase Field Crystal
Sunday,	Equation
September 19,	Amanda Diegel, Mississippi State University
10:30-12:30	4 Extended Galerkin methods in finite element exterior cal-
Room: Libry 4041	culus
	Yuwen Li, Penn State University
MS15: Mathematical Modeling, Analysis and Applications (Part I)

ORGANIZERS: Thomas Hagen, University of Memphis

Talks & Speakers:	1. Recent results on the uniform observability of filtered approximations for piezoelectric beam equations Ozkan Ozer, Western Kentucky University
Scheduled at:	2. Local null controllability for a bacterial infection in a
Parallel Session 1	chronic wound Stanhan Cuffay, Calliamilla High School
Saturday,	Stephen Guney, Contervite High School
September 18,	3. Surjectivity results for monotone operators perturbed by
3:30-5:30	compact operators in reflexive spaces
Room: Libry 4127	Claudio Morales, University of Alabama in Huntsville
	4. Free-boundary problems in film forming flows
	Thomas Hagen, University of Memphis

MS15: Mathematical Modeling, Analysis and Applications (Part II)

Organizers: Th	omas Hagen, University of Memphis	
Talks & Speakers:	1. Analysis of the models for blown film extrusion: qua cylinderical and thin-shell MD Fayaz Ahamed, University of Memphis	asi-
Scheduled at:	2. Modelling human balance using intermittent feedback co	on-
Parallel Session 3 Saturday,	trol Lashika Rajapaksha, University of Texas at Dallas	
September 19, 10:30–12:00	3. Fluid-structure interaction with Kelvin-Voight dampi analyticity, spectral analysis, exponential decay	ng:

Rasika Mahawattege, University of Memphis

10:30-12:00Room: Libry 4127

MS16: Recent Advances in Nonlinear Wave Propagation and Interaction (Part I)

Organizers: Ilija Qi H	Jegdic, Texas Southern University an, Texas A&M University San Antonio
Talks & Speakers:	1. Discontinuous Galerkin method for black oil problem: con- vergence and analysis Loic Cappanera, University of Houston
SCHEDULED AT: Parallel Session 1 Saturday.	2. Mathematical analysis and numerical studies for the modi- fied Buckley-Leverett equations Ying Wang, University of Oklahoma
September 18, 10:00–12:00	3. Stability of vortex lines attached to a thin airfoil Jun Chen, Yichun University
Room: Libry 3133	4. The effect of the asymmetric Ekman term on the phe- nomenology of the two-layer quasigeostropic model Elefterios Gkioulekas, University of Texas at Rio Grande Valley

MS16: Recent Advances in Nonlinear Wave Propagation and Interaction (Part II)

Organizers: Ilija Qi H	Jegdic, Texas Southern University Ian, Texas A&M University San Antonio
Talks & Speakers:	 On entire solutions to eikonal-type partial differential equa- tions Qi Han, Texas A&M University San Antonio
SCHEDULED AT: Parallel Session 2 Saturday, September 18, 3:30–5:30 Room: Libry 3133	 Semi-hyperbolic patches for the unsteady transonic small disturbance equation Katarina Jegdic, University of Houston Bistability in deterministic and stochastic SLIAR-type models with imperfect and waning vaccine protection Evan Milliken, University of Louisville
	4. TBD Zhaosheng Feng, University of Texas Rio Grande Valley

MS16: Recent Advances in Nonlinear Wave Propagation and Interaction (Part III)

Organizers: II Q	ja Jegdic, Texas Southern University i Han, Texas A&M University San Antonio
Talks & Speakers	: 1. Properties of a coupled compressible Flow-plate dynamics Pelin Guven Geredeli, <i>Iowa State University</i>
Scheduled at:	2. Stability analysis of interactive fluid and multilayered struc- ture PDE dynamics
Parallel Session 3 Sunday, September 19,	 George Avalos, University of Nebraska Lincoln 3. Controlling refraction using sub-wavelength resonators Yue Chen, Auburn University Montgomery
10:30–1:00 Room: Libry 313	3 4. Large-time behavior of 2D incompressible MHD system with partial dissipation Wen Feng, Niagara University
	5. Study of chaotic vibration phenomenon of the non-strictly hyperbolic equation Jing Tian, Towson University

MS17: Modeling and Numerical Methods for Image Problems

ORGANIZERS:	Wei Zhu,	University of Alabama at Tuscaloosa
Talks & Speake	RS: 1.	Image decomposition into structure, harmonic and oscilla- tory Components Sung Ha Kang, <i>Georgia Institute of Technology</i>
Scheduled at:	2.	 A novel regularization based on the error function for sparse recovery Weihong Guo, Case Western Reserve University Learnable descent algorithm for nonsmooth nonconvex optimization with applications in image reconstruction
Parallel Session	. 3	
Sunday,		
September 19,	3.	
10:30-12:30		
Room: Libry 30	033	Xiaojing Ye, Georgia State University
	4.	First-order image restoration models for staircase reduction and contrast preservation

Wei Zhu, University of Alabama at Tuscaloosa

MS18: Advances in Memory Efficient Numerical Algorithms for Kinetic Problems

ORGANIZERS: Stefan Schnake, Oak Ridge National Laboratory

Talks & Speakers:	1. Implicit methods with reduced memory for time-dependent radiation transport problems Dmitry Anistratov, North Carolina State University
Scheduled at:	2. Low-memory, discrete ordinates, discontinuous Galerkin methods for radiative transport
Parallel Session 3	
Sunday,	Zheng Sun, University of Alabama
September 19,	3. A Hybrid decomposition method for the BGK equation
10:30-12:30	Minwoo Shin, University of Notre Dame
Room: Libry 4033	4. Residual based rank adaptive algorithms for dynamic low-
	rank approximation
	Stefan Schnake, Oak Ridge National Laboratory

MS19: Recent Advances in Iterative Solvers for Numerical Optimization and Nonlinear Systems (Part I)

ORGANIZERS: William Kong, Oak Ridge National Laboratory Paul Laiu, Oak Ridge National Laboratory

TALKS & SPEAKERS:

1. Iteration complexity of a proximal augmented Lagrangian method for constrained nonconvex composite programming

William Kong, Oak Ridge National Laboratory

- 2. Simple and optimal methods for stochastic variational inequalities Georgios Kotsalis, *Georgia Tech*
- 3. Neural projected Fokker-Planck equations Wuchen Li, University of South Carolina
- 4. Dynamic filtering for Anderson acceleration iteration Sara Pollock, *University of Florida*

Scheduled at:
Parallel Session 1
Saturday,
September 18,

Room: Mell 3520

10:00-12:00

MS19: Recent Advances in Iterative Solvers for Numerical Optimization and Nonlinear Systems (Part II)

Organizers: Will	iam Kong, Oak Ridge National Laboratory
Paul	Laiu, Oak Ridge National Laboratory
Talks & Speakers:	 An infeasible-start framework for convex quadratic opti- mization Paul Laiu, , Oak Ridge National Laboratory
SCHEDULED AT:	2. First order methods for some structured nonconvex func-
Parallel Session 3	tion constrained optimization problems
Sunday,	Digvijay Boob, Southern Methodist University
September 19, 10:30–12:00 Room: Mell 4520	3. Stochastic dual dynamic programming algorithms Shixuan Zhang, <i>Georgia Tech</i>

CP: Contributed Presentations (Part I)

CHAIR: Thor	mas Hamori, University of South Carolina
Talks & Speakers:	1. On a class of nonlocal macroscopic models Thomas Hamori, University of South Carolina
Scheduled at:	2. Construction of orthonormal polynomial wavelets and its application in solving SBVPs
Parallel Session 1	Diksha Tiwari, University of Vienna
Saturday, September 18, 10:00–12:00 Mell 4510A	3. Multiscale simulations and convergence analysis for up- scaled multi-continuum flows Tina Mai, Duy Tan University at Da Nang (Vietnam) and Texas A&M University at College Station (USA)
	4. Nonconforming time discretization based on Robin trans- mission conditions for the Stokes-Darcy system Hemanta Kunwar, <i>Clemson University</i>
	5. Lehmer close pair differences to their next-door solutions Kate Johnson, University of California Davis

6. Efficient algorithms for computation of MHD flow ensemble Muhammad Mohebujjaman, Texas A&M International University

CP: Contributed Presentations (Part II)

CHAIR: Kwadwo Antwi-Fordjour, Samford University

Talks & Speakers:	1. Dynamics of a predator-prey model with generalized func- tional response and mutual interference Kwadwo Antwi-Fordjour, <i>Samford University</i>
Scheduled at:	2. Learning nonlinear level sets for functions approximations on sparse data through goal-driven pseudo-reversible neural network Yuankai Teng, University of South Carolina
Saturday, September 18.	
10:00–12:00 Mell 4520	3. A multistep spectral method for time-dependent PDEs Bailey Rester, <i>The University of Southern Mississippi</i>
	4. On the stochastic sigmoid Beverton-Holt model Quinten McKinney, University of Alabama in Huntsville
	5. Early signs of regime shift and major population fluctuation in a two-timescale ecosystem

Susmita Sadhu, Georgia College & State University

6. Revealing the Russian Information Operation Networks structure using a predictive model Sachith Dassanayaka, *Texas Tech University*

CP: Contributed Presentations (Part III)

CHAIR: Fan Bai, Florida State University

TALKS & SPEAKERS: 1. Take-away impartial combinatorial game on different geo-

	Molena Nguyen, North Carolina State University
Scheduled at:	2. SPDE-Net A neural network way to solve Singularly Per-
Parallel Session 2	turbed Partial Differential Equations Sangeeta Yadav, Indian Institute of Science
Saturday,	
September 18,	3. Partitioned solution of a coupled ROM-FEM model for a
3:30-5:10	transmission problem
Mell $4510A$	Amy de Castro, Clemson University and SIP at Sandia National Labs
	4. A theoretical investigation of a frequency-dependent regu-
	lation of axonal growth
	Fan Bai, Florida State University

metric and discrete structures

5. Fast geometric method for approximating high dimensional kernel matrices Difeng Cai, *Emory University*

CP: Contributed Presentations (Part IV)

CHAIR: Kwadwo Antwi-Fordjour, Samford University

Talks & Speakers:	1. Steklov-Poincaré analysis of the basic three-domain stent problem Irving Martinez, <i>Emory University</i>
Scheduled at:	 A least-squares conjugate-gradient finite element method solver for velocity-current MHD equations K. Daniel Brauss, Francis Marion University
Parallel Session 2	
Saturday,	
September 18,	3. Deep neural network for nonlinear regression and its appli-
3:30-5:10	cations in climate and turbulence modeling Dongwei Chen, <i>Clemson University</i>
Mell 4520	
	4. Even and odd decomposition of the Bernstein polynomial
	opera-tors in $C[-1,1]$
	Ted Kilgore, Auburn University

Poster Presentations

Talks & Speakers:	1. Convergence of a Diffuse Interface Poisson-Boltzmann (PB) Model to the Sharp Interface PB Model: a Unified Regu- larization Formulation
Scheduled at:	 Mark McGowan, University of Alabama 2. A FFT accelerated high order finite difference method for elliptic boundary value problems over irregular domains Yiming Ren, University of Alabama
Saturday, September 18, 6:00–8:00	
	3. Damped waves propagation on moving meshes: An appli- cation in cardiac electrophysiology simulation

Cesar Acosta-Minoli, Universidad del Quindío



4 Abstracts of Mini-symposia and Contributed Talks

MS1: Reduced Order Modeling in the Age of Data (Part I)

ORGANIZERS: Traian Iliescu, Virginia Tech Alessandro Veneziani, Emory University Omer San, Oklahoma State University

DESCRIPTION: This minisymposium aims at giving a survey of recent developments in reduced order modeling, with a special emphasis on data-driven modeling and machine learning. Computational modeling, numerical analysis, and applications to realistic engineering, geophysical, and biomedical problems will be covered in this minisymposium. Both achievements and open problems in reduced order modeling will be discussed.

TALKS 1. Data-driven variational multiscale reduced order models

DETAILS:

Changhong Mou, Virginia Tech

ABSTRACT. We propose a new data-driven reduced order model (ROM) framework that centers around the hierarchical structure of the variational multiscale (VMS) methodology and utilizes data to increase the ROM accuracy at a modest computational cost. The VMS methodology is a natural fit for the hierarchical structure of the ROM basis: In the first step, we use the ROM projection to separate the scales into three categories: (i) resolved large scales, (ii) resolved small scales, and (iii) unresolved scales. In the second step, we explicitly identify the VMS-ROM closure terms, i.e., the terms representing the interactions among the three types of scales. In the third step, we use available data to model the VMS-ROM closure terms. Thus, instead of phenomenological models used in VMS for standard numerical discretizations (e.g., eddy viscosity models), we utilize available data to construct new structural VMS-ROM closure models. Specifically, we build ROM operators (vectors, matrices, and tensors) that are closest to the true ROM closure terms evaluated with the available data. We test the new data-driven VMS-ROM in the numerical simulation of four test cases: (i) the 1D Burgers equation with viscosity coefficient $\nu = 10^{-3}$; (ii) a 2D flow past a circular cylinder at Reynolds numbers Re = 100, Re = 500, and Re = 1000; (iii) the quasi-geostrophic equations at Reynolds number Re = 450 and Rossby number Ro = 0.0036; and (iv) a 2D flow over a backward facing step at Reynolds number Re = 1000. The numerical results show that the data-driven VMS-ROM is significantly more accurate than standard ROMs.

2. Stochastic closure model via parametric inference

Fei Lu, Johns Hopkins University

ABSTRACT. Stochastic closure models aim to make predictions with uncertainty quantified. We achieve this goal by accounting for the effects of the unresolved scales in a statistical learning framework. A fundamental idea is the approximation of the discretetime flow map for the dynamics of the resolved variables. The flow map, which encodes the effects of the unresolved scales, is a functional of the resolved scales, thus its inference faces the curse of dimensionality. We investigate a semi-parametric approach that derives parametric models from the structure of the full model. We show that this approach leads to effective reduced models for deterministic and stochastic PDEs, such as the Kuramoto-Sivashisky equation to viscous stochastic Burgers equations. In particular, we highlight the shift from the nonlinear Galerkin method to statistical inference, and discuss maximal space-time reduction.

3. Dynamics informed data-driven closures for chaotic systems

Honghu Liu, Virginia Tech

ABSTRACT. In this talk, we will discuss an approach to parameterize the unresolved small scale dynamics using the resolved large scales for forced dissipative systems. We will show that efficient parameterizations can be explicitly determined as parametric deformations of dynamic/geometric objects called invariant manifolds. The minimizers are objects, called the optimal parameterizing manifolds, that are intimately tied to the conditional expectation of the original system. We will highlight, within a variational framework, a simple semi-analytic approach to determine such manifolds based on backward-forward auxiliary systems and short DNS data. Concrete examples arising from geophysical considerations will also be presented to illustrate the effectiveness of the approach.

4. Ill-effects of model inconsistency in reduced order models of incompressible flowss

Leo Rebholz, Clemson University

ABSTRACT. We study the error that arises from using different formulations in a finite element numerical scheme that generates the snapshots and the reduced order model built from those snapshots. We focus on Navier-Stokes equations, and show show how this inconsistency arises, how it affects overall error, and give results of several numerical tests that show ROMs that are consistent with the FE schemes that built them outperform those that are not.

5. Interpolatory tensorial reduced-order models for para-metric dynamical systems

Maxim Olshanskii, University of Houston

MS1: Reduced Order Modeling in the Age of Data (Part II)

Organizers:	Traian Iliescu, Virginia Tech	
	Alessandro Veneziani, Emory University	
	Omer San, Oklahoma State University	
Description:	This minisymposium aims at giving a survey of recent developments in reduced order modeling, with a special emphasis on data-driven modeling and machine learning. Computational modeling, numerical analysis, and applications to realistic engineering, geophysical, and biomedical problems will be covered in this minisymposium. Both achievements and open problems in reduced order modeling will be discussed.	

TALKS1. A hybrid variational multiscale and machine learning approach for non-
linear model order reduction

Shady Ahmed, Oklahoma State University

ABSTRACT. The variational multiscale framework (VMS) is motivated by the locality of energy transfer and enabled by the hierarchy of the underlying structures. Thus, VMS appears to be a natural solution for the closure problem in projection-based reduced order models (ROMs). Applications of VMS in ROM often focus on the use of phenomenological closure models by analogy with finite elements and large eddy simulations. Recently, datadriven VMS-ROMs have been explored, where a polynomial-like structure was considered to represent the interactions between different scales. We extend this by investigating whether neural networks can reveal the nonlinear processes and correlations as represented by the mutual interactions between various batches of resolved and unresolved scales. Moreover, we embed the locality of energy transfer into the learning and inference process of the neural network in a physics-guided machine learning (PGML) framework. We showcase the applicability of the proposed PGML-VMS-ROM using a set of prototypical flow problems with strong nonlinearity.

2. Modified neural ordinary differential equations for stable learning of chaotic dynamics.

Romit Maulik, Argonne National Laboratory

ABSTRACT. In recent times, several deep learning techniques have been used for learning dynamical systems from data. One state-of-the-art technique is the method of neural ordinary differential equations (NODEs) which learns the right hand side of a system of differential equations using a neural network. However, we observe that a basic implementation of NODEs for learning chaotic dynamics is shown to lead to unstable surrogate models. To remedy this, we introduce a novel decomposition of the NODE into a linear and nonlinear term that promotes long-term stability and robustness into the surrogate. The linear term may be specified by utilizing a dictionary or through a multipoint stencil prescribe through a convolutional layer. We observe that our novel NODE is able to learn the chaotic dynamics of the Kuramoto-Sivashinsky equations and provide models that are stable and robust to noise for long durations. Moreover, the prescription of a linear term also allows for the identification of an approximate inertial manifold directly from the data which can be used for further model-order reduction of the surrogate.

3. Physics-guided machine learning for projection-based reduced-order modeling

Suraj Pawar, Oklahoma State University

ABSTRACT. The unprecedented amount of data generated from experiments, field observations, and large-scale numerical simulations at a wide range of spatio-temporal scales have enabled the rapid advancement of deep learning models in the field of fluid mechanics. Although these methods are proven successful for many applications, there is a grand challenge of improving their *generalizability*. This is particularly essential when datadriven models are employed within outer-loop applications like optimal control where the unseen operating conditions are common. In this study, we put forth a physics-guided machine learning (PGML) framework that integrates the interpretable physics-based model with a deep learning model. Leveraging a concatenated neural network design from multimodal data sources, the PGML framework is capable of enhancing the generalizability of data-driven models and effectively protect against or inform about the inaccurate predictions resulting from extrapolation. We illustrate the improved generalizability of the PGML framework against a purely data-driven approach through the injection of physics information from Galerkin projection model into long-short term memory (LSTM) architecture. Our quantitative analysis shows that the overall model uncertainty can be reduced through the PGML approach especially for test data coming from a distribution different than the training data. This work builds a bridge between physics-based theories and data-driven modeling paradigm and paves the way for using hybrid physics and machine learning modeling approaches for next-generation digital twin technologies.

4. Data-driven realistic wind data generation for safe operation of small unmanned air vehicles in urban environment

Rohit Vuppala, Oklahoma State University

ABSTRACT. Unmanned Air Vehicles(UAV) are increasingly being used as an efficient means for transportation of goods, surveillance, disaster management, etc over complex terrains. One major application for Unmanned Air Systems(UAS) is the Urban Air Mobility concept where, small Unmanned Air Systems(sUAS) are inclined to be majorly used due to space constraint in densely packed urban environment. However, for widespread usage and adoption in urban areas, physical damage to goods and injuries to passengers, caused by unanticipated wind gusts is a major challenge for sUAS. Predicting gust occurrence in real-time or close to real-time continues to be a challenge for such low-altitude operating applications. Furthermore, generating realistic wind data to test various algorithms for their safe operation like control and path planning, obstacle avoidance also poses a significant challenge for researchers. In this work we present a preliminary work for a method to efficiently generate realistic wind data for urban environments using high fidelity Large Eddy Simulation (LES) data for safe operation of small Unmanned Air Vehicles. A non-intrusive data-driven approach is utilised in achieving these results. We consider a single building in neutral atmospheric conditions for simplicity and as a demonstration of the method. Reduced Order Modeling approach (ROM) coupled with Recurrent Neural Networks, Long Short Term Memory (LSTM) specifically is used to generate computationally low cost realistic wind data. Predictions for future time-steps from the model, without the need of computationally expensive CFD simulations pave a path forward for future work on wind field predictions and for safe aware navigation of sUAS in urban spaces.

MS1: Reduced Order Modeling in the Age of Data (Part III)

ORGANIZERS:	Traian Iliescu, Virginia Tech
	Alessandro Veneziani, Emory University
	Omer San, Oklahoma State University

DESCRIPTION: This minisymposium aims at giving a survey of recent developments in reduced order modeling, with a special emphasis on data-driven modeling and machine learning. Computational modeling, numerical analysis, and applications to realistic engineering, geophysical, and biomedical problems will be covered in this minisymposium. Both achievements and open problems in reduced order modeling will be discussed.

TALKS1. Some applications of model reduction in cardiovascular mathematicsDETAILS:Alessandro Veneziani, Emory University

2. An efficient reduced order modeling method for Lagrangian data assimilation of turbulent flows

Nan Chen, University of Wisconsin-Madison

ABSTRACT. Lagrangian data assimilation of complex nonlinear turbulent flows is an important but computationally challenging topic. In this article, an efficient data-driven statistically accurate reduced-order modeling algorithm is developed that significantly accelerates the computational efficiency of Lagrangian data assimilation. The algorithm starts with a Fourier transform of the high-dimensional flow field, which is followed by an effective model reduction that retains only a small subset of the Fourier coefficients corresponding to the energetic modes. Then a linear stochastic model is developed to approximate the nonlinear dynamics of each Fourier coefficient. Effective additive and multiplicative noise processes are incorporated to characterize the modes that exhibit Gaussian and non-Gaussian statistics, respectively. All the parameters in the reduced order system, including the multiplicative noise coefficients, are determined systematically via closed analytic formulae. These linear stochastic models succeed in forecasting the uncertainty and facilitate an extremely rapid data assimilation scheme. The new Lagrangian data assimilation is then applied to observations of sea ice floe trajectories that are driven by atmospheric winds and turbulent ocean currents. It is shown that observing only about 30 non-interacting floes in a 200km x 200km domain is sufficient to recover the key multi-scale features of the ocean currents. The additional observations of the floe angular displacements are found to be suitable supplements to the center-of-mass positions for improving the data assimilation skill. In addition, the observed large and small floes are more useful in recovering the large- and small-scale features of the ocean, respectively. The Fourier domain data assimilation also succeeds in recovering the ocean features in the areas where cloud cover obscures the observations. Finally, the multiplicative noise is shown to be crucial in recovering extreme events.

3. Modeling ice sheets with deep operator networks

Mauro Perego, Sandia National Laboratories

ABSTRACT. A significant contribution to sea level rise comes from the mass loss of Greenland and Antarctic ice sheets, which can be computed by modeling ice sheet dynamics. At the glacier scale, ice behaves like a highly viscous shear thinning fluid. Several efforts over the last decades focused on efficiently solving the steady state Stokes-like flow equations governing the ice flow, which still represents the most computationally expensive part of an ice sheet model. Flow equations need to be solved at each time step. While time steps can be as little as a week, typical temporal periods of interest range from a few decades to several millennia. Further, deterministic initialization of ice sheets, performed w/ PDE-constrained optimization, requires the solution of thousands of these steady state equations, making ice sheet initialization challenging and expensive. At the moment, Bayesian inference approaches and uncertainty quantification (UQ) are not computationally tractable at the ice sheet scale, due to the large dimensionality of the parameter space and the cost of the forward Stokes model. In this work we propose to create a surrogate model for the ice flow equations. A key requirement for the surrogate is that it has to depend on high-dimensional parameter fields, such as the basal friction coefficient that determines the basal sliding or the bed topography. This will allow us to use the model for inference and for UQ. In this talk we use Deep Operator Networks (DeepONets) to create a surrogate for the flow model. DeepONets rely on approximation theory of nonlinear operators and have proven to be effective in modeling parameter-dependent PDEs problems. We train the DeepONet using data generated by finite element computation models and present preliminary results obtained for simplified glacier geometries.

