5th Annual Meeting

SIAM TX-LA Section

November 4–6, 2022

University of Houston, Houston, TX, USA

PROGRAM & ABSTRACTS

Organized by

Department of Mathematics, University of Houston
SIAM TX-LA

Sponsored by

Society for Industrial and Applied Mathematics

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University of Houston Organizing Committee

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John Zweck, Department of Mathematical Sciences, The University of Texas at Dallas

Program Summary

Friday, November 4, 2022

02:00–05:30 **Registration** Location: CBB (Main Entrance)

03:00–05:00 **Mini-symposia** p6

04:00–05:00 **Career Panel** Location: CEMO 100D

Panelists: Dr. Detlef Hohl (Shell)
Dr. Youzuo Lin (Los Alamos National Laboratory)
Dr. Rami Nammour (TotalEnergies)
Dr. Annalisa Quanini (University of Houston)
Dr. Carol Woodward (Lawrence Livermore National Laboratory)

05:00–05:30 **Refreshments** Location: CBB (Main Entrance)

05:30–06:30 **Plenary lecture** Location: CEMO 100D p31

Title: Content-based image retrieval for industrial material with deep learning
Speaker: Dr. Detlef Hohl, Chief Scientist
Computation and Data Science
Shell

Saturday, November 5, 2022

08:00–11:00 **Registration** Location: CBB (Main Entrance)

08:30–10:30 **Mini-symposia** p8

10:30–11:00 **Coffee Break** Location: Houston Room, Student Center South

11:00–12:00 **Plenary Lecture** Location: CEMO 100D p31

Title: Time integration methods and software for scientific simulations
Speaker: Dr. Carol Woodward, Distinguished Member of the Technical Staff
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory

12:30–01:30 **Poster Session and Lunch** Location: Houston Room, Student Center South p111
12:30–01:30 **Mentoring Event** Location: Houston Room, Student Center South

01:30–03:30 **Mini-symposia** p13

01:30–03:30 **Tutorial** Location: CEMO 100D p110

03:30–04:30 **Plenary Lecture** Location: CEMO 100D p31

Title: Beyond forward simulations: From reduced-order models to digital twins with computational science
Speaker: Dr. Karen E. Willcox, Director
Oden Institute for Computational Engineering and Sciences
The University of Texas at Austin

04:30–06:30 **Mini-symposia** p18

06:30–07:30 **Banquet** Location: Houston Room, Student Center South

07:30– **Poster Session** Location: Houston Room, Student Center South p111

Sunday, November 6, 2022

08:30–10:30	**Mini-symposia**	p22
10:30–11:00	**Coffee Break** Location: Houston Room, Student Center South	
11:00–12:00	**Plenary Lecture** Location: CEMO 100D **Title: Some recent results on wave turbulence theory** **Speaker: Dr. Minh-Binh Tran**, Assistant Professor Department of Mathematics Texas A&M	p31
12:00–01:00	**Lunch** Location: Houston Room, Student Center South	
01:00–03:00	**Mini-symposia**	p26

Program

Mini-symposia: Friday 03:00–05:00

Special Topics in Mathematical Biology
Organizers: Summer Atkins & Hayriye Gulbudak p85
Location: CBB 118

(a) *Complexities of the Cytoskeleton: Integration of Scales*.
Keisha Cook (School of Mathematical and Statistical Sciences, Clemson University, Clemson, South Carolina, USA).

(b) *Population dynamics under environmental and demographic stochasticity*.
Alexandru Hening[1]*, Weiwei Qi[2], Zhongwei Shen[2] and Yingfei Yi[2] (1: Department of Mathematics, Texas A&M University, College Station, Texas, USA. 2: Department of Mathematics, University of Alberta, Edmonton, CA).

(c) *Effect of cross-immunity in a multi-strain cholera model*.
Leah LeJeune*, Cameron Browne (Department of Mathematics, University of Louisiana at Lafayette, Lafayette, Louisiana, USA).