4. Adaptive surrogate modeling for variational inference with normalizing flow

Daniele E. Schiavazzi, University of Notre Dame

ABSTRACT. Development of fast inference procedures where the parameters of a numerical model can be quickly learned from data, would facilitate the integration of modelbased diagnostics in the clinical routine. Sampling-based approaches such as Markov chain Monte Carlo (MCMC) typically require a significant number of pointwise evaluations from the posterior distribution, and may become computationally intractable when each of these evaluations is associated with the solution of a computationally expensive model. Unlike MCMC, new approaches combining variational inference with invertible auto-regressive transformations [1] are characterized by a computational cost that grows only linearly with the dimensionality of the latent variable space [2], providing a more efficient approach for density estimation. Moreover, the cost of computing an expensive likelihood may be mitigated by using a lightweight surrogate model, which approximates the true model response at a fixed number of "pre-training" locations. This approach might, however, generate significant bias in the estimated parameters, particularly for a surrogate that is insufficiently accurate around the true posterior modes. To improve the computational speed without sacrificing accuracy, we propose an optimization strategy that alternatively updates the parameters of a collection of auto-regressive transformations and the weights of a deep neural network surrogate. Additionally, we propose an efficient, memory-aware, sampling weighting scheme for the loss function. Finally, we present a number of numerical experiments including closed form models such as the Sobol function, and lumped parameter models of the human cardiovascular system. In particular, we focus on the performance of the proposed approach for situations where the underlying model lacks identifiability, and where introducing a mean field approximation is simply not acceptable in light of the posterior dependency among parameters. Reference: [1] Papamakarios G. et al, Masked Autoregressive Flow for Density Estimation. arXiv preprint arXiv:1705.07057, 2017. [2] Rezende D. et al, Variational Inference with Normalizing Flows. In International Conference on Machine Learning, pages 1530–1538. PMLR, 2015.

MS2: Recent Developments in Nonlocal Continuum Modeling (Part I)

ORGANIZERS: James Scott, University of Pittsburgh Pablo Seleson, Oak Ridge National Laboratory

DESCRIPTION: The efficacy of nonlocal continuum models in describing behavior across a variety of applications, such as mechanics, diffusion, and image processing, has been demonstrated in recent years. The peridynamics continuum mechanics model, nonlocal diffusion equations, and fractional PDEs are some notable examples. A variety of recent developments will be presented at this minisymposium, giving attendees a broad picture of the state-of-the-art of nonlocal continuum modeling. Topics will include advances in mathematical analysis of nonlocal models, innovations in numerical methods and computational implementations of nonlocal models, and new applications of nonlocal models to engineering and scientific problems.

TALKS 1. Nonlocal brittle fracture modeling with applied traction forces

DETAILS: Robert Lipton, Louisiana State University

ABSTRACT. A hallmark of fracture modeling using peridynamics is the numerical emergence of cracks though the use of nonlocal modeling. Here, local interactions between neighboring points result in global consequences like the emergence of fracture surfaces. Emergent phenomena can be modeled non-locally and examples include motion of flocks of birds modeled through the Cuker Smale model. We provide a peridynamics model for calculating dynamic fracture. The force interaction is derived from a double well strain energy density function. The fracture set emerges from the model and is part of the dynamics. The material properties change in response to evolving internal forces eliminating the need for a separate phase field to model the fracture set. In the limit of zero nonlocal interaction, it is seen that the model reduces to a sharp crack evolution characterized by the classic Griffith free energy of brittle fracture with elastic deformation satisfying the linear elastic wave equation off the crack. The non-local model is seen to encode the well known kinetic relation between crack driving force and crack tip velocity. A rigorous connection between the nonlocal fracture theory and the wave equation posed on cracking domains given in Dal Maso and Toader is found. This is joint work with Prashant Jha.

2. Regularity theory for nonlocal space-time master equations

Pablo Raúl Stinga, Iowa State University

ABSTRACT. The parabolic Signorini problem in elasticity gives rise to nonlinear problems driven by fractional powers of parabolic operators in divergence form. We report on our novel regularity theory for these types of nonlocal space-time equations. Our results include Harnack inequalities, and interior and global Schauder estimates. This is joint work with Animesh Biswas (Iowa State University) and José L. Torrea (Universidad Autónoma de Madrid, Spain).

3. Relaxation phenomena in the localized limit of nonlocal energies motivated by bond-based peridynamics

James M. Scott, Columbia University

ABSTRACT. We investigate properties of minimizers for a class of nonlocal nonconvex functionals that arise in peridynamics as well as the persistence of these properties in minimizers of the localized limit. We demonstrate geometric rigidity in the spirit of Reshetnyak for these nonlocal nonconvex functionals. This rigidity result states that any minimizing convergent sequence must converge to an affine map with gradient in the set of rotations. However, this result does not hold for any corresponding localized energy obtained from the vanishing horizon limit. In the topology of uniform convergence, the zero-set of the localized functional is infinite-dimensional, and includes non-affine maps. In the topology of Γ -convergence, we prove an integral representation for the localized Γ -limit. We then employ convex integration techniques to show that the localized strain energy density vanishes for any "short map;" that is, any deformation tensor with principal strains less than or equal to 1. These relaxation phenomena further quantify the discrepancy between classical nonlinear hyperelastic stored energy functionals and functionals obtained from the localized limit of nonlinear bond-based peridynamics.

4. One-side fractional diffusion equations and their finite element approximations

Mitchell Sutton, University of Tennessee, Knoxville

ABSTRACT. This talk is concerned with analyzing a class of fractional calculus of variations problems and their associated Euler-Lagrange (fractional differential) equations. Unlike the existing fractional calculus of variations which is based on the classical notion of fractional derivatives, the fractional calculus of variations considered in this talk is based on a newly developed notion of weak fractional derivatives and their associated fractional order Sobolev spaces. Since fractional derivatives are direction-dependent, using one-sided fractional derivatives and their combinations leads to new types of fractional differential equations; including new one-side fractional Laplace operators. Throughout the talk, we will establish the well-posedness and regularities for these equations as well as a new finite element method for approximating their solutions.

MS2: Recent Developments in Nonlocal Continuum Modeling (Part II)

ORGANIZERS: James Scott, University of Pittsburgh

Pablo Seleson, Oak Ridge National Laboratory

DESCRIPTION: The efficacy of nonlocal continuum models in describing behavior across a variety of applications, such as mechanics, diffusion, and image processing, has been demonstrated in recent years. The peridynamics continuum mechanics model, nonlocal diffusion equations, and fractional PDEs are some notable examples. A variety of recent developments will be presented at this minisymposium, giving attendees a broad picture of the state-of-the-art of nonlocal continuum modeling. Topics will include advances in mathematical analysis of nonlocal models, innovations in numerical methods and computational implementations of nonlocal models, and new applications of nonlocal models to engineering and scientific problems.

TALKS 1. Overall equilibrium in the coupling of peridynamics and classical continuum mechanics DETAILS: tinuum mechanics

William Oates, Florida State University

2. A symmetric force-based method for the atomistic-to-continuum coupling

Elaine Gorom, University of North Carolina at Challotte

3. Overall equilibrium in the coupling of peridynamics and classical continuum mechanics

Pablo Seleson, Oak Ridge National Laboratory

ABSTRACT. Coupling peridynamics based computational tools with those using classical continuum mechanics can be very beneficial, because it can provide a means to generate a computational method that combines the efficiency of classical continuum mechanics with the capability to simulate crack propagation, typical of peridynamics. This talk presents an overlooked issue in this type of coupled computational methods: the lack of overall equilibrium. This can be the case even if the coupling strategy satisfies the usual numerical tests involving rigid body motions as well as uniform and linear strain distributions. We focus our investigation on the lack of overall equilibrium in an approach to couple peridynamics and classical continuum mechanics recently proposed by the authors. In our examples, the magnitude of the out-of-balance forces is a fraction of a per cent of the applied forces, but it cannot be assumed to be a numerical round-off error. We show analytically and numerically that the main reason for the existence of out-of-balance forces is a lack of balance between the local and nonlocal tractions at the coupling interface. This usually results from the presence of high-order derivatives of displacements in the coupling zone. This is a joint work with Greta Ongaro, Ugo Galvanetto, Tao Ni, and Mirco Zaccariotto.

4. A Petrov-Galerkin method for nonlocal convection-dominated diffusion problems

Xiaochuan Tian, UC San Diego

ABSTRACT. We present a Petrov-Gelerkin (PG) method for a class of nonlocal convectiondominated diffusion problems. There are two main ingredients in our approach. First, we define the norm on the test space as induced by the trial space norm, i.e., the optimal test norm, so that the inf-sup condition can be satisfied uniformly independent of the problem. We show the well-posedness of a class of nonlocal convection-dominated diffusion problems under the optimal test norm with general assumptions on the nonlocal diffusion and convection kernels. Second, following the framework of Cohen et al. (2012), we embed the original nonlocal convection-dominated diffusion problem into a larger mixed problem so as to choose an enriched test space as a stabilization of the numerical algorithm. In the numerical experiments, we use an approximate optimal test norm which can be efficiently implemented in 1d, and study its performance against the energy norm on the test space. We conduct convergence studies for the nonlocal problem using uniform hand p-refinements, and adaptive h-refinements on both smooth manufactured solutions and solutions with sharp gradient in a transition layer. In addition, we confirm that the PG method is asymptotically compatible. This is a joint work with Yu Leng, Leszek Demkowicz, Hector Gomez and John Foster.

MS2: Recent Developments in Nonlocal Continuum Modeling (Part III)

ORGANIZERS: James Scott, University of Pittsburgh Pablo Seleson, Oak Ridge National Laboratory

DESCRIPTION: The efficacy of nonlocal continuum models in describing behavior across a variety of applications, such as mechanics, diffusion, and image processing, has been demonstrated in recent years. The peridynamics continuum mechanics model, nonlocal diffusion equations, and fractional PDEs are some notable examples. A variety of recent developments will be presented at this minisymposium, giving attendees a broad picture of the state-of-the-art of nonlocal continuum modeling. Topics will include advances in mathematical analysis of nonlocal models, innovations in numerical methods and computational implementations of nonlocal models, and new applications of nonlocal models to engineering and scientific problems.

TALKS1. A fast numerical method for a state-based PD modelDETAILS:Hong Wang, University of South Carolina

2. Convergence studies in meshfree peridynamic wave and crack propagation

Marco Pasetto, Oak Ridge National Laboratory

3. An RBF quadrature rule approach for solving nonlocal continuum models

Isaac Lyngaas, Oak Ridge National Laboratory

ABSTRACT. Nonlocal continuum models have gained interest as alternatives to traditional PDE models due to their capability of handling solutions with discontinuities and their ease of modeling anomalous diffusion. The typical approach used for approximating these time-dependent nonlocal integro-differential models is to use finite element or discontinuous Galerkin methods; however these approaches can be quite computationally intensive especially when solving problems in more than one dimension due to the approximation of the nonlocal integral. In this work, a method based on using radial basis functions is presented to generate accurate quadrature rules for the nonlocal integral appearing in the model. These quadrature rules are then coupled with a finite difference approximation to find the time-dependent terms. The viability of the method is demonstrated through various numerical tests on time dependent nonlocal diffusion, nonlocal anomalous diffusion and nonlocal advection problems. In addition to nonlocal problems with continuous solutions.

4. The evolution of the peridynamics co-authorship network

Biraj Dahal, Georgia Institute of Technology

ABSTRACT. Peridynamics is a relatively new field in continuum mechanics that has developed over the past 20 years. We study the evolution of collaborations in peridynamics since its inception using social network analysis. We construct a network for each year from 2000 to 2019 based on co-authorship between scientists in peridynamics. Our study demonstrates that the peridynamics community has been growing exponentially in size in recent years. Node centrality metrics are used to identify the most collaborative scientists in the community. We compute link recommendations based on both elevating a scientist's position in the network with respect to centrality or closing structural holes in the network identified with persistent homology. In some sense, our work studies the past, present, and future of the peridynamics community.

MS3: Recent Advances in Numerical Methods for PDEs (Part I)

ORGANIZERS: S.S. Ravindran, University of Alabama in Huntsville

DESCRIPTION: The rapid growth and diversity of research in science and engineering over the past decades has spawned many intellectually challenging and computationally intensive PDE problems to be solved. Despite significant progress made in development of efficient computational methods for numerical solution of these problems, many problems still remain open. This minisymposium aims to provide a platform to present recent developments on the novel and efficient numerical methods for solving PDEs, enable in-depth discussions on a variety of computa-tional efforts for solving problems arising in areas of science and engineering from researchers at all stages of their careers.

TALKS 1. High-order multirate time integration for multiphysics PDE systems

DETAILS: Daniel Reynolds, Southern Methodist University

ABSTRACT. Modern multiphysics applications present numerous challenges for legacy numerical time integration methods, including the presence of multiple processes that act on disparate time scales, and that combine stiff and nonstiff, as well as linear and nonlinear equations. Although when considered in isolation, optimal methods may exist for each component, no single algorithm is typically suitable for the combined problem. As a result, practitioners have historically tackled multiphysics problems using ad-hoc operator-splitting techniques, that typically exhibit low accuracy and have questionable numerical stability.

In this talk, we focus on our recent work in constructing novel high-order "multirate" time integration methods for multiphysics applications. These flexible approaches allow each phyical process to be treated using optimal algorithms, while simultaneously providing high accuracy and robust stability. Specifically, we will discuss our work in constructing fourth-order (and higher) multirate methods, as well as those that additionally allow implicit or mixed implicit-explicit treatment at each time scale.

2. Improving accuracy and stability of existing time integrators with nonintrusive post-processing

Victor DeCaria, Oak Ridge National Laboratory

3. Numerical solution of supersonic Euler and magnetohydrodynamic flow past cones

Ian Holloway, Wright State University

ABSTRACT. A numerical scheme is presented for systems of conservation laws on manifolds which arise in high speed aerodynamics and magneto-aerodynamics. The systems are presented in an arbitrary coordinate system on the manifold and involve source terms which account for the curvature of the domain. In order for a numerical method to accurately capture the behavior of the system it is solving, the equations must be discretized in a way that is not only consistent in value, but also models the appropriate character of the system. Such a discretization is presented which preserves the tensorial transformation relationships involved in formulating equations in a curved space. A numerical method is demonstrated using this discretization to solve the conical Euler and Ideal Magnetohydrodynamic equations. To the presenter's knowledge, this is the first demonstration of a numerical solver for the conical Ideal MHD equations.

4. A low Mach number model and associated numerical algorithm for simulating complex multiphase flows with mass transfer in a cryogenic fuel tank

Mark Sussman, Florida State University

5. Low rank CP tensor decomposition for model order reduction

Carmeliza Navasca, University of Alabama at Birmingham

ABSTRACT. Model order reduction techniques such as the POD and the Reduced Basis Methods are typically used to solve the problems requiring one to query an expensive yet deterministic computational solver once for each parameter node. In this work, we propose a tensor-based model reduction algorithm to achieve significant computational savings in expensive high fidelity numerical solvers. Dimension reduction techniques are often used when the high-dimensional tensor has relatively low intrinsic rank compared to the ambient dimension of the tensor. We formulate an ℓ_1 regularized optimization problem with an appropriate choice of the regularization parameter by embedding the flexible hybrid method into the framework of the canonical polyadic tensor decomposition to offset the computational burden processing large amount of data. More specifically, assuming tensor A as the collection of the solutions on sampled parameters and selecting the snapshots (reduced bases) for the low rank approximation of the solution manifold, we employ our algorithm to give a prior knowledge of rank(A) denoted R, and then we run our proposed algorithms to approximate A and build up the reduced bases. We demonstrate the efficacy of our algorithms on the two-dimensional diffusion equation that induces a solution manifold that requires many more snapshots to achieve small error. Our proposed approach demonstrates outstanding performance on the model reduction example when compared to the POD.

MS3: Recent Advances in Numerical Methods for PDEs (Part II)

ORGANIZERS: S.S. Ravindran, University of Alabama in Huntsville

DESCRIPTION: The rapid growth and diversity of research in science and engineering over the past decades has spawned many intellectually challenging and computationally intensive PDE problems to be solved. Despite significant progress made in development of efficient computational methods for numerical solution of these problems, many problems still remain open. This minisymposium aims to provide a platform to present recent developments on the novel and efficient numerical methods for solving PDEs, enable in-depth discussions on a variety of computa-tional efforts for solving problems arising in areas of science and engineering from researchers at all stages of their careers.

TALKS1. New finite difference methods on irregular grids for solving Maxwell's
equations

Yingjie Liu, Georgia Institute of Technology

ABSTRACT. This talk is based on joint works with Dr. Xin Wang and Mr. Haiyu Zou. We have developed new, simple and efficient second order finite difference methods for solving Maxwell's equations on non-staggered irregular grids with large CFL numbers (greater than or equal to 1 in one, two or three dimensions). The methods don't need to compute the local characteristic information for the hyperbolic system and are easy to implement on unstructured meshes. The schemes can be naturally adapted to the perfectly matched layers (PML) for absorbing boundaries. BFECC had been applied to schemes for scalar advection equations to improve their stability and order of accuracy. In this talk similar theoretical results for systems will be introduced. These results are robust for irregular meshes and for nonlinear equations. We apply BFECC to the central difference scheme (unstable if used along), Lax-Friedrichs scheme or a combination of them for the Maxwell's equations and obtain second order accurate schemes with large CFL numbers. The method is further applied to schemes based on the least-squares linear interpolation on non-orthogonal, non-staggered irregular grids to obtain second order stabilized versions. The application to scattering around perfect electric conductors with curved boundaries and corners will also be discussed. Numerical examples are presented to demonstrate the robustness of the new schemes.

2. Scalable time-stepping for nonlinear PDEs through Krylov subspace spectral methods

James Lambers, The University of Southern Mississippi

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

3. Robust architectures, initialization, and training for deep neural networks via the adaptive basis interpretation

Mamikon Gulian, Sandia National Laboratories

ABSTRACT. Deep neural networks (DNNs) hold intriguing potential for scientific problems. For example, training a DNN to solve a partial differential equation using a physicsinformed loss is analogous to using an optimizer to construct a mesh, approximation space, and a representation within the approximation space all at the same time. With sufficient hyperparameter tuning, DNNs have shown remarkable success for scientific problems using off-the-shelf architectures and optimizers, e.g., in reduced-order modeling and nonlinear partial differential equations. In comparison to the classical numerical approaches, however, they are prone to instability and irreproducibility, and as a rule do not exhibit of convergence with respect to network size. In support of utilizing DNNs for scientific computing, we introduce the adaptive basis interpretation of DNNs as well as a novel initialization and a Least Squares/Gradient Descent optimizer that greatly reduce training error and yield consistent improvement in training error as the size of the DNN increases. Motivated by recent proofs of optimal approximation rates of DNNs, we then introduce Partition of Unity networks (POU-Nets) which incorporate partitions of unity and polynomial approximants directly into the architecture. Classification architectures of the type used to learn probability measures are used to build a mesh-free partition of space, while polynomial spaces with learnable coefficients are associated to each partition, resulting in hp-element-like approximation.

4. Fractional deep neural network and inverse problems

Deepanshu Verma, Emory University

ABSTRACT. In this talk, we discuss a novel Deep Neural Network (DNN), which allows connectivity between all the layers. The latter is accomplished by using fractional time derivatives. We apply the resulting fractional-DNN to learn the parameter-to-solution map in parameterized partial differential equations (PDEs). Subsequently, we use this approximation to solve Bayesian inverse problems using Markov Chain Monte Carlo. A speedup of 100x over the existing approaches is observed. Several numerical examples are carried out to demonstrate the efficacy of our approach.

MS3: Recent Advances in Numerical Methods for PDEs (Part III)

ORGANIZERS: S.S. Ravindran, University of Alabama in Huntsville

DESCRIPTION: The rapid growth and diversity of research in science and engineering over the past decades has spawned many intellectually challenging and computationally intensive PDE problems to be solved. Despite significant progress made in development of efficient computational methods for numerical solution of these problems, many problems still remain open. This minisymposium aims to provide a platform to present recent developments on the novel and efficient numerical methods for solving PDEs, enable in-depth discussions on a variety of computa-tional efforts for solving problems arising in areas of science and engineering from researchers at all stages of their careers.

TALKS 1. Adaptive two-grid finite element algorithms for linear and nonlinear DETAILS: problems

Yi Zhang, University of North Carolina at Greensboro

ABSTRACT. We propose some efficient and accurate adaptive two-grid finite element algorithms for linear and nonlinear partial differential equations. We will discuss the reliability and efficiency of the proposed residual-type a posteriori error estimators, as well as the convergence of the corresponding adaptive algorithms. We will also present numerical results to gauge the performance of the proposed methods.

2. A decoupled, linear, and unconditionally energy stable finite element method for a two-phase ferrohydrodynamics model

Xiaoming He, Missouri University of Science and Technology

ABSTRACT. In this talk, we present numerical approximations of a phase-field model for two-phase ferrofluids, which consists of the Navier-Stokes equations, the Cahn-Hilliard equation, the magnetostatic equations, as well as the magnetic field equation. By combining the projection method for the Navier-Stokes equations and some subtle implicitexplicit treatments for coupled nonlinear terms, we construct a decoupled, linear, fully discrete finite element scheme to solve the highly nonlinear and coupled multi-physics system efficiently. The scheme is provably unconditionally energy stable and leads to a series of decoupled linear equations to solve at each time step. Through numerous numerical examples in simulating benchmark problems such as the Rosensweig instability and droplet deformation, we demonstrate the stability and accuracy of the numerical scheme.

3. Sparse discretization of optimal control problems with PDEs

Evelyn Herberg, George Mason University

ABSTRACT. We look at different sparse optimal control problems with PDEs, analyse their sparsity structure and employ variational discretization to achieve sparsity on the discrete level. Especially, we consider optimal control problems with measure controls. Due to the measures on the right hand side of the partial differential equation, we consider a very weak solution theory for the state equation and need an embedding into the continuous functions for the pairings to make sense. Furthermore, we employ Fenchel duality to formulate the predual problem and give results on solution theory of both the predual and the primal problem. Numerical experiments highlight the sparsity features of our discrete approach and verify the convergence results.

- 4. Meshfree methods for problems with variable-order Laplacian Yanzhi Zhang, *Missouri University of Science and Technology*
- 5. A fast algorithm for parameter-dependent and random PDEs Xiaobing Feng, University of Tennessee at Knoxville

MS4: Modeling and Numerical Methods for Coupled PDE Systems (Part I)

ORGANIZERS: Xiaoming He, Missouri University of Science and Technology Xiaofeng Yang, University of South Carolina

DESCRIPTION: Coupled PDE systems play a key role in many multi-physics problems. The modeling and the sub-sequent development of efficient and stable numerical algorithms remain challenging for coupled PDEs due to a number of factors, including the nonlinear coupling of different dynamics, the multi-ple scales involved, and unconditionally stable high order methods. This mini-symposium aims to provide a forum for researchers from different fields to discuss recent advances on the modeling and numerical methods for coupled PDE systems.

TALKS1. A divergence-free finite element method for the Stokes problem with
boundary correction

Michael Neilan, University of Pittsburgh

ABSTRACT. In this talk we discuss a boundary correction finite element method for the Stokes problem based on the Scott-Vogelius pair on Clough-Tocher splits. The velocity space consists of continuous piecewise quadratic polynomials, and the pressure space consists of piecewise linear polynomials without continuity constraints. A Lagrange multiplier space that consists of continuous piecewise quadratic polynomials with respect to boundary partition is introduced to enforce (normal) boundary conditions and to mitigate the lack of pressure-robustness. We prove that the method converges with optimal order and the velocity approximation is divergence free. This is joint work with Baris Otus and Haoran Liu (Pitt).

2. Cell-average based neural network method for hyperbolic and parabolic partial differential equations

Jue Yan, Iowa State University

ABSTRACT. In this talk, we present the cell-average based neural network (CANN) method for partial differential equations. The CANN method is motivated by finite volume scheme and based on the integral or weak formulation of partial differential equations. A simple feed forward network is forced to learn the solution average evolution between two neighboring time steps. Offline supervised training is carried out to obtain the optimal network parameter set, which uniquely identifies one finite volume like neural network method. Once well trained, the network method is implemented as a finite volume scheme, thus is mesh dependent. Different to traditional numerical methods, our method can be relieved from the explicit scheme CFL restriction and can adapt to any time step size for solution evolution. First convergence order is observed for parabolic PDE and second convergence orders are observed for hyperbolic PDE. The cell-average based neural network method can sharply evolve contact discontinuity with almost zero numerical diffusion introduced. Shock and rarefaction waves are well captured for nonlinear hyperbolic conservation laws.