Challenges and opportunities in computational science and engineering: Perspectives from data-driven learning and model reduction
Organizers: Ionut Farcas, Marco Tezzele & Aniketh Kalur p97
Location: CBB 120

(a) *Reduced Order Modeling for a LES filtering approach*.
M. Girfoglio[1], A. Quaini[2] & G. Rozza[1] (1: International School for Advanced Studies, 2: University of Houston).

(b) *Adaptive Model Order Reduction for Turbulent Reacting Flows*.
Cheng Huang[1] (1: University of Kansas).

(c) *A low-order nonlinear model of a stalled airfoil from data: Exploiting sparse regression with physical constraints*.
A. Leonid Heide[1], Katherine J. Asztalos[2], Scott T. M. Dawson[2] & Maziar S. Hemati[1] (1: University of Minnesota, 2: Illinois Institute of Technology).

(d) *Dimensionality reduction for spatial-temporal fields beyond POD and CNN*.
Shaowu Pan[1,2], Steve Brunton[2] & Nathan Kutz[2] (1: Rensselaer Polytechnic Institute, 2: University of Washington, Seattle).

Scientific Deep Learning
Organizers: Hai Nguyen, Tan Bui-Thanh & C. G. Krishnanunni p93
Location: CBB 122

(a) *Deep Learning of the Evolution of Unknown Systems*.
Victor Churchill and Dongbin Xiu (The Ohio State University).

(b) *Development of a Physics-Informed Machine Learning Method for Pressure Transient Test*.
Daniel Badawi and Eduardo Gildin (Petroleum Engineering Department, Texas A&M University).

(c) *Learning Data-driven Subgrid-Scale Models: Stability, Extrapolation, and Interpretation*.
Pedram Hassanzadeh, Yifei Guan, Ashesh Chattopadhyay and Adam Subel (Rice University).

(d) *Deep Learning Enhanced Geophysical Inversion Schemes*.
Jiefu Chen, Yanyan Hu, Xuqing Wu and Yueqin Huang (University of Houston).

Mathematics and Computation in Biomedicine
Organizers: Sebastian Acosta and Charles Puelz p62
Location: CBB 124

(a) *Stochastics epidemic models with infection-age dependent infectivity in large populations*.
Guodong (Gordon) Pang (Rice University).

(b) *On the endemic behavior of a competitive tri-virus SIS networked model*.
Sebin Gracy, Mengbin Ye, Brian D.O. Anderson, and Cesar A. Uribe (Rice University).

(c) *Mechanistic models of Alzheimer's disease*.
Travis B. Thompson (Texas Tech University).

(d) *Image-calibrated dynamic system for tau propagation in Alzheimer's disease*.
Zheyu Wen, Ali Ghafouri, George Biros (The University of Texas at Austin).

High Order Methods for Computational Hydrodynamics
Organizers: Madison Sheridan & Bennett Clayton p89
Location: CBB 214

(a) *Energy stable state redistribution cut-cell discontinuous Galerkin methods for wave propagation*.
Christina G. Taylor[1] and Jesse Chan[1] (1: Rice University).

(b) *Robust and efficient approximation of the compressible Navier-Stokes equations*.
Matthias Maier (1: Department of Mathematics, Texas A&M University).

(c) *A second order invariant domain preserving method for the compressible Euler equations with a tabulated equation of state*.
Bennett Clayton[1], Jean-Luc Guermond[1], Matthias Maier[1], Bojan Popov[1], Eric Tovar[2] (1: Department of Mathematics, Texas A&M University 3368 TAMU, College Station, TX 77843, USA. 2: X Computational Physics, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM, 87545, USA).

(d) *High-order methods for nonlinear wave equations in second order form*.
Thomas Hagstrom (Southern Methodist University).

Recent advances in large-scale inverse problems: Numerics, theory, and applications
Organizer: Alexander Mamonov, Andreas Mang & Daniel Onofrei p33
Location: CEMO 101

(a) *Inverse problems of subsurface flows with low permeability fault structures*.
Jeonghun (John) Lee (Department of Mathematics, Baylor University).

(b) *Spatio-temporal quantification of pathological tau spreading in Alzheimer's disease*.
Zheyu Wen, Ali Ghafouri & George Biros (Oden Institute, The University of Texas at Austin).