3. Hybridization and postprocessing in FEEC

Ari Stern, Washington University in St. Louis

ABSTRACT. Finite element exterior calculus (FEEC) unifies several families of conforming finite element methods for Laplace-type problems, including the scalar and vector Poisson equations. This talk presents a framework for hybridization of FEEC, which recovers known hybrid methods for the scalar Poisson equation and gives new hybrid methods for the vector Poisson equation. We also generalize Stenberg postprocessing, proving new superconvergence estimates. Based on joint work with Gerard Awanou, Maurice Fabien, and Johnny Guzman (arXiv:2008.00149).

4. Structure-preserving discontinuous Galerkin methods for Hamiltonian partial differential equations: Energy conservation and multisymplecticity

Zheng Sun, The University of Alabama

ABSTRACT. In this talk, we present and study discontinuous Galerkin (DG) methods for one-dimensional multi-symplectic Hamiltonian partial differential equations. We particularly focus on semi-discrete schemes with spatial discretization only, and show that the proposed DG methods can simultaneously preserve the multi-symplectic structure and energy conservation with a general class of numerical fluxes, which includes the well-known central and alternating fluxes. Applications to the wave equation, the Benjamin–Bona–Mahony equation, the Camassa–Holm equation, the Korteweg–de Vries equation and the nonlinear Schrödinger equation are discussed. Some numerical results are provided to demonstrate the accuracy and long time behavior of the proposed methods. Numerically, we observe that certain choices of numerical fluxes in the discussed class may help achieve better accuracy compared with the commonly used ones including the central fluxes.

MS4: Modeling and Numerical Methods for Coupled PDE Systems (Part II)

ORGANIZERS: Xiaoming He, Missouri University of Science and Technology

Xiaofeng Yang, University of South Carolina

DESCRIPTION: Coupled PDE systems play a key role in many multi-physics problems. The modeling and the sub-sequent development of efficient and stable numerical algorithms remain challenging for coupled PDEs due to a number of factors, including the nonlinear coupling of different dynamics, the multi-ple scales involved, and unconditionally stable high order methods. This mini-symposium aims to provide a forum for researchers from different fields to discuss recent advances on the modeling and numerical methods for coupled PDE systems.

TALKS 1. Boundary control for fluid mixing: analysis and computation

DETAILS: Weiwei Hu, University of Georgia

ABSTRACT. The question of what velocity fields effectively enhance or prevent transport and mixing, or steer a scalar field to a desired distribution, is of great interest and fundamental importance to the fluid mechanics community. In this talk, we mainly discuss the problem of optimal mixing of an inhomogeneous distribution of a scalar field via active control of the flow velocity, governed by the Stokes or the Navier-Stokes equations. Specifically, we consider that the velocity field is steered by a control input which acts tangentially on the boundary of the domain through the Navier slip boundary conditions. This is motivated by mixing within a cavity or vessel by rotating or moving walls. Our main objective is to design a Navier slip boundary control that optimizes mixing at a given final time. Non-dissipative scalars governed by the transport equation will be of our main focus in this talk. A rigorous proof of the existence of an optimal controller and the first-order necessary conditions for optimality will be derived. Computational challenges in solving the optimality conditions will be addressed. Finally, numerical experiments will be presented to demonstrate our ideas and control designs.

2. Optimal control of volume-preserving mean curvature flow

Shawn Walker, Louisiana State University

ABSTRACT. We develop a framework and numerical method for controlling the full spacetime tube of a geometrically driven flow. We consider an optimal control problem for the mean curvature flow of a curve or surface with a volume constraint, where the control parameter acts as a forcing term in the motion law. The control of the trajectory of the flow is achieved by minimizing an appropriate tracking-type cost functional. The gradient of the cost functional is obtained via a formal sensitivity analysis of the space-time tube generated by the mean curvature flow. We show that the perturbation of the tube may be described by a transverse field satisfying a parabolic equation on the tube. We propose a numerical algorithm to approximate the optimal control and show several results in two and three dimensions demonstrating the efficacy of the approach.

3. Variational discretization for optimal control with BV functions based on the mixed formulation

Evelyn Herberg, George Mason University

ABSTRACT. We consider optimal control of an elliptic two-point boundary value problem governed by functions of bounded variation (BV). The cost functional is composed of a tracking term for the state and the BV-seminorm of the control. We use the mixed formulation for the state equation together with the variational discretization approach, where we use the classical lowest order Raviart-Thomas finite elements for the state equation. Consequently the variational discrete control is a piecewise constant function over the finite element grid. We prove error estimates for the variational discretization approach in combination with the mixed formulation of the state equation and confirm our analytical findings with numerical experiments.

4. Variational data assimilation of parabolic interface equation

Xuejian Li, Missouri University of Science and Technology

ABSTRACT. In this report we propose and analyze a numerical method of variational data assimilation(VDA) for a second order parabolic interface equation on a two-dimensional bounded domain. By using Tikhonov regularization we formulate the data assimilation problem into an optimization problem. Existence, uniqueness, and stability of the optimal solution are then established. The standard adjoint operation is utilized to derive the first order continuous optimality system. To numerically solve the data assimilation problem, a finite element discretization is designed for spatial approximation and the backward Euler scheme is used in the temporal discretization. The convergence with the optimal error estimate is proved with special attention paid to the recovery of Galerkin orthogonality. In addition, due to the extreme computational cost in VDA, we focus more on reducing the CPU memory requirement and simulation time by developing a variety of efficient algorithms. Finally, numerical results are provided to validate the proposed method.

MS4: Modeling and Numerical Methods for Coupled PDE Systems (Part III)

ORGANIZERS: Xiaoming He, Missouri University of Science and Technology

Xiaofeng Yang, University of South Carolina

DESCRIPTION: Coupled PDE systems play a key role in many multi-physics problems. The modeling and the sub-sequent development of efficient and stable numerical algorithms remain challenging for coupled PDEs due to a number of factors, including the nonlinear coupling of different dynamics, the multi-ple scales involved, and unconditionally stable high order methods. This mini-symposium aims to provide a forum for researchers from different fields to discuss recent advances on the modeling and numerical methods for coupled PDE systems.

TALKS1. Finite element/holomorphic operator-value function approach for non-
linear eigenvalue problems

Jiguang Sun, Michigan Technological University

ABSTRACT. We propose a new approach combining the holomorphic operator value function and finite elements for some nonlinear eigenvalue problems. The eigenvalue problem is formulated as the eigenvalue problem of a holomorphic Fredholm operator function of index zero. Finite element methods are used for discretization. The convergence of eigenvalues/eigenvectors is proved using the abstract approximation theory for holomorphic operator functions. Then the spectral indicator method is extended to compute the eigenvalues. The proposed approach is employed to compute the band structures of frequency-dependent photonic crystals.

2. A locking-free 2-field finite element solver for poroelasticity

James Liu, Colorado State University

ABSTRACT. In this talk, I will present a new 2-field finite element solver for linear poroelasticity on quadrilateral meshes. The Darcy flow is discretized for fluid pressure by a lowest-order weak Galerkin (WG) finite element method, which establishes the discrete weak gradient and numerical velocity in the lowest-order Arbogast-Correa space. The linear elasticity is discretized for solid displacement by the enriched Lagrangian finite elements with a special treatment for the volumetric dilation. These two types of finite elements are coupled through the implicit Euler temporal discretization to solve poroelasticity problems. Numerical results along with main ideas for error analysis will be presented to demonstrate the accuracy and locking-free property of this new solver. This talk is based on a series of joint work with several collaborators.

3. A simple flux-recovery on quadtree meshes

Shuhao Cao, Washington University in St. Louis

ABSTRACT. Flux-recovery is an important tool in adaptive mesh refinement for simulations of PDE systems with complex material interfaces. Quadtree meshes are widely used in industry and national labs due to its preferable numerical properties over simplicial meshes. However, if there are multilevel irregular hanging nodes, flux recovery in compatible spaces is difficult. In this work, we present a simple flux recovery approach that adopts H(div)-conforming virtual elements, in which arbitrary levels of hanging nodes need no specific ad hoc treatment and are seen as regular nodes in polygons.

4. A nonconforming hybridized model for the 2D vector Laplacian

Mary Barker, Washington University in St. Louis

ABSTRACT. A nonconforming method for the 2D vector Laplacian is introduced. In the lowest-order case, our method is a hybridization of the P1-nonconforming method introduced by Brenner, Cui, Li, and Sung in 2008. Along with the method, some a priori estimates are given and numerical results which illustrate optimal convergence in problems with low regularity.

MS5: PDE, Dynamical Systems and Applications (Part I)

ORGANIZERS: Selim Sukhtaiev, Auburn University		
	Maggie Han, Auburn University	
	Wenxian Shen, Auburn University	
DESCRIPTION	The topics to be discussed in this mini-symposium lie at the interface of partial differ- ential equa-tions, dynamical systems and their applications in mathematical physics, biology and engineering. Concretely, the following themes will be covered: (1). Sta- bility of nonlinear waves, patterns, on coherent structures arising in Hamiltonian sys- tems; (2). Statistical behavior of thermodynamic systems via Boltzmann equation; (3). Mathematical modeling and analysis of the movement of biological cells in response to chemical gradients.	
TALKS 1. DETAILS:	Multi-strain epidemic model Rachidi B. Salako, University of Nevada, Las-Vegas	
	ABSTRACT. In this talk, we discuss a multi-strain epidemic model with diffusion and en- vironmental heterogeneity. We investigate how the local distributions of the transmission and recovery rates affect the dynamics of the disease. In particular, we show that creating a common safety area against all strains and lowering the diffusion rate of the susceptible subgroup will reduce the number of infected populations. Numerical simulations will be presented to illustrate our theoretical findings.	
2.	Embedded eigenvalues for the Neumann-Poincaré operator Stephen Shipman, <i>Louisiana State University</i>	
	ABSTRACT. The PDEs governing sub-wavelength quasi-static scattering and resonance in small particles are intimately connected to the spectral theory of the Neumann-Poincaré (NP) boundary-integral operator in potential theory. In two and three dimensions, we prove the existence of scatterers for which the NP operator has eigenvalues embedded in its continuous spectrum. These eigenvalues arise due to a combination of a sharp point and symmetry in the scatterer. This is joint work with Wei Li (DePaul) and Karl-Mikael Perfekt (NTNU).	

3. The essential spectrum of breathing pulses in a femtosecond laser

John Zweck, The University of Texas at Dallas

ABSTRACT. The pulses in recent generations of experimental femtosecond fiber lasers breathe periodically from round trip to round trip, rather than being stationary nonlinear waves. The modeling of these lasers is based on a version of the nonlinear Schrödinger equation with saturable gain, together with models of discrete devices such as optical filters and saturable absorbers. We characterize the stability of breather solutions of the model in terms of the spectrum of the monodromy operator, which is the linearization of the round trip operator about the breather. Using evolution semigroup theory, we establish existence and regularity properties for the monodromy operator and derive a formula essential spectrum. We verify this formula by comparison with a fully numeric method for an experimental fiber laser. We also demonstrate the effect that the saturable absorber has on pulse stability.

This work is joint with Vrushaly Shinglot, Yuri Latushkin, and Curtis Menyuk and is supported by the NSF under Grant DMS-2106203.

4. Traveling wave solutions for two species competitive chemotaxis systems

Tahir Bachar Issa, San Jose State University

ABSTRACT. This talk foucs on existence/non-existence of traveling wave solutions for two species chemotaxis systems with Lotka-Volterra competition reaction terms. First, under appropriate conditions on the parameters in such a system, we establish the existence of traveling wave solutions of the system connecting two spatially homogeneous equilibrium solutions with wave speed greater than some critical number c^* . Next, we show the non-existence of such traveling waves with speed less than some critical number c_0^* , which is independent of the chemotaxis. Finally, under suitable hypotheses on the coefficients of the reaction terms, we obtain explicit range for the chemotaxis sensitivity coefficients ensuring $c^* = c_0^*$, which implies that the minimum wave speed exists and is not affected by the chemoattractant.

5. Isentropic approximation

Ronghua Pan, Georgia Tech

ABSTRACT. In the study of compressible flows, the isentropic model was often used to replace the more complicated full system when the entropy is near a constant. This is based on the expectation that the corresponding isentropic model is a good approximation to the full system when the entropy is sufficiently close to the constant. We will discuss the mathematical justification of isentropic approximation in Euler flows and in Navier-Stokes-Fourier flows. This is based on the joint work with Y. Chen, J. Jia, and L. Tong.

MS5: PDE, Dynamical Systems and Applications (Part II)

ORGANIZERS:	Selim Sukhtaiev, Auburn University
	Maggie Han, Auburn University
	Wenxian Shen, Auburn University

DESCRIPTION: The topics to be discussed in this mini-symposium lie at the interface of partial differential equa-tions, dynamical systems and their applications in mathematical physics, biology and engineering. Concretely, the following themes will be covered: (1). Stability of nonlinear waves, patterns, on coherent structures arising in Hamiltonian systems; (2). Statistical behavior of thermodynamic systems via Boltzmann equation; (3). Mathematical modeling and analysis of the movement of biological cells in response to chemical gradients.

TALKS1. Small breathers of nonlinear Klein-Gordon equations via exponentiallyDETAILS:small homoclinic splitting

Chongchun Zeng, Georgia Institute of Technology

ABSTRACT. Breathers are temporally periodic and spatially localized solutions of evolutionary PDEs. They are known to exist for integrable PDEs such as the sine-Gordon equation, but are believed to be rare for general nonlinear PDEs. When the spatial dimension is equal to one, exchanging the roles of time and space variables (in the so-called spatial dynamics framework), breathers can be interpreted as homoclinic solutions to steady solutions and thus arising from the intersections of the stable and unstable manifolds of the steady states. In this talk, we shall study small breathers of the nonlinear Klein-Gordon equation generated in an unfolding bifurcation as a pair of eigenvalues collide at the original when a parameter (temporal frequency) varies. Due to the presence of the oscillatory modes, generally the finite dimensional stable and unstable manifolds do not intersect in the infinite dimensional phase space, but with an exponentially small splitting (relative to the amplitude of the breather) in this singular perturbation problem of multiple time scales. This splitting leads to the transversal intersection of the center-stable and center-unstable manifolds which produces small amplitude generalized breathers with exponentially small tails. Due to the exponential small splitting, classical perturbative techniques cannot be applied. We will explain how to obtain an asymptotic formula for the distance between the stable and unstable manifold of the steady solutions. This is a joint work with O. Gomide, M. Guardia, and T. Seara.

2. TBD

Zhiwu Lin, Georgia Institute of Technology

3. Spectral decomposition and decay to grossly determined solutions for a simplified BGK model

Alim Sukhtayev, Miami University

ABSTRACT. For a simplified 1D BGK model we show that H^1 solutions decay exponentially in L^2 to a subclass of the class of grossly determined solutions as defined by Truesdell and Muncaster in the context of Boltzmann's equation. In the process, we determine the spectrum and generalized eigenfunctions of the associated non-selfadjoint linearized operator and derive the associated generalized Fourier transform and Parseval's identity. Notably, our analysis makes use of rigged space techniques originating from quantum mechanics, as adapted by Ljance and others to the nonselfadjoint case.

4. Modeling density dependent dispersal and habitat fragmentation via reaction diffusion equations

Jerome Goddard, Auburn University Montgomery

ABSTRACT. Dispersal is broadly defined as movement from one habitat patch to another and typically is considered to encompass three stages: 1) emigration, 2) inter-patch movement, & 3) immigration. Dispersal can have both beneficial and detrimental effects on the persistence of spatially structured systems. Recent empirical results indicate that certain organisms' emigration from a patch is dependent on density of their own species or even an interacting species—known as density dependent emigration. To date, little is known about the patch-level consequences of such dispersal strategies. In this talk, we will give a brief overview of density dependent emigration and its modeling history, discuss a framework built upon reaction diffusion equations designed to model patch-level effects of density dependent emigration, and share some recent advances. Several methods from nonlinear analysis will be employed such as time map analysis (quadrature method) and linearized stability analysis.

MS5: PDE, Dynamical Systems and Applications (Part III)

ORGANIZERS: Selim Sukhtaiev, Auburn University Maggie Han, Auburn University Wenxian Shen, Auburn University

DESCRIPTION: The topics to be discussed in this mini-symposium lie at the interface of partial differential equa-tions, dynamical systems and their applications in mathematical physics, biology and engineering. Concretely, the following themes will be covered: (1). Stability of nonlinear waves, patterns, on coherent structures arising in Hamiltonian systems; (2). Statistical behavior of thermodynamic systems via Boltzmann equation; (3). Mathematical modeling and analysis of the movement of biological cells in response to chemical gradients.

TALKS1. Delayed model for the transmission and control of COVID-19 — the
role of Fangcang shelter hospital in Wuhan

Guihong Fan, Columbus State University

ABSTRACT. The ongoing coronavirus disease 2019 (COVID-19) epidemic poses a huge threat to global public health. Motivated by China's experience to use Fangcang shelter hospitals (FSHs) successfully combat the epidemic, we proposed a two-stage delay model considering the average waiting time of patients' admission to study the impact of hospital beds and centralized quarantine on mitigating and control of the outbreak. We calculated the basic reproduction number and defined the relative contribution indices of either type of the hospitals, and analyzed the sensitivity of the average waiting times of patients before being admitted into the hospitals. We conclude that while designated hospitals save the life of severely infected individuals, the FSHs played a key role in mitigating and eventually stopped the epidemic. We also quantified some key epidemiological indicators, such as the final sizes of infections and deaths, the peak size and time, and the maximum occupation of beds in FSHs. Our study suggests that for a region or country still struggling with COVID-19, when possible, it is essential to increase testing capacity and use centralized quarantine to massively reduce the severity and magnitude of the epidemic that follows. This is a collaborated work with Dr. Juan Li and Prof. Huaiping Zhu.

2. Nonlocal dispersal equations with almost periodic dependence

Maria Amarakristi Onyido, Auburn University

ABSTRACT. We discuss the principal spectral theory of nonlocal dispersal operators with almost periodic dependence We investigate the principal spectral theory from two aspects: top Lyapunov exponents and generalized principal eigenvalues. Among others, we provide various characterizations of the top Lyapunov exponents and generalized principal eigenvalues, establish the relations between them, and study the effect of time and space variations on them. This is a joint work with Prof. Wenxian Shen

3. Long transient dynamics in stochastic systems

Zhongwei Shen, University of Alberta

ABSTRACT. Transient dynamics, often observed in multi-scale systems, are roughly defined to be interesting dynamical behaviours over finite time scales. For a class of randomly perturbed dynamical systems that arise in chemical reactions and population dynamics, and that exhibit persistence dynamics over finite time periods and extinction dynamics in the long run, we use quasi-stationary distributions (QSDs) to rigorously capture transient states governing the long transient persistence dynamics. We study the noise-vanishing asymptotic of QSDs to gain information about transient states and investigate the dynamics near transient states to understand transient dynamical behaviours as well as the global multiscale dynamics.

4. Global stability analysis of some classes of predator-prey models Wenzhang Huang, University of Alabama in Huntsville

ABSTRACT. The main purpose of this chapter is to present a recently developed approach in the studies of the global stability of a positive (co-existence) equilibrium for several classes of predator-prey systems. By identifying the important property of a key function this approach enables us to show that the global and local stability of the positive equilibrium, whenever it exists, is equivalent. We believe that the technique introduced here has the potential to be extended to study the global stability of the positive equilibrium for larger classes of predator-prey models.

5. Traveling wave solutions for multi-species predator-prey systems Shangbing Ai, University of Alabama in Huntsville

ABSTRACT. We present recent results on the existence of traveling wave solutions for some multi-species predator-prey systems. We first discuss an existence theorem on weak traveling wave solutions of a general multi-species predator-prey system. We then apply this theorem to some concrete predator-prey systems such as an SIS system for spread of infectious disease and a generalized Lotka-Volterra system and prove by means of Lyapunov functions that the weak traveling wave solutions of these systems are also traveling wave solutions.

MS6: Recent Developments on Partial Differential Equations and Applications (Part I)

ORGANIZERS: Loc Nguyen, University of North Carolina at Charlotte

Dinh-Liem Nguyen, Kansas State University

DESCRIPTION: The area of Partial Differential Equations (PDEs) is an important research topic in both pure and applied mathematics. It is also an interdisciplinary area that involves Physics, Engineering, Biology, and many other fields. The goal of this mini-symposium is to bring together researchers working on different aspects of the field to discuss recent and new results in the field such as (1) the existence of unique or multiple solutions to PDEs, (2) regularity theory for PDEs, and (3) inverse problems for PDEs. Another goal of the mini-symposium is to promote idea exchange as well as potential fu-ture collaborations.

TALKS1. Optimal rates of convergence in periodic homogenization of linear ellip-
tic equations in non-divergence form

Hung Tran, University of Wisconsin-Madison

ABSTRACT. I will discuss the basic theory and recent progress in the study of optimal rates of convergence in periodic homogenization of linear elliptic equations in non-divergence form. Some open questions will be addressed as well.

2. Infinite series asymptotic expansions for solutions of dissipative nonlinear differential equations

Luan Hoang, Texas Tech University

ABSTRACT. We study the precise asymptotic behavior of a non-trivial solution that converges to zero, as time tends to infinity, of dissipative systems of nonlinear ordinary differential equations. The nonlinear term of the equations may not possess a Taylor series expansion about the origin. This absence technically cripples previous proofs in establishing an asymptotic expansion, as an infinite series, for such a decaying solution. In the current paper, we overcome this limitation and obtain an infinite series asymptotic expansion, as time goes to infinity. This series expansion provides large time approximations for the solution with the errors decaying exponentially at any given rates. The main idea is to shift the center of the Taylor expansions for the nonlinear term to a non-zero point. Such a point turns out to come from the non-trivial asymptotic behavior of the solution, which we prove by a new and simple method. Our result applies to different classes of non-linear equations that have not been dealt with previously. This is joint work with Dat Cao (Minnesota State University, Mankato) and Thinh Kieu (University of North Georgia, Gainesville Campus).

3. Orthogonality sampling method for electromagnetic inverse scattering problems

Dinh-Liem Nguyen, Kansas State University

ABSTRACT. We study the precise asymptotic behavior of a non-trivial solution that converges to zero, as time tends to infinity, of dissipative systems of nonlinear ordinary differential equations. The nonlinear term of the equations may not possess a Taylor series expansion about the origin. This absence technically cripples previous proofs in establishing an asymptotic expansion, as an infinite series, for such a decaying solution. In the current paper, we overcome this limitation and obtain an infinite series asymptotic expansion, as time goes to infinity. This series expansion provides large time approximations for the solution with the errors decaying exponentially at any given rates. The main idea is to shift the center of the Taylor expansions for the nonlinear term to a non-zero point. Such a point turns out to come from the non-trivial asymptotic behavior of the solution, which we prove by a new and simple method. Our result applies to different classes of non-linear equations that have not been dealt with previously. This is joint work with Dat Cao (Minnesota State University, Mankato) and Thinh Kieu (University of North Georgia, Gainesville Campus).

4. A system of first order H-J equations related to an optimal debt management problem

Tien Khai Nguyen, North Carolina State University

ABSTRACT. Consider a system of first order Hamilton-Jacobi equations with discontinuous coefficients, arising from a model of deterministic optimal debt management in an infinite time horizon, with exponential discount and currency devaluation. The existence of an equilibrium solution is obtained by a suitable concatenation of backward solutions to the system of Hamilton-Jacobi equations. A detailed analysis of the behavior of the solution as the debt-ratio-income tends to infinity will be discussed.

MS6: Recent Developments on Partial Differential Equations and Applications (Part II)

ORGANIZERS: Loc Nguyen, University of North Carolina at Charlotte

Dinh-Liem Nguyen, Kansas State University

DESCRIPTION: The area of Partial Differential Equations (PDEs) is an important research topic in both pure and applied mathematics. It is also an interdisciplinary area that involves Physics, Engineering, Biology, and many other fields. The goal of this mini-symposium is to bring together researchers working on different aspects of the field to discuss recent and new results in the field such as (1) the existence of unique or multiple solutions to PDEs, (2) regularity theory for PDEs, and (3) inverse problems for PDEs. Another goal of the mini-symposium is to promote idea exchange as well as potential fu-ture collaborations.

TALKS1. Convergence of an inverse iterative scheme for the Hessian eigenvalueDETAILS:Nam Q. Le, Indiana University, Bloomington

ABSTRACT. In this talk, we will first introduce a nondegenerate inverse iterative scheme to solve the eigenvalue problem for the k-Hessian operator on a smooth, bounded domain in Euclidean spaces. We show that the scheme converges, with a rate, to the k-Hessian eigenvalue for all k. We also prove a local L^1 convergence of the Hessian of solutions of the scheme. Hyperbolic polynomials play an important role in our analysis.

2. Imaging of scattering objects from near-field acoustic measurements Thi-Phong Nguyen, *Purdue University*

ABSTRACT. We consider the inverse scattering problem that aims to recover scattering objects from the measured scattered waves generated by a point source. We will discuss some recent results on Direct Sampling Methods for solving the inverse problem. In particular, we propose two imaging functionals that allow us to distinguish an arbitrary point test inside or outside the obstacle without inverting the near-field operator. Each proposed imaging functional relies on the fact that the imaginary part of the Green function at each observation point (i.e, the Bessel function J_0) is approximated by the first order of the inverse distance from the source to the receiver. Similarly to other direct inversion methods, it is very robust with respect to white noise. This is a joint work with Isaac Harris and Dinh-Liem Nguyen.

3. Sampling methods for bi-anisotropic Maxwell's equations

Thu Le, Kansas State University

4. Numerical viscosity solutions to Hamilton-Jacobi equations via a Carleman estimate and the convexification method

Loc Nguyen, University of North Carolina at Charlotte

ABSTRACT. We propose a globally convergent numerical method, called the convexification, to numerically compute the viscosity solution to first-order Hamilton-Jacobi equations through the vanishing viscosity process where the viscosity parameter is a fixed small number. By convexification, we mean that we employ a suitable Carleman weight function to convexify the cost functional defined directly from the form of the Hamilton-Jacobi equation under consideration. The strict convexity of this functional is rigorously proved using a new Carleman estimate. We also prove that the unique minimizer of the this strictly convex functional can be reached by the gradient descent method. Moreover, we show that the minimizer well approximates the viscosity solution of the Hamilton-Jacobi equation as the noise contained in the boundary data tends to zero. Some interesting numerical illustrations are presented.

MS6: Recent Developments on Partial Differential Equations and Applications (Part III)

Organizers: Loc Nguyen, University of North Carolina at Charlotte

Dinh-Liem Nguyen, Kansas State University

DESCRIPTION: The area of Partial Differential Equations (PDEs) is an important research topic in both pure and applied mathematics. It is also an interdisciplinary area that involves Physics, Engineering, Biology, and many other fields. The goal of this mini-symposium is to bring together researchers working on different aspects of the field to discuss recent and new results in the field such as (1) the existence of unique or multiple solutions to PDEs, (2) regularity theory for PDEs, and (3) inverse problems for PDEs. Another goal of the mini-symposium is to promote idea exchange as well as potential fu-ture collaborations.

TALKS1. Convexification-based globally convergent numerical method for a 1DDETAILS:coefficient inverse problem with experimental data

Thuy Le, University of North Carolina at Charlotte

ABSTRACT. To compute the spatially distributed dielectric constant from the backscattering data, we study a coefficient inverse problem for a 1D hyperbolic equation. To solve the inverse problem, we establish a new version of Carleman estimate and then employ this estimate to construct a cost functional which is strictly convex on a convex bounded set with an arbitrary diameter in a Hilbert space. The strict convexity property is rigorously proved. This result is called the convexification theorem and is considered as the central analytical result of this paper. Minimizing this convex functional by the gradient descent method, we obtain the desired numerical solution to the coefficient inverse problems. We prove that the gradient descent method generates a sequence converging to the minimizer and we also establish a theorem confirming that the minimizer converges to the true solution as the noise in the measured data and the regularization parameter tend to zero. Unlike the methods that are based on optimization, our convexification method converges globally in the sense that it delivers a good approximation of the exact solution without requiring any initial guess. Results of numerical studies of both computationally simulated and experimental data are presented.

2. On wellposedness and regularity estimates of solutions to a class of degenerate parabolic equations

Tuoc Phan, University of Tennessee - Knoxville

ABSTRACT. We consider a class of parabolic equations in divergence form in the upperhalf space with Dirichlet boundary condition. The leading coefficients in this class of equations are allowed to be degenerate on the boundary of the domain. Wellposedness and regularity estimates of solutions in suitable weighted Sobolev space are established. The talk is based on the joint work with Hung V. Tran (University of Wisconsin - Madison) and Hongjie Dong (Brown University).
3. Inverse Born series method for a periodic inverse scattering problem Trung Truong, *Kansas State University*

ABSTRACT. Periodic inverse scattering problems have attracted an increasing amount of attention during the past few decades due to their applications in the study of photonic crystals. These problems are known to be non-linear and severely ill-posed. There have been several different approaches to tackle both shape reconstruction and material parameter reconstruction problems. The latter often requires advanced a priori information about the solution, for example, optimization-based methods need a good initial guess. Inverse Born series, on the other hand, is a direct method for reconstructing the material parameter with an analysis that can be rigorously justified under certain conditions. Numerical reconstructions also show high levels of accuracy and stability. This talk focuses on the analysis of the Forward and Inverse Born series as well as their modified versions to solve the periodic inverse scattering problem. Corresponding numerical results will also be presented. This is joint work with Dinh-Liem Nguyen and Colin Williams.

4. Convexification and experimental data for a 3D inverse scattering problem with the moving point source

Vo Anh Khoa, Florida A&M University, Tallahassee

ABSTRACT. Reconstruction of physical properties of a medium from boundary measurements is one of the substantially challenging inverse scattering problems. In this talk, we present a convexification method to find the dielectric constant as an unknown coefficient of a three-dimensional Helmholtz equation for the case when the backscattering data are generated by a point source running along an interval of a straight line and the wavenumber is fixed. Using a special Fourier basis, the method of this work strongly relies on a new derivation of a boundary value problem for a system of coupled quasilinear elliptic equations. We then introduce a cost functional in the partial finite difference, weighted by a suitable Carleman weight function. This numerical setting allows us to verify the performance of the method using experimental data in which the spatial discretization is fixed. The experimental data were collected using a microwave scattering facility at The University of North Carolina at Charlotte.

MS7: Recent Developments and Applications in Computational Biology (Part I)

ORGANIZERS: Shan Zhao, University of Alabama Xinfeng Liu, University of South Carolina

DESCRIPTION: Due to the rapid developments of mathematical models and computational algorithms, computation-al biology has become a significant approach to understand the biological phenomena. This mini-symposium will focus on continuous type math models including PDEs and ODEs, which help to better understand biological experiments and predict more information. A variety of biological applications at multiple scales, such as at molecular, cell and tissue levels, will be considered. Empha-sis will be placed not only on mathematical theories and methods, but also on biological simulations and software developments closely integrated with experiments.

TALKS 1. Synchronization properties of scale-free networks of pituitary cells

DETAILS: Richard Bertram Florida State University

ABSTRACT. Pituitary cells secrete hormones that regulate most functions of the body. Like neurons, they exhibit electrical activity, and it is this activity that regulates hormone secretion. In particular, bursts of electrical impulses evoke secretion, while isolated impulses do not. We and others have developed and analyzed mathematical models of the various types of pituitary cells, based on experimental data from dispersed cells. However, in vivo the cells are found in networks of electrically-coupled cells of the same type. Some experimental work using pituitary slices has examined the functional connectivity of pituitary cells in their native networks, but no mathematical modeling work of pituitary networks has been done. We have begun such an analysis, focusing on general questions that would be of relevance to the interpretation of the in vivo data, and the extrapolation of data from dispersed cells to the network level. In this presentation, we provide preliminary modeling results on these questions, and interpret these preliminary findings in a biological context.

2. MicroRNAs govern bistable cell differentiation and lineage segregation via noncanonical feedback

Tian Hong, The University of Tennessee, Knoxville

ABSTRACT. Your abstract starts here. Positive feedback driven by transcriptional regulation has long been considered a key mechanism underlying cell lineage segregation during embryogenesis. Using the developing spinal cord as a paradigm, we found that canonical, transcription-driven feedback cannot explain robust lineage segregation of motor neuron subtypes marked by two cardinal factors, Hoxa5 and Hoxc8. We propose a feedback mechanism involving elementary microRNA-mRNA reaction circuits that differ from known feedback loop-like structures. Strikingly, we show that a wide range of biologically-plausible post-transcriptional regulatory parameters are sufficient to generate bistable switches, a hallmark of positive feedback. Using embryonic stem cell differentiation and mouse genetics, we corroborate that microRNA-mRNA circuits govern tissue boundaries and hysteresis upon motor neuron differentiation with respect to transient morphogen signals. Our findings reveal a previously underappreciated feedback mechanism that may have widespread functions in cell fate decisions and tissue patterning.

3. Mathematical modeling, computation and experimental investigation of dynamical heterogeneity in breast cancer

Xinfeng Liu, University of South Carolina

ABSTRACT. Solid tumors are heterogeneous in composition. Cancer stem cells (CSCs) are a highly tumorigenic cell type found in developmentally diverse tumors that are believed to be resistant to standard chemotherapeutic drugs and responsible for tumor recurrence. Thus understanding the tumor growth kinetics is critical for development of novel strategies for cancer treatment. For this talk, I shall introduce mathematical modeling to study Her2 signaling for the dynamical interaction between cancer stem cells (CSCs) and nonstem cancer cells, and our findings reveal that two negative feedback loops are critical in controlling the balance between the population of CSCs and that of non-stem cancer cells. Furthermore, the model with negative feedback suggests that over-expression of the oncogene HER2 leads to an increase of CSCs by regulating the division mode or proliferation rate of CSCs.

4. Modeling the transmission dynamics of COVID-19

Jin Wang, University of Tennessee at Chattanooga

ABSTRACT. We present a compartmental modeling framework based on systems of differential equations to investigate the transmission and spread of COVID-19. We focus our attention on the presence of multiple transmission routes, the evolution of disease transmission rates, the prevalence of underlying health conditions in host populations, and their impacts on the transmission dynamics of COVID-19. We discuss both analytical and numerical results.

MS7: Recent Developments and Applications in Computational Biology (Part II)

ORGANIZERS:	Shan Zhao, University of Alabama
	Xinfeng Liu, University of South Carolina
Description:	Due to the rapid developments of mathematical models and computational algorithms, computation-al biology has become a significant approach to understand the biological phenomena. This mini-symposium will focus on continuous type math models including PDEs and ODEs, which help to better understand biological experiments and predict more information. A variety of biological ap-plications at multiple scales, such as at molecular, cell and tissue levels, will be considered. Empha-sis will be placed not only on mathematical theories and methods, but also on biological simulations and software developments closely integrated with experiments.

TALKS 1. Micro-macro coupling of fluid dynamics in complex fluids

DETAILS: Paula Vasquez, University of South Carolina

2. A hybrid model for simulating sprouting angiogenesis in biofabrication Yi Sun, University of South Carolina

ABSTRACT. We present a 2D hybrid model to study sprouting angiogenesis of multicellular aggregates during vascularization in biofabrication. This model is developed to describe and predict the time evolution of angiogenic sprouting from endothelial spheroids during tissue or organ maturation in a novel biofabrication technology-bioprinting. Here we employ typically coarse-grained continuum models (reaction-diffusion systems) to describe the dynamics of vascular-endothelial-growth-factors, a mechanical model for the extra-cellular matrix based on the finite element method and couple a cellular Potts model to describe the cellular dynamics. The model can reproduce sprouting from endothelial spheroids and network formation from individual cells.

3. A regularization approach for biomolecular electrostatics involving singular charge sources and diffuse interfaces

Shan Zhao, University of Alabama

ABSTRACT. Both the sharp interface and diffuse interface Poisson-Boltzmann (PB) models have been presented in the literature for studying electrostatic interactions between a solute molecule and its surrounding solvent environment. In the mathematical analysis and numerical computation for these PB models, a significant challenge is due to singular charge sources in terms of Dirac delta distributions. For sharp interface case, this difficulty is often overcome by using a regularization method. However, the development of regularization method for diffuse interface models is highly nontrivial, because the fundamental solution with a space dependent dielectric function is unattainable. In our recent study, by means of a novel dual decomposition, the first regularization formulation has been developed to capture the singularity analytically for diffuse interface PB models. The well-posedness of the proposed regularization has been analyzed rigorously. Moreover, when the underlying diffuse interface approaches to a sharp interface, the regularization of the diffuse interface PB model has been shown to converge to that of the sharp interface case. The proposed algorithm has been validated by comparing with existing PB models for calculating electrostatic free energies of proteins, and benchmarked with experimental data in estimating salt affinities. This talk is based on joint works with Yuanzhen Shao (University of Alabama) and Emil Alexov (Clemson University).

4. Determination of protein-membrane interface using surface phase field with random potential

Yongcheng Zhou, Colorado State University

MS8: Modeling and Data Science in Quantitative Biology: Predictions and Descriptions (Part I)

ORGANIZERS: Bhargav Karamched, Florida State University

DESCRIPTION: Biological processes are incredibly complex, posing a plethora of challenges that obfuscate underly-ing mechanisms and render outcomes unpredictable. For example: How do bacteria coordinate ac-tivity across large spatial domains that exceed the correlation lengths of their communication signals? How do vesicles reach specific locations in a cell in a timely fashion? What are optimal methods to prevent spread of disease? Obtaining answers to such questions via experimental methods often requires significant time and money. Hence, there is a growing need for theoretical investigation to guide experimentalists with predictions and uncover underlying mechanisms. Theoretical models have a longstanding tradition of capturing fundamental dynamics of biological processes. Moreover, the emergence of data science and machine learning as powerful tools to match theoretical models to data has improved theoretical models' predictive power. Thus, modeling and data science together are valuable for improving understanding in biological science. This mini-symposium will feature talks by young academics on how theoretical models of different areas in biology uncover underly-ing mechanisms and how machine learning and data science have helped make novel, sometimes counterintuitive, predictions.

TALKS 1. Delay-induced uncertainty in a paradigmatic glucose-insulin model

DETAILS: Bhargav Karamched, Florida State University

ABSTRACT. Medical practice in the intensive care unit is based on the supposition that physiological systems such as the human glucose-insulin system are predictable. In this talk, we will show that delay within the glucose-insulin system can induce sustained temporal chaos, rendering the system unpredictable. Specifically, we exhibit such chaos for the paradigmatic Ultradian glucose-insulin model. This well-validated, finite-dimensional model represents feedback delay as a three-stage filter. Using the theory of rank one maps from smooth dynamical systems, we precisely explain the nature of the resulting delay-induced uncertainty (DIU). We develop a recipe one may use to diagnose DIU in a general oscillatory dynamical system. For infinite-dimensional delay systems, no analog of the theory of rank one maps exists. Nevertheless, we show that the geometric principles encoded in our DIU recipe apply to such systems by exhibiting sustained temporal chaos for a linear shear flow. Our results are potentially broadly applicable because delay is ubiquitous throughout mathematical physiology.

2. Management strategies using optimal control for disease outbreaks

George Lytle, University of Montevallo

ABSTRACT. The spread of pathogens transcends geographical boundaries; yet, our management of infectious diseases typically occurs within distinct geo-political units. In this preliminary report, we explore the ramifications of controlling continuous disease processes within discrete management units. Specifically, we investigate the extent to which optimal controls and public health outcomes vary under different governance structures. We study two hypothetical diseases similar to cholera and ebola. This is joint work with Julie Blackwood, Kyle Dahlin, Christina Edholm, Lindsey Fox, Margaret Grogan, Brandon Hollingsworth, Emily Howerton, Suzanne Lenhart, and Katriona Shea.

3. Data-driven approaches for predicting and reconstructing cardiac electrical dynamics

Elizabeth Cherry, Georgia Institute of Technology

ABSTRACT. Integration of data to enhance or even replace mechanistic mathematical models of physical and biological processes is an important focus of modern scientific analysis. In this talk, we consider two such approaches within the context of complex cardiac electrical dynamics, which can range from period-2 rhythms in single cells to spiral and scroll waves of electrical activity. First, we illustrate the use of data assimilation (specifically, an ensemble Kalman filter) to reconstruct one- and three-dimensional time series of observed and unobserved variables in cardiac electrical dynamics. Second, we show that machine-learning approaches can successfully predict single-cell cardiac voltage data and compare the performance of recurrent neural networks and echo state networks in such forecasting tasks.

4. Fast-slow analysis of a stochastic mechanism for electrical bursting Mehran Fazli, *Florida State University*

ABSTRACT. Electrical bursting oscillations in neurons and endocrine cells are activity patterns that facilitate the secretion of neuro-transmitters and hormones, and have been the focus of study for several decades. Mathematical modeling has been an extremely useful tool in this effort, and the use of fast-slow analysis has made it possible to understand bursting from a dynamic perspective, and to make testable predictions about changes in system parameters or the cellular environment. It is typically the case that the electrical impulses that occur during the active phase of a burst are due to stable limit cycles in the fast subsystem of equations, or in the case of so-called "pseudo-plateau bursting", canards that are induced by a folded node singularity. In this study, we show an entirely different mechanism for bursting that relies on stochastic opening and closing of a key ion channel. We demonstrate, using fast-slow analysis, how the short-lived stochastic channel openings can yield a much longer response in which single action potentials are converted into bursts of action potentials. Without this stochastic element, the system is incapable of bursting. This mechanism can describe stochastic bursting in pituitary corticotrophs, which are small cells that exhibit a great deal of noise, as well as other pituitary cells such as lactotrophs and somatotrophs that exhibit noisy bursts of electrical activity.

MS8: Modeling and Data Science in Quantitative Biology: Predictions and Descriptions (Part II)

ORGANIZERS: Bhargav Karamched, Florida State University

DESCRIPTION: Biological processes are incredibly complex, posing a plethora of challenges that obfuscate underly-ing mechanisms and render outcomes unpredictable. For example: How do bacteria coordinate ac-tivity across large spatial domains that exceed the correlation lengths of their communication signals? How do vesicles reach specific locations in a cell in a timely fashion? What are optimal methods to prevent spread of disease? Obtaining answers to such questions via experimental methods often requires significant time and money. Hence, there is a growing need for theoretical investigation to guide experimentalists with predictions and uncover underlying mechanisms. Theoretical models have a longstanding tradition of capturing fundamental dynamics of biological processes. Moreover, the emergence of data science and machine learning as powerful tools to match theoretical models to data has improved theoretical models' predictive power. Thus, modeling and data science together are valuable for improving understanding in biological science. This mini-symposium will feature talks by young academics on how theoretical models of different areas in biology uncover underly-ing mechanisms and how machine learning and data science have helped make novel, sometimes counterintuitive, predictions.

TALKS1. Cyclic network structure and multistationarity in biochemical networksDETAILS:Casian Pantea, West Virginia University

ABSTRACT. Multistationarity, or the existence of multiple positive steady states, is a much-studied property of biochemical reaction networks. Multistationarity and bistability are related to the capacity of the system to exhibit switch-like behavior, and are central to important biological phenomena like cell differentiation or apoptosis. It is well-known that the existence of certain cyclic network substructures (positive circuits) are necessary for multistationarity, but not sufficient in general. In this talk we study a class of multistationary positive circuits (cyclic sequestration-transmutation, or CST networks) and we show how their occurrence as substructures in biochemical networks might be sufficient to conclude multistationarity.

2. Modeling and data analysis for filament organization in cells

Maria-Veronica Ciocanel, Duke University

ABSTRACT. Actin filaments are polymers that interact with myosin motor proteins inside cells and play important roles in cell motility, shape, and development. This dynamic network of interacting proteins reshapes and organizes in a variety of structures, including bundles, clusters, and contractile rings. Motivated by observations from roundworm development, we use a stochastic modeling framework to simulate interactions between actin filaments and myosin motor proteins inside cells. We show that methods building on topological data analysis can help distinguish between the filament organization resulting from interactions with different motor proteins. In ongoing work, we are interested in studying the dynamics of an unconventional myosin motor and in developing minimal stochastic models that characterize its protein interactions.

3. Gene expression level classification using conditional random fields.

Xiyuan Liu, Louisiana Tech University

ABSTRACT. The classical methods for the classification problem include hypothesis test with Benjamini-Hochberg method, Hidden Markov Chain Model (HMM), and Support Vector Machine (SVM). One major application of the classification problem is gene expression analysis, for example, detecting the host genes having interaction with pathogen. The classical methods can be applied and have a good performance when the number of genes having interaction with the pathogen is not sparse with respect to the candidate genes. On the other hand, Conditional Random Field (CRF), with an appropriate design, can be applied and have good performance even when it is sparse. In this work, we proposed a modified CRF with a baseline to reduce the number of parameters in CRF. Moreover, we show an application of CRF with the Least Absolute Selection and Shrinkage Operator (LASSO) to classifying barley genes of its reaction to the pathogen.

4. Epidemiology of COVID-19 in Jails

Kellen Myers, Tusculum University

ABSTRACT. Throughout the COVID-19 pandemic, institutions like the criminal justice system have faced challenges mitigating COVID while maintaining at least partial operations. In many localities, e.g. New Jersey, reductions in the jail and/or prison populations were considered. I will briefly summarize a mathematical model exploring the epidemiological impact of such interventions for jails, contrasted with "business as usual." In particular, the model considers not just within-jail dynamics, but spill-over risks for both corrections officers and the broader community. The model demonstrates that operating in a "business as usual" fashion may result in significantly greater disease burden in the community and within the jail. The public health policy implications are clear: Large-scale reductions in arrests and speeding of jail releases are likely to reduce negative health outcomes among incarcerated people, jail staff, and the community at large. I will summarize the policy recommendations for the most effective interventions. Joint work with Lofgren, Lum, Horowitz, Madubuonwu, and Fefferman.

MS9: Deep Learning Methods for Data Driven Models (Part I)

ORGANIZERS: Zhu Wang, University of South Carolina Lili Ju, University of South Carolina

DESCRIPTION: Modern sensor technology and data acquisition capability have led to the explosive production of digital data and information. Data-driven approaches based on model reduction methods or machine learning techniques are powerful tools for extracting important characteristics and essential repre-sentations from the massive data, affecting every branch of science and social life with unprece-dented impact. Although deep learning has achieved tremendous successes in many areas such as computer vision and speech recognition, challenges still exist in many scientific and engineering ar-eas. This mini-symposium will focus on recent advances in data-driven approaches using emerging deep learning algorithms together with their applications in scientific research and engineering.

TALKS1. Alternating the population and control neural networks to solve high-
dimensional stochastic mean-field games

Wuchen Li, University of South Carolina

ABSTRACT. We present APAC-Net, an alternating population and agent control neural network for solving stochastic mean field games (MFGs). Our algorithm is geared toward high-dimensional instances of MFGs that are beyond reach with existing solution methods. We achieve this in two steps. First, we take advantage of the underlying variational primal-dual structure that MFGs exhibit and phrase it as a convex-concave saddle point problem. Second, we parameterize the value and density functions by two neural networks, respectively. By phrasing the problem in this manner, solving the MFG can be interpreted as a special case of training a generative adversarial network (GAN). We show the potential of our method on up to 100-dimensional MFG problems.

2. Neural parametric Fokker-Planck equations

Shu Liu, Georgia Institute of Technology

ABSTRACT. We develop and analyze a numerical method proposed for solving highdimensional Fokker-Planck equations by leveraging the generative models from deep learning. Our starting point is a formulation of the Fokker-Planck equation as a system of ordinary differential equations (ODEs) on finite-dimensional parameter space with the parameters inherited from generative models such as normalizing flows. We call such ODEs "neural parametric Fokker-Planck equations". The fact that the Fokker-Planck equation can be viewed as the 2-Wasserstein gradient flow of the relative entropy (also known as KL divergence) allows us to derive the ODE as the 2-Wasserstein gradient flow of the relative entropy constrained on the manifold of probability densities generated by neural networks. For numerical computation, we design a variational semi-implicit scheme for the time discretization of the proposed ODE. Such an algorithm is sampling-based, which can readily handle computations in higher dimensional space. Moreover, we establish bounds for the asymptotic convergence analysis as well as the error analysis for both the continuous and discrete schemes of the neural parametric Fokker-Planck equation. Several numerical examples are provided to illustrate the performance of the proposed algorithms and analysis.

3. Equivariant neural network in computer vision and scientific computing Wei Zhu, *University of Massachusetts Amherst*

Encoding symmetry information explicitly into the representation learned by a convolutional neural network (CNN) is beneficial for many computer vision and scientific computing tasks. I will present, in this talk, a scaling-translation-equivari- ant (ST-equivariant) CNN with joint convolutions across the space and the scaling group, which is shown to be both sufficient and necessary to achieve equivariance for the regular representation of the scaling-translation group ST. To reduce the model complexity and computational burden, we decompose the convolutional filters under two pre-fixed separable bases and truncate the expansion to low-fre- quency components. A further benefit of the truncated filter expansion is the improved deformation robustness of the equivariant representation, a property which is theoretically analyzed and empirically verified. Numerical experiments demon-strate that the proposed scaling-translation-equivariant network with decomposed convolutional filters (ScDCFNet) achieves significantly improved performance in multiscale image classification and better interpretability than regular CNNs at a reduced model size. Time permitting, I will also highlight the potential of equivar- iant neural networks in scientific computing by respecting conservation and sym- metry constraint in physical models.

4. Solving and learning phase field models using the modified Physics Informed Neural Networks

Jia Zhao, Utah State University

ABSTRACT. In this talk, we introduce some recent results on solving and learning phase field models using deep neural networks. In the first part, we focus on using the deep neural network to design an automatic numerical solver for the Allen-Cahn and Cahn-Hilliard equations by proposing an adaptive physics informed neural network (PINN). In particular, we propose to embrace the adaptive idea in both space and time and introduce various sampling strategies, such that we are able to improve the efficiency and accuracy of the PINN on solving phase field equations. In the second part, we introduce a new deep learning framework for discovering the phase field models from existing image data. The new framework embraces the approximation power of physics informed neural networks (PINN), and the computational efficiency of the pseudo-spectral methods, which we named pseudo-spectral PINN or SPINN. We will illustrate its approximation power by some interesting examples.

MS9: Deep Learning Methods for Data Driven Models (Part II)

ORGANIZERS: Zhu Wang, University of South Carolina

Lili Ju, University of South Carolina

DESCRIPTION: Modern sensor technology and data acquisition capability have led to the explosive production of digital data and information. Data-driven approaches based on model reduction methods or machine learning techniques are powerful tools for extracting important characteristics and essential repre-sentations from the massive data, affecting every branch of science and social life with unprece-dented impact. Although deep learning has achieved tremendous successes in many areas such as computer vision and speech recognition, challenges still exist in many scientific and engineering ar-eas. This mini-symposium will focus on recent advances in data-driven approaches using emerging deep learning algorithms together with their applications in scientific research and engineering.

TALKS 1. Reproducing activation function for deep learning

DETAILS: Chunmei Wang, University of Florida

ABSTRACT. The speaker will propose the reproducing activation function to improve deep learning accuracy for various applications ranging from computer vision problems to scientific computing problems. The idea of reproducing activation functions is to employ several basic functions and their learnable linear combination to construct neuron-wise data-driven activation functions for each neuron. Armed with such activation functions, deep neural networks can reproduce traditional approximation tools and, therefore, approximate target functions with a smaller number of parameters than traditional neural networks. In terms of training dynamics of deep learning, reproducing activation functions activation functions lessening the spectral bias of deep learning. As demonstrated by extensive numerical tests, the proposed reproducing activation function can facilitate the convergence of deep learning optimization for a solution with higher accuracy than existing deep learning solvers for audio/image/video reconstruction, PDEs, and eigenvalue problems.

2. Solving PDEs on unknown manifolds with machine learning

Senwei Liang, Purdue University

ABSTRACT. Solving high-dimensional PDEs on unknown manifolds is a challenging computational problem that commands a wide variety of applications. In this talk, I will introduce a mesh-free computational framework and machine learning theory for solving elliptic PDEs on unknown manifolds, identified with point clouds, based on diffusion maps (DM) and deep learning. The PDE solver is formulated as a supervised learning task to solve a least-squares regression problem that imposes an algebraic equation approximating a PDE (and boundary conditions if applicable). In a well-posed elliptic PDE setting, when the hypothesis space consists of neural networks with either infinite width or depth, we show that the global minimizer of the empirical loss function is a consistent solution in the limit of large training data. When the hypothesis space is a two-layer neural network, we show that for a sufficiently large width, gradient descent can identify a global minimizer of the empirical loss function. Supporting numerical examples demonstrate the convergence of the solutions and the effectiveness of the proposed solver in avoiding numerical issues that hampers the traditional approach when a large data set becomes available, e.g., large matrix inversion.

3. A nonlocal gradient for high-dimensional black-box optimization in scientific machine learning

Guannan Zhang, Oak Ridge National Laboratory,

4. Improved nonlinear level set learning for high-dimensional function approximation

Anthony Gruber, Florida State University

ABSTRACT. Quantities of scientific interest are often presented as real-valued functions on a high-dimensional input space. When measurements are scarce, prediction techniques must avoid overfitting the available data in order to be effective. This talk discusses improvements to the network-based Nonlinear Level set Learning (NLL) method for pointwise prediction and sensitivity analysis. Leveraging geometric information provided by the Implicit Function Theorem, these improvements are shown to yield both faster training and more accurate results when compared to the original NLL method and the linear method of Active Subspaces.

MS10: Theory Meets Practice for Inverse Problems in Imaging Applications (Part I)

ORGANIZERS: Anuj Abhishek, University of North Carolina at Charlotte Taufiquar Khan, University of North Carolina at Charlotte

DESCRIPTION: Inverse Problems are problems wherein the intrinsic properties of an object are to be determined from some indirect measurements of such properties. The field of inverse problems has driven much of technological development over the past few decades. Applications include a number of imaging modalities such as medical imaging, geophysical imaging and non-invasive industrial imag-ing techniques. In the past decade or so there have been significant developments both in the math-ematical theory and applications of inverse problems. The purpose of this mini-symposium would be to bring together people working on different aspects of the field, to encourage interaction be-tween mathematicians and scientists and engineers working directly with the applications.

TALKS1. A new nonlinear sparse optimization framework for two-photon photoa-
coustic computed tomography.

Souvik Roy, University of Texas at Arlington

ABSTRACT. In this talk, we present a new approach to reconstruct sparse optical coefficients in two-photon phtoacoustic computed tomography (2P-PACT). 2P-PACT is a hybrid imaging tomographic technique that uses near infrared light and the data from the photoacoustic phenomenon to obtain cross-sectional images of the distribution of the optical coefficients in an object. This can be mathematically formulated as an inverse problem. Existing mathematical reconstruction algorithms for 2P-PACT inversion either require more data for better reconstructions or suffer from loss of contrast in optical coefficient distributions representing holes and inclusions. We, thus, develop a new and efficient 2P-PACT inversion algorithm based on a partial differential equation (PDE)-constrained sparse optimization method. We provide a new proof of existence and uniqueness of a solution to the underlying photon-propagation equation, given by a semi-linear PDE. Furthermore, a proximal method, involving a Picard solver for the semi-linear PDE and its adjoint, is used to solve the optimization problem. Several numerical experiments demonstrate the effectiveness of our method. This is a joint work with Madhu Gupta and Rohit Kumar Mishra.

2. TBD

Shyla Kupis, Clemson University

3. On accelerating iterative gradient type methods for solving electrical impedance tomography problem

Sanwar Uddin Ahmad, Colorado State University

ABSTRACT. Electrical impedance tomography (EIT) is an imaging modality that determines the internal conductivity and permittivity distribution based on the voltage measurements made on an object's surface when currents are applied. Due to its noninvasiveness, non-ionizing characteristics and cost effectiveness, EIT is gaining a lot of attention in recent years. Gradient type methods have been extensively studied and used for solving the inverse EIT problem. However, these methods suffer greatly due to the high computational cost at every iteration. In this presentation, we discuss the implementation of computing the Jacobian and the step-length parameter for reducing the computational cost. Results are shown with timing for experimental data sets collected with the ACT 5 system.

4. Adaptive estimation of function from Exponential radon transform data Sakshi Arya, *Pennsylvania State University*

ABSTRACT. In this talk, we propose a locally adaptive strategy for estimating a function from its Exponential Radon Transform (ERT) data, without any knowledge of the smoothness of functions that are to be estimated. We build a non-parametric kernel type estimator and show that for a class of functions comprising a wide Sobolev regularity scale, our proposed strategy follows the minimax optimal rate up to a log n factor. We also show that there does not exist a pointwise optimal adaptive estimator and in fact the rate achieved by the proposed estimator is the adaptive rate of convergence.

MS10: Theory Meets Practice for Inverse Problems in Imaging Applications (Part II)

ORGANIZERS: Anuj Abhishek, University of North Carolina at Charlotte Taufiquar Khan, University of North Carolina at Charlotte

DESCRIPTION: Inverse Problems are problems wherein the intrinsic properties of an object are to be determined from some indirect measurements of such properties. The field of inverse problems has driven much of technological development over the past few decades. Applications include a number of imaging modalities such as medical imaging, geophysical imaging and non-invasive industrial imag-ing techniques. In the past decade or so there have been significant developments both in the math-ematical theory and applications of inverse problems. The purpose of this mini-symposium would be to bring together people working on different aspects of the field, to encourage interaction be-tween mathematicians and scientists and engineers working directly with the applications.

TALKS 1. Streak artefacts in X-ray tomography

DETAILS: Yiran Wang, Emory University

ABSTRACT. In X-ray CT scan with metal objects, it is known that direct application of the filtered back-projection formula leads to streak artefacts in the reconstruction. An outstanding problem is to identify the cause of the artefacts and reduce them. In 2017, Seo *et al* characterized the artefacts mathematically using wave front sets. It is interesting that the artefacts are generated from certain nonlinear interactions of the X-ray transform. In this talk, we show how to analyze such phenomena quantitatively using microlocal techniques. We will also discuss the connection of the artefacts and the geometry of the metal objects.

2. From static to dynamic inverse problems: new edge-preserving methods for image reconstruction

Mirjeta Pasha, Arizona State University

ABSTRACT. In this talk we consider efficient methods for computing solutions to dynamic inverse problems, where both the quantities of interest and the forward operator (measurement process) may change at different time instances but we want to solve for all the images simultaneously. We are interested in large-scale ill-posed problems that are made more challenging by their dynamic nature and, possibly, by the limited amount of available data per measurement step. To remedy these difficulties, we apply regularization methods that enforce simultaneous regularization in space and time (such as edge enhancement at each time instant and proximity at consecutive time instants) and achieve this with low computational cost and enhanced accuracy. More precisely, we develop iterative methods based on a majorization-minimization (MM) strategy with quadratic tangent majorant, which allows the resulting least squares problem to be solved with a generalized Krylov subspace (GKS) method; the regularization parameter can be defined automatically and efficiently at each iteration. Numerical examples from a wide range of applications, such as limited-angle computerized tomography (CT), space-time image deblurring, and photoacoustic tomography (PAT), illustrate the effectiveness of the described approaches.

3. An optimal Bayesian estimator for a stochastic problem of diffuse optical tomography

Anuj Abhishek, UNC Charlotte

ABSTRACT. Studying coefficient inverse problems in a stochastic setting has increasingly gained in prominence in the past couple of decades or so. In this talk, we will present some results that were obtained for a Bayesian estimator built from the noisy data obtained in a simplified Diffuse Optical Tomography (DOT) Model. We establish the rate of convergence of such an estimator in the supremum norm loss and show that it is optimal. This work extends the approach proposed by Abraham and Nickl in a recent article (On Statistical Calderon problems) and applies it the problem in DOT setting.

MS11: Recent Progress of Classical and Deep Learning Methods in Inverse Problems and Imaging (Part I)

Organizers: Xiaojing Ye, Georgia State University

Yang Yang, Michigan State University

DESCRIPTION: Inverse problems seek to infer causal factors from observations. They arise naturally in a wide range of scientific fields, especially in imaging sciences and technologies. Classical approaches to-wards inverse problems explore the relation between causal factors and observations using tools from various mathematical branches including partial differential equations, functional analysis, op-timization, numerical analysis, and probability theory. On the other hand, recent decades have wit-nessed an emerging trend of using deep learning (DL) methods to solve inverse problems. Com-pared to classical approaches, DL methods shed new light on solving several fundamental challeng-es in inverse problems such as the curse of dimensionality and ill-posedness. The aim of this mini-symposium is to bring together applied mathematicians in the area of inverse problems to discuss recent progress of classical and DL methods. The minisymposium is expected to promote the de-velopment of novel ideas and new research collaborations through knowledge dissemination and discussion.

TALKS 1. Structure probing neural network deflation

DETAILS: Chunmei Wang, University of Florida

ABSTRACT. Deep learning is a powerful tool for solving nonlinear differential equations, but usually, only the solution corresponding to the flattest local minimizer can be found due to the implicit regularization of stochastic gradient descent. The speaker will discuss a network-based structure probing deflation method to make deep learning capable of identifying multiple solutions that are ubiquitous and important in nonlinear physical models. First, we introduce deflation operators built with known solutions to make known solutions no longer local minimizers of the optimization energy landscape. Second, to facilitate the convergence to the desired local minimizer, a structure probing technique is proposed to obtain an initial guess close to the desired local minimizer. Together with neural network structures carefully designed, the new regularized optimization can converge to new solutions efficiently. Due to the mesh-free nature of deep learning, the proposed method is capable of solving high-dimensional problems on complicated domains with multiple solutions, while existing methods focus on merely one or two-dimensional regular domains and are more expensive in operation counts. Numerical experiments also demonstrate that the proposed method could find more solutions than exiting methods.

2. Optimal transport for parameter identification of chaotic dynamics via invariant measures

Yunan Yang, New York University

ABSTRACT. Parameter identification determines the essential system parameters required to build real-world dynamical systems by fusing crucial physical relationships and experimental data. However, the data-driven approach faces many difficulties, such as discontinuous or inconsistent time trajectories and noisy measurements. The ill-posedness of the inverse problem comes from the chaotic divergence of the forward dynamics. Motivated by the challenges, we shift from the Lagrangian particle perspective to the state space flow eld's Eulerian description. Instead of using pure time trajectories as the inference data, we treat statistics accumulated from the Direct Numerical Simulation (DNS) as the observable. The continuous analog of the latter is the physical invariant probability measure, a distributional solution of the stationary continuity equation. Thus, we reformulate the original parameter identification problem as a data-fitting, PDE-constrained optimization problem.

3. Deep learning theory for PDEs: approximation, optimization, and generalization

Haizhao Yang, Purdue University

ABSTRACT. The remarkable success of deep learning in computer science has evinced potentially great applications of deep learning in computational and applied mathematics. Understanding the mathematical principles of deep learning is crucial to validating and advancing deep learning-based PDE solvers. We present a few thoughts on the theoretical foundation of this topic for high-dimensional partial differential equations including approximation, optimization, and generalization. Though our analysis is not a complete story and there are many missing pieces to make it well-justified, it may still be helpful to provide some insights into deep learning.

4. Model predictions in epidemiology by using stable parameter estimation and real data

Alexandra Smirnova, Georgia State University

ABSTRACT. Our goal is to solve a nonlinear constrained optimization problem given some noisy (and possibly incomplete) measurements of the state observation operator. A hybrid regularized predictor-corrector scheme is introduced that builds upon all-at-once formulation, recently developed by Kaltenbacher and her co-authors for general constrained least squares problems (2016), the generalized profiling methods by Ramsay, Hooker, Campbell, and Cao (2007) for estimating parameters in nonlinear ordinary differential equations, and the so-called traditional route for solving nonlinear ill-posed problems, pioneered by A. Bakushinsky (1991). Similar to all-at-once approach, our proposed algorithm does not require an explicit deterministic or stochastic trajectory of system evolution. At the same time, the predictor-corrector framework of the new method avoids the difficulty of dealing with large solution spaces resulting from all-at-once make-up, which inevitably leads to oversized Jacobian and Hessian approximations. Therefore our predictor-corrector algorithm (PCA) has the potential to save time and storage, which is critical when multiple runs of the iterative scheme are carried out for uncertainty quantification. The new algorithm takes full advantage of the iterative regularization framework and it is not limited to the constraints in the form of differential equations (or systems of differential equations). To assess numerical efficiency of novel PCA, two parameter estimation inverse problems in epidemiology are considered. All experiments are carried out with real data on COVID-19 pandemic in Netherlands and Spain.

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MS11: Recent Progress of Classical and Deep Learning Methods in Inverse Problems and Imaging (Part II)

ORGANIZERS: Xiaojing Ye, Georgia State University

Yang Yang, Michigan State University

DESCRIPTION: Inverse problems seek to infer causal factors from observations. They arise naturally in a wide range of scientific fields, especially in imaging sciences and technologies. Classical approaches to-wards inverse problems explore the relation between causal factors and observations using tools from various mathematical branches including partial differential equations, functional analysis, op-timization, numerical analysis, and probability theory. On the other hand, recent decades have wit-nessed an emerging trend of using deep learning (DL) methods to solve inverse problems. Com-pared to classical approaches, DL methods shed new light on solving several fundamental challeng-es in inverse problems such as the curse of dimensionality and ill-posedness. The aim of this mini-symposium is to bring together applied mathematicians in the area of inverse problems to discuss recent progress of classical and DL methods. The minisymposium is expected to promote the de-velopment of novel ideas and new research collaborations through knowledge dissemination and discussion.

TALKS 1. Neural primal dual methods for mean field games

DETAILS: Wuchen Li, University of South Carolina

ABSTRACT. We present APAC-Net, an alternating population and agent control neural network for solving stochastic mean field games (MFGs). Our algorithm is geared toward high-dimensional instances of MFGs that are beyond reach with existing solution methods. We achieve this in two steps. First, we take advantage of the underlying variational primal-dual structure that MFGs exhibit and phrase it as a convex-concave saddle point problem. Second, we parameterize the value and density functions by two neural networks, respectively. By phrasing the problem in this manner, solving the MFG can be interpreted as a special case of training a generative adversarial network (GAN). We demonstrate the potential of our method on up to 100-dimensional MFG problems.

- 2. Quantitative PAT with simplified P_N approximation Yimin Zhong, *Duke University*
- **3.** Machine learning techniques for inverse problems in sonar imaging Christina Frederick, *New Jersey Institute of Technology*

ABSTRACT. In this talk we discuss machine learning for inverse problems in high frequency underwater acoustics, where the goal is to recover detailed characteristics of the seafloor from measured backscatter data generated from SONAR systems. The key to successful inversion is the use of accurate forward modeling that captures of the dependence of the backscatter on seafloor properties, such as sediment type, roughness, and thickness of layers.

To enable a rapid, remote, and accurate recovery of the seafloor, we propose an approach that combines high fidelity forward modeling and simulation of the entire physical wave propagation and scattering process and machine learning strategies. The idea is to partition large underwater acoustic environments, on the order of kilometers in spatial width, into much smaller "template" domains, a few meters in spatial width, in which the sediment layer can be described using a limited number of parameters. Hybrid prediction models can be created by embedding localized simulations of Helmholtz equations on each template domain in a large-scale geometric optics model for larger domains. To solve the inverse problem, machine learning strategies applied to a reference library of acoustic templates can be used to estimate the seafloor parameters that describe the full domain.

4. Geometry inspired DNNs on manifold-structured data

Rongjie Lai, Rensselaer Polytechnic Institute

MS12: Recent Developments of Numerical Methods for Fluid Flows and Applications (Part I)

ORGANIZERS: Thi-Thao-Phuong Hoang, Auburn University

DESCRIPTION: Numerical simulation of fluid flows is a topic of great interest with a wide range of applications. The goal of this mini-symposium is to bring together mathematicians and scientists to present cutting-edge research on efficient numerical schemes, their analysis and application to the numerical solution of various problems in fluid dynamics.

TALKS1. A weighted least-squares finite element method for Biot's consolidationDETAILS:problem

Hyesuk Lee, Clemson University

ABSTRACT. In this talk we consider a weighted least-squares method for a poroelastic structure governed by Biot's consolidation model. The quasi-static model equations are converted to a first-order system of four-field, and the least-squares functional is defined for the time discretized system. We consider two different sets of weights for the functional and show its coercivity and continuity properties, from which an a priori error estimate for the primal variables is derived. Numerical experiments are provided to illustrate the performance of the proposed method.

2. Efficient methods for non-Newtonian fluids

Sara Pollock, University of Florida

ABSTRACT. Non-Newtonian fluids arise in many applications, including industrial manufacturing and food production. Commonly used models include grade-two and Bingham fluids. The more complicated stress-strain relationship in these models in comparison to their Newtonian counterparts create challenges for their numerical simulation. We will discuss some recent advances in non-Newtonian modeling and numerical simulation using finite elements.

3. An artificial compressibility CNLF method for the Stokes-Darcy model and application in ensemble simulations

Ying Li, University of Florida

ABSTRACT. We propose and analyze an efficient, unconditionally stable, second order convergent, artificial compressibility Crank-Nicolson leap-frog (CNLFAC) method for numerically solving the Stokes-Darcy equations. The method decouples the fully coupled Stokes-Darcy system into two smaller subphysics problems, which reduces the size of the linear systems to be solved, at each time step, and allows parallel computing of the two subphysics problems. It also decouples the computation of the velocity and pressure in the free flow region. The pressure only needs to be updated at each time step without solving a Poisson equation, avoiding pressure errors in boundary layers due to imposing artificial boundary conditions. We prove that the method is unconditionally long time stable and second order convergent. We also propose an unconditionally stable ensemble algorithm based on the CNLFAC method. The ensemble algorithm results in a common coefficient matrix for all realizations and consequently allows the use of efficient direct or iterative solvers to reduce the computational cost. Numerical experiments are provided to illustrate the second-order convergence and unconditional stability of the CNLFAC method. Moreover, the CNLFAC ensemble algorithm is demonstrated to reduce the computational time of a CNLF nonensemble algorithm by 95% in our tests.

4. High-Order multirate explicit time-stepping schemes for the baroclinicbarotropic split dynamics in primitive equations

Rihui Lan, University of South Carolina

ABSTRACT. In order to treat the multiple time scales of ocean dynamics in an efficient manner, the baroclinic-barotropic splitting technique has been widely used for solving the primitive equations for ocean modeling. In this paper, we propose second and thirdorder multirate explicit time-stepping schemes for such split systems based on the strong stability-preserving Runge-Kutta (SSPRK) framework. Our method allows for a large time step to be used for advancing the three-dimensional (slow) baroclinic mode and a small time step for the two-dimensional (fast) barotropic mode, so that each of the two mode solves only need satisfy their respective CFL condition to maintain numerical stability. It is well known that the SSPRK method achieves high-order temporal accuracy by utilizing a convex combination of forward-Euler steps. At each time step of our method, the baroclinic velocity is first computed by using the SSPRK scheme to advance the baroclinic-barotropic system with the large time step, then the barotropic velocity is specially corrected by using the same SSPRK scheme with the small time step to advance the barotropic subsystem with a barotropic forcing interpolated based on values from the preceding baroclinic solves. Finally, the fluid thickness and the sea surface height perturbation is updated by coupling the predicted baroclinic and barotropic velocities. Temporal truncation error analyses are also carried out for the proposed schemes. Two benchmark tests drawn from the "MPAS-Ocean" platform are used to numerically demonstrate the accuracy and parallel performance of the proposed schemes.

MS12: Recent Developments of Numerical Methods for Fluid Flows and Applications (Part II)

ORGANIZERS: Thi-Thao-Phuong Hoang, Auburn University

DESCRIPTION: Numerical simulation of fluid flows is a topic of great interest with a wide range of applications. The goal of this mini-symposium is to bring together mathematicians and scientists to present cutting-edge research on efficient numerical schemes, their analysis and application to the numerical solution of various problems in fluid dynamics.

TALKS1. Stabilized integrating factor Runge-Kutta method and unconditional
preservation of maximum bound principle

Lili Ju, University of South Carolina

ABSTRACT. Maximum bound principle (MBP) is an important property for a large class of semilinear parabolic equations, in the sense that their solution preserves for all time a uniform pointwise bound in absolute value imposed by the initial and boundary conditions. It has been a challenging problem on how to design unconditionally MBP-preserving time stepping schemes for these equations, especially the ones with order greater than one. We combine the integrating factor Runge-Kutta (IFRK) method with the linear stabilization technique to develop a stabilized IFRK (sIFRK) method, and successfully derive the sufficient conditions for the proposed method to preserve MBP unconditionally in the discrete setting. We then elaborate some sIFRK schemes with up to the third order accuracy, which are proven to be unconditionally MBP-preserving by verifying these conditions. In addition, it is shown that many strong stability preserving sIFRK (SSP-sIFRK) schemes do not satisfy these conditions, except the first-order one. Various numerical experiments are also carried out to demonstrate the performance of the proposed method.

2. Exponential integrators for meteorological equations

Vu Thai Luan, Mississippi State University

ABSTRACT. The existence of vastly different time scales (known as stiffness) in atmospheric phenomena has posed a major challenge in developing efficient, stable, and accurate time integration methods for meteorological models over the past 70 years. In this talk, we propose the use of stiffly accurate exponential integrators, which are designed for large-scale stiff systems. They are fully explicit, in that they do not require iterative nonlinear solvers, and show unconditional linear stability. For accuracy and efficiency purposes, we construct efficient exponential schemes of high orders. Moreover, we propose an efficient modification to one of the state-of-the-art algorithms for implementing exponential integrators. Numerical experiments based on a suite of challenging tests problems performed with the shallow water models on a geodesic icosahedral grid confirm that the proposed schemes enable accurate solutions at much longer time-steps than the semi-implicit schemes (which have been widely used), proving more efficient as the desired accuracy decreases or as the problem nonlinearity increases. The talk is based on joint works with Janusz A. Pudykiewicz (Environment Canada) and Daniel R. Reynolds (SMU).

3. Pressure robust scheme for incompressible flow

Lin Mu, University of Georgia

ABSTRACT. In this talk, we shall introduce the recent development regarding the pressure robust weak Galerkin finite element method (FEM) for solving incompressible flow. Weak Galerkin (WG) Method is a natural extension of the classical Galerkin finite element method with advantages in many aspects. For example, due to its high structural flexibility, the weak Galerkin finite element method is well suited to most partial differential equations on the general meshing by providing the needed stability and accuracy. In this talk, the speaker shall discuss the new divergence preserving schemes in designing the robust numerical schemes. Due to the viscosity independence in the velocity approximation, our scheme is robust with small viscosity and/or large permeability, which tackles the crucial computational challenges in fluid simulation. We shall discuss the details in the implementation and theoretical analysis. Several numerical experiments will be tested to validate the theoretical conclusion.

4. Geometric multigrid for massively parallel, adaptive, large scale Stokes flow problems

Timo Heister, Clemson Unversity

ABSTRACT. We present a large scale, parallel geometric multigrid method for Stokes flow on adaptively refined meshes. The motivation is the simulation of convection in the Earth's mantle. The governing equations are solved using the Finite Element method on adaptively refined meshes, which allows us to resolve features at high resolution, without intractable computational cost.

Nevertheless, linear systems can become quite large (100+ million unknowns), so efficient, parallel solvers are necessary. We are implementing massively-parallel, matrix-free, geometric Multigrid solvers to solve the Stokes part of the governing equations.

The solver is implement in the open source mantle convection code ASPECT that is built on the open source deal. II finite element library. We will show benchmark results that confirm far better performance and scalability compared to the algebraic multigrid solvers built on assembled matrices, that were used in ASPECT until now. We can show good scalability to 100,000+ cores and 100s of billions of unknowns.

MS13: Surrogate Modeling for High-dimensional Problems and Applications (Part I)

ORGANIZERS: Hoang Tran, Oak Ridge National Laboratory Armenak Petrosyan, Georgia Tech

DESCRIPTION: The approximations of high-dimensional systems from data play a pivotal role in a wide variety of mathematical and scientific problems including uncertainty quantification, control and optimization, statistical inference and data processing. Such problems often require repetitive, expensive measurements (for instance, ensemble of complex numerical simulations or time-consuming physical experiments), thus, it would be very beneficial to have access to an accurate surrogate model, which can be used in place of the original model, to approximate the input-output relationship of interest. This mini-symposium aims at bringing together people working on the theory and methods for surrogate modeling and high-dimensional approximation, in particular, but not restricted to, nonlinear approximation, sparse recovery, low-rank approximation and deep neural networks, showcasing the latest results on both methodology and applications.

TALKS 1. Robust identification of differential equations from noisy data

DETAILS: Sung-Ha Kang, Georgia Institute of Technology

ABSTRACT. Identifying unknown differential equations from given discrete time dependent data is a challenging problem. Noisy data make such identification particularly challenging. In this talk, we present robust methods against a high level of noise which approximate the underlying noise-free dynamics well. This approach is fundamentally based on numerical PDE techniques, and we introduce successively denoised differentiation and utilize subspace pursuit time evolution error for PDE identification.

2. Plateau phenomenon in gadient descent training of ReLU networks: explanation, quantification, and avoidance

Yeonjong Shin, Brown University

ABSTRACT. Gradient-based optimization methods result in the loss function decreases rapidly at the beginning of training but then, after a relatively small number of steps, significantly slow down. The loss may even appear to stagnate over the period of a large number of epochs, only to then suddenly start to decrease fast again for no apparent reason. This so-called plateau phenomenon manifests itself in many learning tasks. In this talk, we will present our mathematical analysis that identifies and quantifies the root causes of the plateau phenomenon. Based on the insights gained from the mathematical analysis we propose a new iterative training method, the Active Neuron Least Squares (ANLS), characterized by the explicit adjustment of the activation pattern at each step, which is designed to enable a quick exit from a plateau.

3. Optimal transport methods in nonlinear dimensionality reduction

Keaton Hamm, University of Texas at Arlington

ABSTRACT. The manifold hypothesis, that high-dimensional data lives on or near a lowdimensional embedded manifold, is ubiquitous in machine learning theory and practice. For imaging data, the data appears as vectors in high-dimensional Euclidean space, where the vectors are acquired from some imaging operator mapping a functional space, such as L_2 to Euclidean space. It is thus unclear that Euclidean distance between the image vectors contains sufficient semantic meaning to understand the structure of the data manifold. We propose treatment of the functional data as a set of probability measures, and use pairwise Wasserstein distances to compute similarity. We then utilize these distances in the ISOMAP algorithm for nonlinear dimensionality reduction. The proposed algorithm, called WassMap, can be shown to recover translation and dilational functional manifolds up to global isometry, and further experiments on synthetic data show its success on a variety of other kinds of image manifolds.

4. A bandit-learning approach to multifidelity approximation

Yiming Xu, University of Utah

ABSTRACT. Multifidelity approximation is an important technique in scientific computation and simulation. In this talk, we introduce a bandit-learning approach for leveraging data of varying fidelities to achieve precise estimates of the parameters of interest. Under a linear model assumption, we formulate a multifidelity approximation as a modified stochastic bandit, and analyze the optimal regret for a class of policies which uniformly explore each model before exploiting. Utilizing the estimated conditional mean-squared error (MSE), we propose a consistent algorithm, adaptive Explore-Then- Commit (AETC), and establish a corresponding trajectory-wise optimality result. The main advantage of our approach is that we require neither hierarchical model structure nor a priori knowledge of statistical information (e.g., correlations) about or between models. Instead, the AETC algorithm requires only knowledge of which model is a trusted high-fidelity model, along with (relative) computational cost estimates of querying each model.

MS13: Surrogate Modeling for High-dimensional Problems and Applications (Part II)

ORGANIZERS: Hoang Tran, Oak Ridge National Laboratory Armenak Petrosyan, Georgia Tech

DESCRIPTION: The approximations of high-dimensional systems from data play a pivotal role in a wide variety of mathematical and scientific problems including uncertainty quantification, control and optimization, statistical inference and data processing. Such problems often require repetitive, expensive measurements (for instance, ensemble of complex numerical simulations or time-consuming physical experiments), thus, it would be very beneficial to have access to an accurate surrogate model, which can be used in place of the original model, to approximate the input-output relationship of interest. This mini-symposium aims at bringing together people working on the theory and methods for surrogate modeling and high-dimensional approximation, in particular, but not restricted to, nonlinear approximation, sparse recovery, low-rank approximation and deep neural networks, showcasing the latest results on both methodology and applications.

TALKS1. Gaussian process and Bayesian optimization – Bridging the gap betweenDETAILS:theory and practice in materials science

Anh Tran, Sandia National Laboratories

ABSTRACT. Gaussian process (GP) has been one of the cornerstones in non-parametric Bayesian machine learning methods. Using GP as an underlying surrogate model, Bayesian optimization (BO) aims to balance exploration and exploitation and refine the GP model as the optimization progresses. With a solid mathematical foundation, these two methods have been widely adopted across multiple disciplines. While they are among one of the most popular data-driven approaches, there are many limitations in the classical GP and BO that do not naturally fit in the practical settings. In this talk, we discuss a wide range of extensions, including multi-objective, multi-fidelity, mixed-integer, parallel, scalable, and high-dimensional from theoretical and computational perspectives. We conclude the talk with real-world engineering applications for materials and manufacturing.

2. TBD

Oleksander Vlasiuk, Vanderbilt University

3. Non-convex analysis of matching and embedding of image keypoints Vahan Huroyan, *University of Arizona*

ABSTRACT. We address two important subproblems of Structure from Motion Problem. The first subproblem is known as Multi-way Matching, where the input includes multiple sets, with the same number of objects and noisy measurements of fixed one-to-one correspondence maps between the objects of each pair of sets. Given only noisy measurements of the mutual correspondences, the Multi-way Matching problem asks to recover the correspondence maps between pairs of them. The desired output includes the original fixed correspondence maps between all pairs of sets. The second subproblem is called Multi-Perspective Simultaneous Embedding (MPSE). The input for MPSE assumes a set of pairwise distance matrices defined on the same set of objects and possibly along with the same number of projection operators. MPSE embeds points in 3D so that the pairwise distances are preserved under the corresponding projections. Our proposed algorithm for the Multi-way Matching problem iteratively solves the associated non-convex optimization problem. We prove that for a specific noise model, if the initial point of our proposed iterative algorithm is good enough, the algorithm linearly converges to the unique solution. Numerical experiments demonstrate that our method is much faster and more accurate than the state-of-the-art methods. For MPSE, we propose a heuristic algorithm and provide an extensive quantitative evaluation with datasets of different sizes, as well as several examples that illustrate the quality of the resulting solutions.

4. Learning high-dimensional Hilbert-valued functions with deep neural networks from limited data

Nick Dexter, Simon Fraiser University

ABSTRACT. The approximation of solutions to parameterized partial differential equations (PDEs) is a key challenge in computational uncertainty quantification problems for engineering and science. In these problems, the solution is a function of both the physical and parametric variables, taking values in an infinite-dimensional Hilbert or Banach space. Compressed sensing (CS) has recently been extended to allow approximation of Hilbert-valued functions, and exponential rates of convergence for CS-based polynomial approximations have been established. However, the application of deep neural networks (DNNs) to such problems presents many potential benefits over the polynomial based approach. DNNs with ReLU activation functions have been shown to emulate virtually every known approximation scheme, and optimal approximation rates have been established for such networks on a wide array of function classes including holomorphic and piecewise smooth functions. In this work we present theoretical results on learning highdimensional Hilbert-valued functions from limited datasets by DNNs. We also present numerical results demonstrating the efficacy of such approaches on function and parametric PDE approximation problems.

MS14: Numerical Methods and Deep Learning for Nonlinear PDEs (Part I)

ORGANIZERS: Chunmei Wang, University of Florida Sara Pollock, University of Florida

DESCRIPTION: Numerical Methods for partial differential equations and their analysis are important and challenging topics in applied and computational mathematics. Deep learning is a method of data analysis that automates analytical model building, which is a branch of artificial intelligence based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention. This mini-symposium is focused on recent developments in numerical methods and deep learning for PDEs with an focus on nonlinear PDEs, including new developments in finite element methods, deep learning and relevant applications. The goal of this mini-symposium is to bring together leading researchers in the field of numerical methods and deep learning to discuss and disseminate the latest results and envisage future challenges in traditional and new areas of science. The topics of the mini-symposium cover a broad range of numerical methods and deep learning, including but not limited to finite element methods, interior penalty method, extended Galerkin methods, vector-cloud neural networks, weak adversarial networks, etc. A wide range of application fields will also be covered, such as poroelasticity, electroporoelasticity, and phase field crystal equations.

TALKS 1. On the equations of electroporoelasticity

DETAILS: A. J. Meir, Southern Methodist University

ABSTRACT. Complex coupled problems are mathematical models of physical systems (or physically motivated problems) which are governed by partial differential equations and which involve multiple components, complex physics or multi-physics, as well as complex or coupled domains, or multiple scales. One such phenomenon is electroporoelasticity.

After introducing the equations of electroporoelasticity (the equations of poroelasticity coupled to Maxwell's equations) which have applications in geoscience, hydrology, and petroleum exploration, as well as various areas of science and technology, I will describe some recent results and challenges.

2. Solving high-dimensional PDEs using weak adversarial networks Xiaojing Ye, *Georgia State University*

ABSTRACT. We introduce a weak adversarial network (WAN) approach to numerically solve a variety of inverse problems involving high-dimensional partial differential equations (PDEs). The weak formulation of the PDEs for the given inverse problem is leveraged, where the solution and the test function are parameterized as deep neural networks. Then, the weak formulation and the boundary conditions induce a minimax problem of a saddle function of the network parameters. The weak solution network and the test function network are two players in a zero-sum game. As the parameters are alternatively updated, the solution network gradually approaches the weak solution of the inverse problem. The oretical justifications are provided on the convergence of the proposed algorithm. The proposed method is completely mesh-free without any spatial discretization, and is particularly suitable for problems with high dimensionality and low regularity on solutions.

3. Learning nonlocal constitutive PDE models with vector-cloud neural networks

Jiequn Han, Flatiron Institute

ABSTRACT. Constitutive models are widely used for modeling complex systems in science and engineering, when first-principle-based, well-resolved simulations are prohibitively expensive. For example, in fluid dynamics, constitutive models are required to describe nonlocal, unresolved physics such as turbulence and laminar-turbulent transition. However, traditional constitutive models based on PDEs often lack robustness and are too rigid to accommodate diverse calibration datasets. We propose a frame-independent, nonlocal constitutive model based on a vector-cloud neural network that represents the physics of PDEs and meanwhile can be learned with data. The model predicts the closure variable at a point based on the flow information in its neighborhood. Such nonlocal information is represented by a group of points, each having a feature vector attached to it, and thus the input is referred to as vector cloud. The cloud is mapped to the closure variable through a frame-independent neural network, invariant both to coordinate translation and rotation and to the ordering of points in the cloud. As such, the network can deal with any number of arbitrarily arranged grid points and thus is suitable for unstructured meshes in fluid simulations. The merits of the proposed network are demonstrated for scalar transport PDEs on a family of parameterized periodic hill geometries. The vector-cloud neural network is a promising tool not only as nonlocal constitutive models and but also as general surrogate models for PDEs on irregular domains.

4. Deep network approximation via function composition Networks Shijun Zhang, National University of Singapore

MS14: Numerical Methods and Deep Learning for Nonlinear PDEs (Part II)

ORGANIZERS: Chunmei Wang, University of Florida Sara Pollock, University of Florida

DESCRIPTION: Numerical Methods for partial differential equations and their analysis are important and challenging topics in applied and computational mathematics. Deep learning is a method of data analysis that automates analytical model building, which is a branch of artificial intelligence based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention. This mini-symposium is focused on recent developments in numerical methods and deep learning for PDEs with an focus on nonlinear PDEs, including new developments in finite element methods, deep learning and relevant applications. The goal of this mini-symposium is to bring together leading researchers in the field of numerical methods and deep learning to discuss and disseminate the latest results and envisage future challenges in traditional and new areas of science. The topics of the mini-symposium cover a broad range of numerical methods and deep learning, including but not limited to finite element methods, interior penalty method, extended Galerkin methods, vector-cloud neural networks, weak adversarial networks, etc. A wide range of application fields will also be covered, such as poroelasticity, electroporoelasticity, and phase field crystal equations.

TALKS 1. Transition path theory with low complexity models

DETAILS: Yuehaw Khoo, University of Chicago

2. Large eddy simulation reduced order models

Traian Iliescu, Virginia Tech

ABSTRACT. We present reduced order models (ROMs) that are constructed by using ideas from large eddy simulation (LES) and variational multiscale (VMS) methods. These LES-ROMs are built by using ROM spatial filters, e.g., the ROM projection and the ROM differential filter. The LES-ROMs capture the large scale ROM features and model the interaction between these large scales and the small scale ROM features. We present results for LES-ROMs in the numerical simulation of under-resolved engineering flows (e.g., flow past a cylinder and turbulent channel flow) and the quasi-geostrophic equations (which model the large scale ocean circulation).

3. A C0 interior penalty method for the phase field crystal equation Amanda E. Diegel, *Mississippi State University*

ABSTRACT. We present a C0 interior penalty finite element method for the sixth-order phase field crystal equation. We demonstrate that the numerical scheme is uniquely solvable, unconditionally energy stable, and convergent and benchmark our method against numerical experiments previously established in the literature.

4. Extended Galerkin methods in finite element exterior calculus

Yuwen Li, The Pennsylvania State University

ABSTRACT. In this talk, I present a novel discontinuous Galerkin (dG) discretization framework for the Hodge Laplace equation in finite element exterior calculus. The proposed dG methods satisfy unifying discrete inf-sup conditions and quasi-optimal a priori error estimates. In addition, those dG methods are shown to be hybridizable. The material in the talk is based on a joint work with Qingguo Hong and Jinchao Xu.

MS15: Mathematical Modeling, Analysis and Applications (Part I)

ORGANIZERS: Thomas Hagen, University of Memphis

DESCRIPTION: This mini-symposium will feature diverse presentations which explore novel developments in mathematical modeling of continuum mechanical processes and introduce significant techniques for the analytical and computational prediction of their behavior. It will bring together junior mathematicians with more senior researchers and lead to a fruitful exchange of new ideas and objectives.

TALKS1. Recent results on the uniform observability of filtered approximationsDETAILS:for piezoelectric beam equations

Ahmet Ozkan Ozer, Western Kentucky University

ABSTRACT. Space-discretized Finite-Difference approximations of the system of "noncompactly" coupled PDE model of piezoelectric beam model are studied. Even though the PDE model is shown to be exactly observable with two boundary observations, its approximations do not retain uniform exact observability with respect to the mesh parameter $h \rightarrow 0$. This is mainly due to the loss of the uniform gap among two branches of eigenvalues. To obtain a uniform gap, and therefore, a uniform observability result with respect to mesh parameter, a direct Fourier-filtering method is adopted to eliminate artificial high-frequency eigenvalues of the approximated model. Both the discrete multipliers and Ingham's theorem are utilized for proving main results. The main hurdle in proving the discrete energy estimates is the non-identical wave speeds and con-compact coupling of the wave system.Current projects and future directions will be briefly discussed.

2. Local existence and null-controllability for a PDE-ODE model concerning a bacterial infection in a radially-symmetric, chronic wound Stephen Guffey, *Collierville High School*

ABSTRACT. In this work, we discuss results for a differential equation model for a bacterial infection in a radially-symmetric, chronic wound. The goal of the current work is the following: show the model produces a unique solution in a suitable setting and then determine whether one can drive the system to the origin using controllers contained in a small subdomain of the wound. The model consists of three parabolic-like partial differential equations along with a single vector-valued ordinary differential equation. Of the critical features of the model, one of the most challenging is the nonlinear coupling describing chemotactic attraction between the neutrophils and a chemoattractant distributed throughout the wound. Lower order nonlinearities, describing various coupling phenomena, present further mathematical difficulties including the potential for our system to become singular. In this talk, we discuss the existence and positivity of the mild solutions. We also discuss the local null-controllability using compactly-supported controllers. A critical step in this argument is the control of the linearized system about the origin, for which we apply appropriate Carleman-type estimates. These give us an appropriate surjectivity condition that allows us to invoke the implicit function theorem for the nonlinear problem.

3. Surjectivity results for monotone operators perturbed by compact operators in reflexive spaces

Claudio Morales, University of Alabama in Huntsville

ABSTRACT. Let X be a reflexive space and let $A : C \to X^*$ be a maximal monotone operator. Suppose $C : K \to X^*$ is compact with K being closed and bounded with nonempty interior. One of the questions that we are interested in resolving is, under what conditions the operator A + C is surjective? Various additional results will be discussed in this presentation.

4. Free-boundary problems in film forming flows

Thomas Hagen, The University of Memphis

ABSTRACT. The manufacture of thin plastic sheets makes use of film forming flows, including cast-film extrusion. During manufacture a polymer melt is fed through a die, stretched into a thin fluid sheet and solidified. For highly viscous materials various mathematical models of this forming process were developed to study instabilities and other physical phenomena that put restrictions on the manufacturing process.

In this talk I will give a brief overview of mathematical aspects encountered even in simple, stationary flows of cast-film extrusion. The model reduces to a set of coupled nonlinear ordinary differential equations subject to boundary conditions. It features a free boundary which has to be determined as part of the solution. Quite unexpectedly, a sharp criterion for the model parameters governs existence of solutions when a pulling force is prescribed. When a velocity boundary condition is imposed, uniqueness of solutions is found via a maximum principle and a monotonicity argument.

MS15: Mathematical Modeling, Analysis and Applications (Part II)

ORGANIZERS: Thomas Hagen, University of Memphis

DESCRIPTION: This mini-symposium will feature diverse presentations which explore novel developments in mathematical modeling of continuum mechanical processes and introduce significant techniques for the analytical and computational prediction of their behavior. It will bring together junior mathematicians with more senior researchers and lead to a fruitful exchange of new ideas and objectives.

TALKS1. Analysis of the models for blown film extrusion: quasi-cylindrical and
thin-shellDETAILS:thin-shell

Md Fayaz Ahamed, The University of Memphis

ABSTRACT. Blown film extrusion is the most common process to produce plastic films. Mathematical models for film blowing are given by nonlinear, coupled boundary value problems involving free parameters that have to be found as a part of the solution. The formulation of the problem will be based on treating the liquid bubble as "quasi-cylindrical" and then "thin-shell". I will first talk about the derivation of the governing equations of both types and then discuss possible solutions. The scope for future developments will also be addressed.

2. Modelling human balance using intermittent feedback control

Lashika Rajapaksha, University of Texas at Dallas

ABSTRACT. Risk of falling increases as people age and falls are the leading cause of injury related deaths among older people. Thus, there is a growing interest to understand why falls occur and how to minimize the risk of falling. Recent works indicate that the brain plays an important role in balance control by switching on and off related muscle activities. Assuming that the human body can be modelled as an inverted pendulum subjected to a delayed proportional-derivative controller, the current study aims to determine the effect of an intermittent feedback control strategy on postural balance.

3. Fluid-structure interaction with Kelvin-Voight damping: analyticity, spectral analysis, exponential decay

Rasika Mahawattege, University of Memphis

ABSTRACT. We consider a fluid- structure interaction model defined on a doughnut-like domain. It consists of the dynamic Stokes equations evolving on the exterior sub-domain, coupled with an elastic structure occupying the interior sub-domain. A key factor - a novelty over past literature - is that the structure equation includes a strong (viscoelastic) damping term of Kelvin-Voigt type at the interior. This affects the boundary conditions at the interface between the two media and accounts for a highly unbounded "perturbation". Results include: (i) analyticity of s.c semigroup of contractions defining the overall coupled system, (ii) its (uniform) exponential decay, along with (iii) sharp spectral properties of its generator. Some results are geometry-dependent.

MS16: Recent Advances in Nonlinear Wave Propagation and Interaction (Part I)

ORGANIZERS: Ilija Jegdic, Texas Southern University Qi Han, Texas A&M University San Antonio

DESCRIPTION: The nonlinear wave phenomenon appears in a wide range of applications in sciences and engineering, including fluid dynamics, elastodynamics, electromagnetic, and other fields. The study of partial differential equations modeling nonlinear wave propagation and interaction involves an interplay between the pure mathematical theory, numerical methods, and mathematical physics. An interesting feature of these equations is that solutions could become irregular even for smooth initial and boundary data and one of the challenges in the study of such solutions is to select physically meaningful solutions. Recently, there has been lot of progress in the study of these equations and the purpose of this mini-symposium is to bring together mathematicians working on various problems both from theoretical and numerical perspectives. Some of the topics to be discussed include analysis of solutions to eikonal-type equations; study of existence, uniqueness, and stability of subsonic flows past an airfoil governed by the Euler gas dynamics equations; analysis of solutions to the two-layer quasigeotropic model; as well as convergence analysis of a large time step numerical method for conservation laws and numerical schemes for modified Buckley-Leverett equations and the black oil problem in porous media.

TALKS1. Discontinuous Galerkin method for black oil problem: convergence and
applications

Loic Cappanera, University of Houston

ABSTRACT. We introduce and analyze an original discretization technique for threecomponent three-phase flow problems in heterogeneous porous media. The method uses discontinous Galerkin finite element for the space discretization and a sequential implicit formulation for the time marching. The formulation is based on a compositional model and uses the liquid pressure, aqueous and vapor saturations as primary unknowns. Effects of mass transfer between phases are not considered such that the aqueous, liquid and vapor phases are respectively composed of water, oil and gas. We show that the discrete problem is well-posed and we establish a priori error estimates to show that our algorithm converges with first order. After describing the main steps that allow us establish the convergence of this method, we study the numerical convergence of the algorithm with smooth manufactured solutions involving gravity effects and variable density. The robustness of the method is then shown on highly heterogeneous reservoirs setups where the absolute permeability is generated randomly and present ratio of magnitude up to 10^3 .

2. Mathematical analysis and numerical studies for the modified Buckley-Leverett equations

Ying Wang, University of Oklahoma

3. Stability of vortex lines attached to a thin airfoil

Jun Chen, Yichun University

ABSTRACT. Occurrence of wingtip vortex may cause flight instability and even airplane crash. This type of vortex flow can be described as a vortex line attached to a two dimensional airfoil in Euler flow. In this talk, I will introduce background, setup and the main result of our problem about the stability of the vortex lines. Some technical details about solving the problem, such as elliptic estimates and application of the implicit function theorem will be explained.

4. The effect of the asymmetric Ekman term on the phenomenology of the two-layer quasigeostrophic model

Eleftherios Gkioulekas, University of Texas Rio Grande Valley

ABSTRACT. In the two-layer quasi-geostrophic model, the friction between the flow at the lower layer and the surface boundary layer, placed beneath the lower layer, is modeled by the Ekman term, which is a linear dissipation term with respect to the horizontal velocity at the lower layer. The Ekman term appears in the governing equations asymmetrically; it is placed at the lower layer, but does not appear at the upper layer. A variation, proposed by Phillips and Salmon, uses extrapolation to place the Ekman term between the lower layer and the surface boundary layer, or at the surface boundary layer. We present theoretical results that show that in either the standard or the extrapolated configurations, the Ekman term dissipates energy at large scales, but does not dissipate potential enstrophy. It also creates an approximately symmetric stable distribution of potential enstrophy between the two layers. The behavior of the Ekman term changes fundamentally at small scales. Under the standard formulation, the Ekman term will unconditionally dissipate energy and also dissipate, under very minor conditions, potential enstrophy at small scales. However, under the extrapolated formulation, there exist small "negative regions", which are defined over a two-dimensional phase space, capturing the distribution of energy per wavenumber between baroclinic energy and barotropic energy, and the distribution of potential enstrophy per wavenumber between the upper layer and the lower layer, where the Ekman term may inject energy or potential enstrophy.

MS16: Recent Advances in Nonlinear Wave Propagation and Interaction (Part II)

ORGANIZERS: Ilija Jegdic, Texas Southern University

Qi Han, Texas A&M University San Antonio

DESCRIPTION: The nonlinear wave phenomenon appears in a wide range of applications in sciences and engineering, including fluid dynamics, elastodynamics, electromagnetic, and other fields. The study of partial differential equations modeling nonlinear wave propagation and interaction involves an interplay between the pure mathematical theory, numerical methods, and mathematical physics. An interesting feature of these equations is that solutions could become irregular even for smooth initial and boundary data and one of the challenges in the study of such solutions is to select physically meaningful solutions. Recently, there has been lot of progress in the study of these equations and the purpose of this mini-symposium is to bring together mathematicians working on various problems both from theoretical and numerical perspectives. Some of the topics to be discussed include analysis of solutions to eikonal-type equations; study of existence, uniqueness, and stability of subsonic flows past an airfoil governed by the Euler gas dynamics equations; analysis of solutions to the two-layer quasigeotropic model; as well as convergence analysis of a large time step numerical method for conservation laws and numerical schemes for modified Buckley-Leverett equations and the black oil problem in porous media.

TALKS 1. On entire solutions to eikonal-type partial differential equations

DETAILS: Qi Han, Texas A&M University San Antonio

2. Semi-hyperbolic patches for the unsteady transonic small disturbance equation

Katarina Jegdic, University of Houston - Downtown

ABSTRACT. We consider a two-dimensional Riemann problem for the unsteady transonic small disturbance equation resulting in diverging rarefaction waves. We write the problem in self-similar coordinates and we obtain a mixed type hyperbolic-elliptic system. We resolve the one-dimensional discontinuities in the far field and we formulate the problem in a semi-hyperbolic patch that is between the hyperbolic and the elliptic regions. A semihyperbolic patch is known as a region where one family out of two nonlinear families of characteristics starts on a sonic curve and ends on a transonic shock. We use a characteristic decomposition to prove existence of a smooth local solution in this semi-hyperbolic patch and we obtain various properties of global smooth solutions.

3. Bistability in deterministic and stochastic SLIAR-type models with imperfect and waning vaccine protection

Evan Milliken, University of Louisville

ABSTRACT. Various vaccines have been approved for use to combat COVID-19 that offer imperfect immunity and could furthermore wane over time. We analyze the effect of vaccination in an SLIARS model with demography by adding a compartment for vaccinated individuals and considering disease-induced death, imperfect and waning vaccination protection as well as waning infections-acquired immunity. When analyzed as systems of ordinary differential equations, the model is proven to admit a backward bifurcation. A continuous time Markov chain (CTMC) version of the model is simulated numerically and compared to the results of branching process approximations. While the CTMC model detects the presence of the backward bifurcation, the branching process approximation does not. The special case of an SVIRS model is shown to have the same properties.

4. TBD

Zhaosheng Feng, University of Texas Rio Grande Valley

MS16: Recent Advances in Nonlinear Wave Propagation and Interaction (Part III)

ORGANIZERS: Ilija Jegdic, Texas Southern University

Qi Han, Texas A&M University San Antonio

DESCRIPTION: The nonlinear wave phenomenon appears in a wide range of applications in sciences and engineering, including fluid dynamics, elastodynamics, electromagnetic, and other fields. The study of partial differential equations modeling nonlinear wave propagation and interaction involves an interplay between the pure mathematical theory, numerical methods, and mathematical physics. An interesting feature of these equations is that solutions could become irregular even for smooth initial and boundary data and one of the challenges in the study of such solutions is to select physically meaningful solutions. Recently, there has been lot of progress in the study of these equations and the purpose of this mini-symposium is to bring together mathematicians working on various problems both from theoretical and numerical perspectives. Some of the topics to be discussed include analysis of solutions to eikonal-type equations; study of existence, uniqueness, and stability of subsonic flows past an airfoil governed by the Euler gas dynamics equations; analysis of solutions to the two-layer quasigeotropic model; as well as convergence analysis of a large time step numerical method for conservation laws and numerical schemes for modified Buckley-Leverett equations and the black oil problem in porous media.

TALKS1. Stability properties of a coupled compressible flow-plate dynamicsDETAILS:Pelin Guven Geredeli, Iowa State University

ABSTRACT. We consider a linearized compressible flow structure interaction PDE model for which the interaction interface might be under the effect of material derivative term. We analyze the stability properties of the solutions via a certain multiplier method in the time domain. In particular, our main (gradient type) multiplier is based upon the solution of a certain Neumann problem, a solution which is sufficiently smooth, even considering the unavoidable boundary interface singularities. We note that the application of this multiplier is practicable and convenient, due to the characterization (compatibility condition) of the invariant finite energy subspace.

2. Stability Analysis of interactive fluid and multilayered structure PDE dynamics

George Avalos, University of Nebraska-Lincoln

ABSTRACT. In this talk, we will discuss our recent work on a certain multilayered structure-fluid interaction (FSI) which arises in the modeling of vascular blood flow. The coupled PDE system under our consideration mathematically accounts for the fact that mammalian veins and arteries are typically composed of various layers of tissues: each layer will generally manifest its own intrinsic material properties, and will moreover be separated from the other layers by thin elastic laminae. Consequently, the resulting modeling FSI system will manifest an additional PDE, which evolves on the boundary interface, so as to account for the thin elastic layer. (This is in contrast to the FSI PDE's which appear in the literature, wherein elastic dynamics are largely absent on the boundary interface.) As such, the PDE system will constitute a coupling of 3D fluid-2D wave-3D elastic dynamics. For this multilayered FSI system, we will in particular present results of wellposedness and stability. This is joint work with Pelin Güven Geredeli of Iowa State University and Boris Muha of the University of Zagreb (Croatia).

3. Controlling refraction using sub-Wavelength resonators

Yue Chen, Auburn University at Montgomery

ABSTRACT. We construct metamaterials from sub-wavelength nonmagnetic resonators and consider the refraction of incoming signals traveling from free space into the metamaterial. The directionality of the transmitted signal and its frequency dependence is shown to be explicitly controlled by sub-wavelength resonances that can be calculated from the geometry of the sub-wavelength scatters.

4. Large-time behavior of 2D incompressible MHD system with partial dissipation

Wen Feng, Niagara University

ABSTRACT. In this talk, we will discuss the decay results on a 2D magnetohydrodynamic (MHD) system with only vertical dissipation. Without the magnetic field, the fluid velocity obeys a 2D anisotropic Navier-Stokes equation and is not known to be stable in the Sobolev setting H^2 due to the potential double exponential growth of its H^2 -norm in time. However, when coupled with the magnetic field in the MHD system, we show that the H^2 -norm of any perturbation near a background magnetic field actually decays algebraically in time. This result demonstrates that the magnetic field indeed stabilizes and damps the electrically conducting fluids. Mathematically this result along with its proof offers a new and effective approach to the large-time behavior on partially dissipated systems of partial differential equations (PDEs). Existing methods are mostly designed for systems with full dissipation and do not apply when the dissipation is anisotropic. This is the joint work with Farzana Hafeez and Jiahong Wu.

5. Study of chaotic vibration phenomenon of the non-strictly hyperbolic equation

Jing Tian, Towson University

ABSTRACT. The study of chaotic vibration for multidimensional PDEs due to nonlinear boundary conditions is challenging. In this talk, we discuss the chaotic oscillation of a two-dimensional non-strictly hyperbolic equation due to an energy-injecting boundary condition and a distributed self-regulating boundary condition. By using the method of characteristics, we give a rigorous proof of the onset of the chaotic vibration phenomenon of the 2D non-strictly hyperbolic equation. We have also found a regime of the parameters when the chaotic vibration phenomenon occurs. Numerical simulations are also provided.

MS17: Modeling and Numerical Methods for Image Problems

ORGANIZERS: Wei Zhu, University of Alabama at Tuscaloosa

DESCRIPTION: In the past three decades, variational and PDE-based models have achieved remarkable progresses in mathematical imaging and have been intensively employed in practical applications such as medical image analysis, remote sensing, and machine vision. Recently, efficient neural network based models were developed to deal with different imaging tasks including image classification, segmentation, recognition, etc. The main goal of this symposium is to bring together researchers interested in the modeling and numerical methods for imaging problems using PDE-based method or deep learning based method.

TALKS1. Image decomposition into structure, harmonic and oscillatory Compo-
DETAILS:nents

Sung-Ha Kang, Georgia Institute of Technology

ABSTRACT. We present a non-convex variational decomposition model which separates a given image into piecewise-constant, smooth and oscillatory components. This decomposition is motivated not only by image denoising and structure separation, but also by shadow and spot light removal. The proposed model clearly separates the piecewise constant structure and smoothly varying harmonic part, thanks to having a separated oscillatory component.

2. A novel regularization based on the error function for sparse recovery Weihong Guo, Case Western Reserve University

ABSTRACT. Regularization plays an important role in solving ill-posed problems by adding extra information about the desired solution, such as sparsity. Many regularization terms usually involve some vector norm, e.g., L1 and L2 norms. We propose a novel regularization framework that uses the error function to approximate the unit step function. It can be considered as a surrogate function for the L0 norm. The asymptotic behavior of the error function with respect to its intrinsic parameter indicates that the proposed regularization can approximate the standard L0, L1 norms as the parameter approaches to 0 and 1; respectively. Statistically, it is also less biased than the L1 approach. We then incorporate the error function into either a constrained or an unconstrained model when recovering a sparse signal from an under- determined linear system. Computationally, both problems can be solved via an iterative reweighted L1 (IRL1) algorithm with guaranteed convergence. A large number of experimental results demonstrate that the proposed approach outperforms the state-of-the-art methods in various sparse recovery scenarios. This is a joint work with Yifei Lou (University of Texas at Dallas), Jing Qin (University of Kenturky) and Ming Yan (Michigan State).

3. Learnable descent algorithm for nonsmooth nonconvex image reconstruction

Xiaojing Ye, Georgia State University

ABSTRACT. We develop a general learning based framework for solving nonsmooth and nonconvex image reconstruction problems. We model the regularization function as the composition of the $l_{2,1}$ norm and a smooth but nonconvex feature mapping parametrized as a deep convolutional neural network. We develop a descent-type algorithm to solve the nonsmooth nonconvex minimization problem by leveraging the Nesterov's smoothing technique and the idea of residual learning, and learn the network parameters such that the outputs of the algorithm match the references in training data. Our method is versatile as one can employ various modern network structures into the regularization, and the resulting network inherits the convergence properties of the algorithm. We also show that the proposed network is parameter-efficient and its performance compares favorably to the state-of-the-art methods in a variety of image reconstruction problems in practice.

4. First-order image restoration models for staircase reduction and contrast preservation

Wei Zhu, University of Alabama, Tuscaloosa

ABSTRACT. In this talk, we will discuss two novel first-order variational models for image restoration. In the literature, lots of higher-order models were proposed to fix the staircase effect. In our first model, we consider a first-order variational model that imposes stronger regularity than total variation on regions with small image gradients in order to achieve staircase reduction. In our second model, we further propose a novel regularizer that presents a lower growth rate than any power function with a positive exponent for regions with large image gradients. Besides removing noise and keeping edges effectively, this regularizer also helps preserve image contrasts during the image restoration process. We employ augmented Lagrangian method (ALM) to minimize both models and provide the convergence analysis. Numerical experiments will be then presented to demonstrate the features of the proposed models..

MS18: Advances in Memory Efficient Numerical Algorithms for Kinetic Problems

ORGANIZERS: Stefan Schnake, Oak Ridge National Laboratory

DESCRIPTION: Current research in popular fields such as plasma physics, semiconductors, radiation transport, and geeral kinetic theory often requires discretization of phase spaces with up to six dimensions. These problems suffer from the so-called curse of dimensionality which makes storage and computational requirements impractical for full resolution numerical approximations. In order to make numerical simulations tractable on modern supercomputers, rsearch has aimed to reduce the memory footprint of such approximations. More mature techniques such as Particle in Cell (PIC) and Monte-Carlo methods reduce memory requirements but can fail to capture physical phenomenon without a large sample size. This minisymposium features more recent techniques that focus on reducing memory requirements of more traditional Eulerian methods. Some techniques employ algorithms to reduce the raw number of degrees of freedom while minimally affecting accuracy; other techniques such as Reduced Order Modeling (ROM) and Dynamic Low-Rank approximation (DLRA) model low-rank features of the problem.

TALKS1. Implicit methods with reduced memory for time-dependent radiationDETAILS:transport problems

Dmitriy Anistratov, North Carolina State University

ABSTRACT. The solution of the Boltzmann transport equation (BTE) depends on 7 independent variables. Temporal discretization schemes for the BTE involve the discrete solution at the previous time level. This requires storing multi-dimensional grid functions that approximate the transport solution on a mesh in the phase space. This talk presents implicit methods with reduced memory (RM) formulated for the BTE, discretized in time with the backward Euler scheme. The grid functions of the transport solution from the previous time level are approximated by techniques based on the low-rank proper orthogonal decomposition. The performance of the implicit methods with RM are demonstrated on solving nonlinear radiation transport problems of high energy density physics. They are applied as a part of multilevel methods defined by hierarchy of equations consisting of the high-order BTE and low-order moment equations. The proposed approach can be extended to various time integration methods. This is joint work with Joseph Coale (NCSU).

2. Low-memory, discrete ordinates, discontinuous Galerkin methods for radiative transport.

Zheng Sun, The University of Alabama

ABSTRACT. The discrete ordinates discontinuous Galerkin $(S_N$ -DG) method is a wellestablished and practical approach for solving the radiative transport equation. In this talk, we present a low-memory variation of the upwind S_N -DG method. The proposed method uses a smaller finite element space that is constructed by coupling spatial unknowns across collocation angles, thereby yielding an approximation with fewer degrees of freedom than the standard method. Like the original S_N -DG method, the low-memory variation still preserves the asymptotic diffusion limit and maintains the characteristic structure needed for mesh sweeping algorithms. While we observe second-order convergence in scattering dominated, diffusive regime, the low-memory method is in general only first-order accurate. To address this issue, we use upwind reconstruction to recover second-order accuracy. For both methods, numerical procedures based on upwind sweeps are proposed to reduce the system dimension in the underlying Krylov solver strategy.

3. A hybrid decomposition method for the BGK Equation

Minwoo Shin, University of Notre Dame

ABSTRACT. We apply the hybrid decomposition method for the Boltzmann equation with the BGK operator in a hyperbolic scaling, which leads to Euler or compressible Navier–Stokes equations in the asymptotic limit. Implicit treatment for the source term is necessary to solve hyperbolic systems with stiff sources. Although it helps the numerical scheme become stable with a large time step size, it is still not obvious to achieve the desired order of accuracy due to the relationship between size of the spatial cell and mean free path. Without asymptotic preserving property, very restricted size of spatial cell is required to resolve mean free path, which is not practical. Our approaches are based on the noncollision-collision decomposition of the BGK equation. We introduce the arbitrary order of nodal discontinuous Galerkin (DG) discretization in space with semi-implicit time stepping method; we employ the backward Euler time integration for the uncollided equation and the 2nd order predictor-corrector scheme for the collided equation, i.e., both source terms in uncollided and collided equations are treated implicitly and only streaming term in the collided equation is solved explicitly. This improves the computational efficiency without the complexity of the numerical implementation. Numerical results are presented for various Knudsen numbers to present the effectiveness and accuracy of our hybrid method. Also, we compare the solutions of the hybrid and non-hybrid scheme.

4. Residual based rank adaptive algorithms for dynamic low-rank approximation

Stefan Schnake, Oak Ridge National Laboratory

ABSTRACT. Numerical discretizations of kinetic equations often suffer from the *curse* of dimensionality which make full resolution computations intractable. A recent and popular technique to reduce the order of complexity for these systems is Koch and Lubich's Dynamic Low-Rank Approximation (DLRA) which seeks to evolve the PDE on a low-rank manifold. Numerical integrators utilizing DLRA accurately capture low-rank features of kinetic systems by adaptively updating the global basis functions in time, but few give indicators for when to adaptively increase the rank of the solution. In this talk, we first present a technique to formulate popular discontinuous Galerkin methods as a semi-discrete matrix-valued ODE with low-memory and computationally efficient evaluations of the discrete operator. Next, we present residual-based indicators for when to increase the rank of a low-rank solution and which basis vectors should be added in order to optimally increase accuracy. Low- and high-rank numerical examples are given at the end of the talk.
MS19: Recent Advances in Iterative Solvers for Numerical Optimization and Nonlinear Systems (Part I)

ORGANIZERS: William Kong, Oak Ridge National Laboratory

Paul Laiu, Oak Ridge National Laboratory

DESCRIPTION: This minisymposium addresses the recent advances in the development and analysis of iterative solvers for numerical optimization and nonlinear systems. Topics may cover but not be limited to: (1) Development of iterative solvers with improved efficiency and robustness; (2) Convergence and complexity analysis of iterative solvers; (3) Application of iterative solvers to scientific problems.

TALKS 1. Iteration complexity of a proximal augmented Lagrangian method for DETAILS: constrained nonconvex composite programming With the second product of t

Weiwei Kong, Oak Ridge National Labs

ABSTRACT. This talk presents and analyzes a nonlinear inner accelerated inexact proximal augmented Lagrangian (NL-IAIPAL) method for solving smooth nonconvex composite optimization problems with nonlinear \mathcal{K} -convex constraints, i.e., the constraints are convex with respect to the order given by a closed convex cone \mathcal{K} . Each NL-IAIPAL iteration consists of inexactly solving a proximal augmented Lagrangian subproblem by an accelerated composite gradient (ACG) method followed by a Lagrange multiplier update. Under some mild assumptions, it is shown that NL-IAIPAL generates an approximate stationary solution of the constrained problem in $\mathcal{O}(\log(1/\rho)/\rho^3)$ ACG iterations, where $\rho > 0$ is a given tolerance. Numerical experiments are given to illustrate the computational efficiency of the presented method.

2. Simple and optimal methods for stochastic variational inequalities

Georgios Kotsalis, Georgia Institute of Technology

ABSTRACT. In this talk we will present a novel operator extrapolation (OE) method for solving deterministic variational inequality (VI) problems. We will show how the OE method can achieve the optimal rate of convergence for solving a variety of VI problems in a much simpler way than existing approaches. We then introduce the stochastic operator extrapolation (SOE) method and establish its optimal convergence behavior for solving different stochastic VI problems. The developed numerical scheme is demonstrated by means of a signal estimation example.

3. Neural projected Fokker-Planck equations

Wuchen Li, University of South Carolina

ABSTRACT. In this talk, we develop and analyze numerical methods for high dimensional Fokker-Planck equations by generative models. Our starting point is a formulation of the Fokker-Planck equation as a system of ordinary differential equations (ODEs) on finite-dimensional parameter space with the parameters inherited from generative models. We call such ODEs neural parametric Fokker-Planck equations. The fact that the Fokker-Planck equation can be viewed as the L2-Wasserstein gradient flow of Kullback-Leibler (KL) divergence allows us to derive the ODEs as the constrained L2-Wasserstein gradient flow of KL divergence on the set of probability densities generated by neural networks. Several numerical examples are provided to illustrate the performance of the proposed algorithms and analysis.

4. Dynamic filtering for Anderson acceleration

Sara Pollock, University of Florida

ABSTRACT. We will overview some recent theoretical advances in understanding how Anderson acceleration can be used to improve convergence and robustness of fixed-point iterations for the solution of nonlinear systems. We will look in particular at a filtering strategy which is suggested by a bound on the residual, and demonstrate it with some numerical examples.

MS19: Recent Advances in Iterative Solvers for Numerical Optimization and Nonlinear Systems (Part II)

ORGANIZERS: William Kong, Oak Ridge National Laboratory Paul Laiu, Oak Ridge National Laboratory

DESCRIPTION: This minisymposium addresses the recent advances in the development and analysis of iterative solvers for numerical optimization and nonlinear systems. Topics may cover but not be limited to: (1) Development of iterative solvers with improved efficiency and robustness; (2) Convergence and complexity analysis of iterative solvers; (3) Application of iterative solvers to scientific problems.

TALKS 1. An infeasible-start framework for convex quadratic optimization

DETAILS: Paul Laiu, Oak Ridge National Laboratory

ABSTRACT. We proposed a framework for solving general convex quadratic programs (CQPs) from an infeasible starting point by invoking an existing *feasible-start* algorithm tailored for *inequality*-constrained CQPs. The central tool is an exact penalty function scheme equipped with a penalty-parameter updating rule. The feasible-start algorithm merely has to satisfy certain general requirements, and so is the updating rule. Under mild assumptions, the framework is proved to converge on CQPs with both inequality and equality constraints and, at a negligible additional cost per iteration, produces an infeasibility certificate, together with a feasible point for an (approximately) ℓ_1 -least relaxed feasible problem, when the given problem does not have a feasible solution.

2. First-order methods for some structured nonconvex function constrained optimization problems

Digvijay Boob, Southern Methodist University

ABSTRACT. In this talk, we provide a new and simple algorithm for a structured nonconvex, possibly nonsmooth, function constrained optimization problem. We provide convergence rate to first-order KKT point under a well-known constraint qualification. Finally, we also show numerical experiments on an application problem that satisfies assumptions of our setting.

3. Iteration complexity of stochastic dual dynamic programming algorithms

Shixuan Zhang, Georgia Institute of Technology

ABSTRACT. In this talk, we discuss the iteration complexity of a class of stochastic dual dynamic programming (SDDP) algorithms for multistage stochastic mixed-integer nonlinear programs (MS-MINLP). Our SDDP algorithmic class encompasses, as important special cases, the traditional SDDP algorithm on multistage stochastic convex optimization and stochastic dual dynamic integer programming (SDDiP). Moreover, several interesting classes of MS-MINLP are identified, where the new algorithms are guaranteed to obtain the global optimum even without the assumption of complete recourse. We then characterize the iteration complexity of the proposed algorithms. In particular, for a (T+1)-stage stochastic MINLP with d-dimensional state spaces, to obtain an ϵ -optimal root node solution, we prove that the number of iterations of the proposed deterministic sampling algorithm is upper bounded by $\mathcal{O}((\frac{2T}{\epsilon})^d)$, and is lower bounded by $\mathcal{O}((\frac{T}{2\epsilon})^d)$ for the nonconvex case or by $\mathcal{O}((\frac{T}{8\epsilon})^{d/2-1})$ for the convex case. This shows that the obtained complexity bounds are rather sharp. It also reveals that the iteration complexity depends polynomially on the number of stages. We further show that the iteration complexity depends linearly on T, if all the state spaces are finite sets, or if we seek a $(T\epsilon)$ -optimal solution when the state spaces are infinite sets, i.e. allowing the optimality gap to scale with T. The iteration complexity study resolves a conjecture by the late Prof. Shabbir Ahmed.

CP: Contributed Presentations (Part I)

CHAIR: Thomas Hamori University of South Carolina

TALKS 1. On a class of nonlocal macroscopic models

DETAILS: Thomas Hamori University of South Carolina

ABSTRACT. Macroscopic models for traffic flow compare the motion of cars through a roadway to the motion of fluids in a stream. One such approach falls into the category of **scalar conservation laws**, based on the notion that traffic mass (cars) is conserved in time. These nonlinear PDE tend to lead to the formation of shocks such as those observed in Burgers equation, representing a traffic jam. Models are typically local, however, nonlocal models have gained interest in recent years. I will present a class of nonlocal traffic models with an Arrhenius type slow down term, inspired by the classical Lighthill-Witham-Richards (LWR) model. I will show there are two critical thresholds on initial data which distinguish solutions which are globally smooth from those which result in a finite time blow-up. While the LWR model experiences finite time blow-up for any nontrivial initial data, our thresholds allow for a class of subcritical initial data for which traffic jams are avoided. This indicates the nonlocal effect can help to prevent shock formations. This is joint work with Dr. Changhui Tan

2. Construction of orthonormal polynomial wavelets and it's application in solving SBVPs

Diksha Tiwari, University of Vienna

ABSTRACT. Capturing solution near the singular point of any nonlinear SBVPs is challenging because coefficients involved in the differential equation blow up near singularities. In this article, we aim to construct a general method based on orthogonal polynomials as wavelets. We discuss multiresolution analysis for wavelets generated by orthogonal polynomials, e.g., Hermite, Legendre, Chebyshev, Laguerre, and Gegenbauer. Then we use these wavelets for solving nonlinear SBVPs. These wavelets can deal with singularities easily and efficiently. To deal with the nonlinearity, we use both Newton's quasilinearization and the Newton-Raphson method. To show the importance and accuracy of the proposed methods, we solve the Lane-Emden type of problems and compare the computed solutions with the known solutions. As the resolution is increased the computed solutions converge to exact solutions or known solutions. We observe that the proposed technique performs well on a class of Lane-Emden type BVPs. As the paper deals with singularity, non-linearity significantly and different wavelets are used to compare the results.

3. Multiscale simulations and convergence analysis for upscaled multicontinuum flows

Tina Mai, Duy Tan University at Da Nang (Vietnam) and Texas A&M University

ABSTRACT. In this paper [1], we consider a challenging problem of simulating fluid flows, in complex multiscale media with multi-continuum background. As an endeavor to solve this issue, model reduction is utilized. In a recent article by Park and Hoang, homogenization was successfully employed, to derive homogenized equations and effective coefficients of a dual-continuum system, having negative interaction coefficients and new convection terms. Nevertheless, some degree of multiscale is still left. This motivates us to come up with a numerical scheme formed on the generalized multiscale finite element method (GMsFEM) and the dual-continuum approach, to accelerate the simulation, increase the accuracy and clearly interpret the interactions between the dual continua. Within our paper, each continuum is considered as a global system and connected to the other all through the media. We take into account the flow exchanges between the dual continua and within each continuum. These multiscale flow dynamics are modeled by the GMsFEM, which systematically builds either uncoupled or coupled multiscale basis (to convey the local characteristics to the global ones). We hence work with a system of two coupled equations accompanied with some interaction terms, and each equation shows one of the fine-grid dual continua. Convergence analysis of the proposed strategy is assisted by the numerical results, which demonstrate the favorable outcomes.

[1] Jun Sur Richard Park, Siu Wun Cheung, Tina Mai, Viet Ha Hoang, Multiscale simulations for upscaled multi-continuum flows, Journal of Computational and Applied Mathematics, 374 (2020) 112782.

4. Nonconforming time discretization based on Robin transmission conditions for the Stokes-Darcy system

Hemanta Kunwar, Clemson University

ABSTRACT. We consider a space-time domain decomposition method based on Schwarz waveform relaxation (SWR) for the time-dependent Stokes-Darcy system. The coupled system is formulated as a time-dependent interface problem based on Robin-Robin transmission conditions, for which the decoupling SWR algorithm is proposed and proved for the convergence. In this approach, the Stokes and Darcy problems are solved independently and globally in time, thus allowing the use of different time steps for the local problems. Numerical tests are presented for both non-physical and physical problems with various mesh sizes and time step sizes to illustrate the accuracy and efficiency of the proposed method.

5. Lehmer close pair differences to their next-door solutions

Kate Johnson, University of California Davis

ABSTRACT. We examine Lehmer's phenomenon; when some of the solutions for the imaginary coefficients of the Riemann zeta function zeros lie extremely close together (e.g., 7005.063 and 7005.101). It has yet to be proved that there exist infinitely many Lehmer pairs. The close pairs are constructed by examining the imaginary solutions of the Riemann hypothesis, a conjecture that all non-trivial zeros of the zeta-function have real part one-half. If the hypothesis is correct all of the non-trivial zeros lie on the critical line $\frac{1}{2}$ + ti. We provide a SAS(R) program that uses a search grid to find the imaginary coordinates as we zoom into the non-trivial zeros of the Riemann's zeta function (SAS/STAT, 2018). We examine the differences between Lehmer 'close together' points and the next-to solutions on the search grid. The search grid consists of examining grids of sets of 2 million imaginary solution points. We determine a good measure of how close the Lehmer points /ordinates should be in order to be considered close; we refine the measure used to define 'closeness' for determining a Lehmer pair; we calculate the difference between the maximum of the Lehmer pair and its next door solution and investigate these differences. We repeat this for differing sets, looking as far out as to the 100-billionth Riemann zeta zero solution. We find some interesting anomalies and trends.

6. Efficient algorithms for computation of MHD flow ensemble

Muhammad Mohebujjaman, Texas A&M International University

ABSTRACT. We propose, analyze, and test a series of fully discrete algorithms for the computation of the MHD flow ensemble. The key features are: (1) The algorithms are stable but decoupled into two identical sub-problems, which can be solved at each time-step simultaneously. (2) At each time-step, the algorithms share their system matrix with all the ensemble members, which saves computer memory, factorization of the system matrix and pre-conditioner are needed to build only once per time-step, saving computational time. We provide rigorous proof of the stability and convergence theorems. Optimal convergence rates are observed with the manufactured solutions. Finally, we test the algorithms on benchmark problems and found them to perform well.

CP: Contributed Presentations (Part II)

CHAIR: Kwadwo Antwi-Fordjour Samford University

TALKS1. Dynamics of a predator-prey model with generalized functional responseDETAILS:and mutual interference

Kwadwo Antwi-Fordjour, Samford University

ABSTRACT. Mutual interference and prey refuge are important drivers of predator-prey dynamics. The "exponent" or degree of mutual interference has been under much debate in theoretical ecology. In the present work, we investigate the interplay of the mutual interference exponent, and prey refuge, on the behavior of a predator-prey model with a generalized Holling type functional response — considering in particular the "non-smooth" case. This model can also be used to model an infectious disease where a susceptible population, moves to an infected class, after being infected by the disease. We investigate dynamical properties of the system and derive conditions for the occurrence of saddle-node, transcritical and Hopf-bifurcations. A sufficient condition for finite time extinction of the prey species has also been derived. In addition, we investigate the effect of a prey refuge on the population dynamics of the model and derive conditions such that the prev refuge would yield persistence of the population. We provide additional verification of our analytical results via numerical simulations. Our findings are in accordance with classical experimental results in ecology (Gause, 1934), that show that extinction of predator and prey populations is possible in a finite time period — but that bringing in refuge can effectively yield persistence.

2. Learning nonlinear level sets for functions approximations on sparse data through goal-driven pseudo-reversible neural network Yuankai Teng, University of South Carolina

ABSTRACT. Due to the curse of dimensionality approximating high-dimensional functions is a computationally challenging task, even for powerful deep neural networks. Inspired by the work of Nonlinear Level-set Learning (NLL) which use RevNet for dimensional reduction, we propose a goal-driven pseudo-reversible neural network for determining active variables of high-dimensional functions based on given sparse data. The proposed method not only relaxes the reversibility requirement in the NLL method, but also introduces novel loss terms to measure the influence of data samples on the function's sensitivity to the active variables. Extensive experimental results show that our method outperforms the NLL and the Active Subspaces methods, especially when the target functions possess critical points.

3. A multistep spectral method for time-dependent PDEs

Bailey Rester, The University of Southern Mississippi

ABSTRACT. Krylov subspace spectral (KSS) methods are high-order accurate, explicit time-stepping methods for partial differential equations (PDEs) with stability characteristic of implicit methods. Unlike other time-stepping approaches, KSS methods compute each Fourier coefficient of the solution from an individualized approximation of the solution operator of the PDE. As a result, KSS methods scale effectively to higher spatial resolution. This talk will present an explicit multistep formulation of KSS methods to provide a "best-of-both-worlds" situation that combines the efficiency of multistep methods with the stability and scalability of KSS methods. The effectiveness of the multistep KSS method will be demonstrated using numerical experiments.

4. On the stochastic Sigmoid Beverton-Holt model

Quinten McKinney, University of Alabama in Huntsville

ABSTRACT. The sigmoid Beverton-Holt equation, given by

$$x_{n+1} = \frac{a_n x_n^\delta}{1 + x_n^\delta} \quad x_0 > 0$$

is studied. We consider the case where $\delta > 0$ is arbitrary and $\{a_n\}_{n \in \mathbb{N}}$ is a random almost periodic sequence bounded from below in a menner dependent on δ . When $\delta > 1$ we prove the existence of exactly two positive almost periodic solutions and discuss the stability of each of these solutions. When $\delta \leq 1$, we prove the existence of a unique almost periodic solution and discuss its stability.

5. Early signs of regime shift and major population fluctuation in a twotimescale ecosystem

Susmita Sadhu, Georgia College & State University

ABSTRACT. A two-trophic ecosystem consisting of two species of predators competing for their common prey with explicit interference competition is considered. With proper rescaling, the model is written as a singularly perturbed system with fast prey dynamics and slow dynamics of the predators. In a parameter regime near singular Hopf bifurcation, chaotic mixed-mode oscillations, featuring concatenation of small and large-amplitude oscillations, are observed as long transients before the system approaches its asymptotic state. To analyze the dynamical cause that initiates a large-amplitude oscillation, the model is reduced to a suitable normal form near the singular-Hopf point. The analysis is then used to determine whether the system exhibits a major population fluctuation, and also predict the timing of the transition to the asymptotic state.

6. Revealing the Russian information operation networks structure using a predictive model

Sachith Dassanayaka, Texas Tech University

ABSTRACT. Information operations by foreign adversaries pose a meaningful threat to democratic processes. Given the increased frequency of this type of threat, understanding those operations is paramount in the effort of combating their influence. Building on existing scholarship on the inner functions within those influence networks on social media, we suggest a new approach to map those type of operations. Using Twitter content identified as part of Russian influence network we created a predictive model to map the network operations. We classify accounts type based on their authenticity function for a sub-sample of accounts and trained AI to identify similar patterns of behavior across the network. Our method model attains 88% prediction accuracy for the test set. We validate our predicted results set by comparing the similarities with the 3 million Russian troll tweets dataset. The result indicates 91% similarity between the two datasets and overall, 82% success within our dataset. The predictive and validation results suggest that our neural network model can use to identify the tweets actors.

CP: Contributed Presentations (Part III)

CHAIR: Fan Bai Florida State University

TALKS1. Take-away impartial combinatorial game on different geometric and dis-
crete structures

Molena Nguyen, North Carolina State University

ABSTRACT. From the standard Take-Away Impartial Combinatorial Game on only Oddly Uniform or Evenly Uniform Hypergraphs in the Ph.D. Dissertation of Dr. Kristen Barnard (an Assistant Professor of Mathematics at Berea College), during this research experience, I found the winning strategy for the standard Take-Away Game on neither Oddly nor Evenly Uniform Hypergraphs. However, these extended neither Oddly nor Even Uniform Hypergraphs must meet the special requirements given. In a standard Take-Away Game, two players take turns to remove the vertices and the hyperedges of a hypergraph. In each turn, a player must remove either only one vertex or only one hyperedge. When one vertex is chosen to be removed, all hyperedges that contain the chosen vertex are also removed. When one hyperedge is chosen to be removed, only that chosen hyperedge is removed. All of the new theorems in this research paper are the extended versions of the theorems in Dr. Kristen Barnard's PhD Dissertation.

2. SPDE-Net A neural network way to solve singularly perturbed partial differential equations

Sangeeta Yadav, Indian Institute of Science

ABSTRACT. Numerical techniques and neural network based PDE solvers are both inadequate to solve singularly perturbed differential equations (SPDE). Both of these techniques give spurious oscillation in the numerical solution in the presence of boundary layers. Stabilization techniques are often employed to reduce the spurious oscillations, but the accuracy of the stabilization technique is limited by the availability of a user chosen stabilization parameter(τ). We introduce SPDE-Net- a neural network cum finite element technique to solve singularly perturbed partial differential equations. In this talk, we will explain our contributions for learning stabilization parameter for Streamline Upwind Petrov Galerkin technique using deep learning. The prediction task is solved in a regression setup. All of the proposed techniques, perform better than state-of-the-art neural network based PDE solvers such as Physics Informed Neural Network (PINNs)

3. Partitioned solution of a coupled ROM-FEM model for a transmission problem

Amy de Castro, Clemson University, SIP at Sandia National Labs

ABSTRACT. Application of reduced order modeling (ROM) on select subdomains can help to increase the computational efficiency of multiphysics simulations. We develop a partitioned scheme for a model interface problem which couples a ROM with a conventional finite element method. The proper orthogonal decomposition (POD) approach is implemented to construct a low-dimensional reduced basis on half the domain and solve the subdomain problem in terms of this basis. The ROM solution is then coupled to the FEM solution using a Lagrange multiplier representing the interface flux. The multiplier at the current time step can be expressed as an implicit function of the state solutions through a Schur complement. As a result, application of an explicit time integration scheme decouples the subdomain problems, allowing their independent solution for the next time step. We present some numerical examples to illustrate this approach.

4. A theoretical investigation of a frequency-dependent regulation of axonal growth

Fan Bai, Florida State University

ABSTRACT. A delayed feedback model is developed based on a frequency-dependent axonal length sensing mechanism, in which two chemical signals interact and oscillate with the help of bidirectional transportation of kinesin and dynein motors. The delays and currents of the motors in the model are derived by analyzing a Totally Asymmetric Simple Exclusion Process (TASEP). Bifurcation analysis of the model shows that signal oscillations emerge via a supercritical Hopf bifurcation due to delayed negative feedback. This results in inhibition of the axonal growth, which becomes stronger as the length increases. The model is tested using two previous experimental manipulations. In one, axon growth rate is reduced by reducing the binding affinity between the motors and one of the signaling molecules. In another, where the density of motors was reduced, caused an increase in the length of the axon. The model replicates both results, and we explain why. In summary, the model demonstrates that axon length can be regulated by information encoded in the frequency of oscillations in signaling molecules carried along axonal microtubules.

5. Fast geometric method for approximating high dimensional kernel matrices

Difeng Cai, Emory Universityy

ABSTRACT. In data science, a major computational bottleneck is how to efficiently manipulate the correlation of large-scale high dimensional data in machine learning tasks. In this talk, we present a novel geometric approach to compute low-rank approximation to kernel matrix with high dimensional data. The algorithm first extracts a small subset of the data and then computes matrix factorization. It does not require any access to the matrix and runs in linear complexity. Theoretically, we derive universal error bounds for the subset selection-based low-rank approximation for kernel matrices, valid for all subset selection schemes. The bound also provides a guideline for choosing good subsets: evenly distributed points are better for approximation. Extensive experiments are performed to demonstrate the advantages of the proposed method. The results show that the new method generates achieves significantly better accuracy, speed, and robustness.

CP: Contributed Presentations (Part IV)

CHAIR: Kwadwo Antwi-Fordjour Samford University

TALKS 1. Steklov-Poincaré analysis of the basic three-domain stent problem

DETAILS: Irving Martínez, Emory University

ABSTRACT. The Steklov-Poincaré problem was previously considered in the artery lumen and wall setting with a single interface. Here the analysis is expanded to incorporate solute behavior in the presence of a fixed-volume, solid, simple stent. In this geometry, a third domain is added to the two-domain structure of wall and artery. Through this intersecting domain volume setting there are three interfaces: lumen-wall, stent-lumen, and wall-stent. Steady-state incompressible Navier-Stokes equations are used to explain the behavior of blood through the lumen, while advection-diffusion dynamics are considered for the solute mechanics across the lumen, wall, and stent. Having a fixed blood velocity value, Steklov-Poincaré decomposition of the advection-diffusion equations is applied locally to each of the interfaces. To unify these instances on a global scale, their overall intersection is explored in a smaller manifold, reducing the problem to one previously solved by Quarteroni, Veneziani, and Zunino. Through finite element analysis (FEM), the solution is discretized and found to be convergent. Finally, computational simulations with one, three, and five stent rings, placed between the volumes of inner and outer cylindrical meshes, were performed using NGSolve, confirming the convergence of the solution and its relation to the coarseness of the mesh.

2. A A least-squares conjugate-gradient finite element method solver for velocity-current MHD equations

K. Daniel Brauss, Francis Marion University

ABSTRACT. Due to the symmetry of weak formulations for the stationary Navier-Stokes equations and the stationary velocity-current magnetohydrodynamic (MHD) equations studied by A.J. Meir and Paul G. Schmidt, we propose a least squares formulation and numerical approximation method for the stationary velocity-current MHD equations. The least squares algorithm is based on the work of Roland Glowinski and fellow authors. The parallel finite element method (FEM) solver utilizes the open-source, C++ software library deal.II to wrap into freely available software libraries: p4est and Trilinos. A block-diagonal preconditioner is utilized for convergence of the conjugate gradient algorithm. The weak formulation, finite-dimensional approximation, and implementation aspects are discussed.

3. Deep neural network for nonlinear regression and its applications in climate and turbulence modeling

Dongwei Chen, Clemson University

ABSTRACT. Deep learning has made extraordinary processes in science and engineering recently. Particularly convolutional neural networks have been successfully applied into image process as convolution could extract features of images and reduce redundant information, improving the computation efficiency. However, due to the localness of convolution kernels and the independence of input features, convolutional neural networks may lose critical information from input variables. Therefore convolutional neural networks are not suitable for nonlinear regression tasks. Based on the architectures of ResNet and DenseNet, this paper develops novel deep neural networks for nonlinear regression. Convolutional layers and pooling layers of the original convolutional neural networks are replaced by fully connected layers, and the residual shortcuts and dense concatenation connection are kept in ResNet and DenseNet, respectively [1, 2]. This avoids gradient vanishing and guarantees feature reuse, and makes the deep regression models have better convergence performance. The new deep regression models are carefully validated on simulated data, and the results give optimal parameters for ResNet regression and DenseNet regression. In addition, we also compare the two optimal regression models with other baseline techniques, such as linear models, decision tree, and support vector machine. It turns out that both DenseNet regression and ResNet model outperform other regression methods listed above. In the end, we apply the DenseNet regression and ResNet regression to predict relative humidity, and the outcome shows high accuracy, which indicates that DenseNet regression and ResNet regression could be used in practice and advance data analysis. Finally, ResNet regression is employed to derive a data-driven model of a subgrid scale (SGS) closure of Large Eddy Simulation (LES) for turbulent premixed combustion [3]. The result illustrates that the proposed data-driven subgrid model to represent the non-linear unresolved terms is a successful approximation. Only fully local values in the filtered domain suffice to yield good agreement with direct numerical simulation (DNS) results. This contrasts with earlier attempts, which use the full LES domain dataset as input to the network.

[1] Chen, Dongwei, Fei Hu, Guokui Nian, and Tiantian Yang. 2020. "Deep Residual Learning for Nonlinear Regression." Entropy 22, no. 2: 193.

[2] Jiang, Chao, Canchen Jiang, Dongwei Chen and Fei Hu. 2021. "Densely connected neural networks for nonlinear regression." Environmental Modelling & Software (under review)

[3] Shin, Junsu, Yipeng Ge, Arne Lampmann, and Michael Pfitzner. "A data-driven subgrid scale model in Large Eddy Simulation of turbulent premixed combustion." Combustion and Flame 231 (2021): 111486.

4. Even and Odd Decomposition of the Bernstein Polynomial Operators in C[-1,1]

Ted Kilgore, Auburn University

ABSTRACT. To decompose the Bernstein polynomial operators in C[-1, 1] into an even part and an odd part may sometimes reduce error. Two different methods for doing such decompositions will be described.

Poster Presentations

TALKS 1. Convergence of a diffuse interface Poisson-Boltzmann (PB) model to DETAILS: the sharp interface PB Model: a unified regularization formulation Mathematical Mathmaterees Mathematical Mathematical Mathematic

Mark McGowan, University of Alabama

ABSTRACT. Both the sharp interface and diffuse interface Poisson-Boltzmann (PB) models have been developed in the literature for studying electrostatic interaction between a solute molecule and its surrounding solvent environment. In the mathematical analysis and numerical computation for these PB models, a significant challenge is due to singular charge sources in terms of Dirac delta distributions. Recently, based on various regularization schemes for the sharp interface PB equation, the first regularization method for the diffuse interface PB model has been developed in [S. Wang, E. Alexov, and S. Zhao, Mathematical Biosciences and Engineering, 18, 1370-1405, (2021)] for analytically treating the singular charges. This work concerns with the convergence of a diffuse interface PB model to the sharp interface PB model, as the diffused Gaussian-convolution surface (GCS) approaches to the sharp solvent accessible surface (SAS). Due to the limitation in numerical algorithm and mesh resolution, such a convergence is impossible to be verified numerically. Through analyzing the weak solution for the regularized PB equations, the convergences for both the reaction-field potential and electrostatic free energy are rigorously proved in this work. Moreover, this study provides a unified regularization for both sharp interface and diffuse interface PB models, and clarifies the connection between this unified formulation and the existing regularizations. This lays a theoretical foundation to develop regularization for more complicated PB models.

2. A FFT accelerated high order finite difference method for elliptic boundary value problems over irregular domains

Yiming Ren, The University of Alabama

ABSTRACT. For elliptic boundary value problems (BVPs) involving irregular domains and Robin boundary condition, no numerical method is known to deliver a fourth order convergence and $O(N \log N)$ efficiency, where N stands for the total degree-of-freedom of the system. Based on the matched interface and boundary (MIB) and fast Fourier transform (FFT) schemes, a new finite difference method is introduced for such problems, which involves two main components. First, a ray-casting MIB scheme is proposed to handle different types of boundary conditions, including Dirichlet, Neumann, Robin, and their mix combinations. By enclosing the concerned irregular domain by a large enough cubic domain, the ray-casting MIB scheme generates necessary fictitious values outside the irregular domain by imposing boundary conditions along the normal direction of the boundary, so that a high order central difference discretization of the Laplacian can be formed. Second, an augmented MIB formulation is built, in which Cartesian derivative jumps are reconstructed on the boundary as auxiliary variables. By treating such variables as unknowns, the discrete Laplacian can be efficiently inverted by the FFT algorithm, in the Schur complement solution of the augmented system. The accuracy and efficiency of the proposed augmented MIB method are numerically examined by considering various elliptic BVPs in two and three dimensions. Numerical results indicate that the new algorithm not only achieves a fourth order of accuracy in treating irregular domains and complex boundary conditions, but also maintains the FFT efficiency.

3. Damped waves propagation on moving meshes: An application in cardiac electrophysiology simulation

Cesar Acosta-Minoli, Universidad del Quindio

ABSTRACT. Research on cardiac electrophysiology driven discovery of the secrets of the heart. This vital organ is in charge of the efficient pumping of blood, which requires that its tissue contracts in coordination in space in such a way that it can change its shape;

An electrical stimulus causes this contraction process that spreads through all cardiac cells coherently and orderly. Disorders in the rhythm of pumping or heart rhythm are known as a disease called arrhythmia, linked to the heart's electrical activity that is diagnosed with the electrocardiogram (ECG).

In this presentation, we develop and implement an algorithm based on a high-order numerical precision method to model the electromechanical activity of the heart. To describe the cardiac electrophysiology activity, we use a two-dimensional hyperbolic monodomain model. Then we discretize by using a discontinuous Galerkin spectral element in space and a Runge Kutta of Williamson. Finally, to simulate the motion of the heart's tissue, we derive the method on moving meshes. We present a time step refinement study to validate approximations. A test problem includes a two-dimensional simulation of a cross-section of the heart.