(c) *An inverse solver for a multispecies tumor growth model*.
Ali Ghafouri & George Biros (Oden Institute, The University of Texas at Austin).

(d) *Deep generative models and accelerated MRI*.
Brett Levac, Alexandros G. Dimaki & Jon Tamir (Department of Electrical and Computer Engineering, The University of Texas at Austin).

Mini-symposia: Saturday 08:30–10:30

Mathematical physics and graph theory

Organizers: R. Han, J. Fillman & S. Shipman p53
Location: CBB 104

(a) *Eigenvalue statistics for the disordered Hubbard model within Hartree-Fock theory*.
Rodrigo Matos (Texas A&M University).

(b) *A spectral statistic of quantum graphs without the semiclassical limit*.
Jon Harrison (Baylor University).

(c) *Limit-Periodic Dirac Operators with Thin Spectra*.
Milivoje Lukić (Rice University).

(d) *Analytic tongue boundaries and Cantor spectrum*.
Long Li (Rice University).

Stability of Solitary Waves with applications to Optics and Fluids

Organizers: Brian Choi & Ross Parker p84
Location: CBB 106

(a) *Pure Quartic Solitons in Novel Laser Designs*.
Sabrina Hetzel (Southern Methodist University).

(b) *Stability of Ginzburg-Landau Solitons via Fredholm determinants of a Green's operator*.
Erika Gallo[1], John Zweck[1], and Yuri Latushkin[2] (1: University of Texas at Dallas, 2: University of Missouri).

(c) *Bright and Dark Multi-Solitons in a Fourth-Order Nonlinear Schrödinger Equation*.
Ross Parker, Alejandro Aceves (Southern Methodist University).

(d) *Continuum limit of 2-d Nonlinear Schr̈dinger Equation*.
Brian Choi, Alejandro Aceves (Southern Methodist University).

Recent Advances in Reduced Order Models

Organizers: Matthias Heinkenschloss p68
Location: CBB 108

(a) *Operator inference for non-intrusive model reduction with quadratic manifolds*.
Rudy Geelen[1] and Stephen Wright[2] and Karen Willcox[1] (1: University of Texas at Austin, 2: University of Wisconsin-Madison).

(b) *A fast and accurate domain-decomposition nonlinear reduced order model using shallow masked autoencoders*.
Alejandro N. Diaz (Rice University).

(c) *Stabilization of linear time-varying reduced order models, a feedback controller approach*.
Rambod Mojgani and Maciej Balajewicz (Rice University).

(d) *The Loewner framework in the time-domain*.
A. C. Antoulas (Rice University Houston and Max-Planck Institute Magdeburg).

Modeling, analysis and numerical simulations involving thin structures

Organizers: F. Marazzato, A. Bonito, A. Quaini, M. Olshanskii & F. Marazzato p41
Location: CBB 110

(a) *A Descent Scheme for Thick Elastic Curves with Self-contact and Container Constraints*.
Shawn Walker (Louisiana State university).

(b) *Finite Element Approximation of a Membrane Model for Liquid Crystal Polymeric Networks*.
Lucas Bouck (University of Maryland).

(c) *The Preasymptotic Model of Prestrained Plates*.
Angelique Morvant (Texas A&M University).

(d) *Mixed quasi-trace surface finite element methods*.
Alan Demlow (Texas A&M University).

Special Topics in Mathematical Biology
Organizers: Summer Atkins & Hayriye Gulbudak p85
Location: CBB 118

(a) *Multistationarity and concentration robustness in biochemical reaction networks*.
Badal Joshi[1], Nidhi Kaihnsa[2], Tung D. Nguyen[3]*, Anne Shiu[3] (1: California State University, San Marcos. 2: Brown University. 3: Texas A&M University).

(b) *A switch point algorithm applied to a harvesting problem*.
S. Atkins [1]*, M. Martcheva[2], and W. Hager[2] (1: Department of Mathematics, Louisiana State University, Baton Rouge, Louisiana, USA. 2: Department of Mathematics, University of Florida, Gainesville, Florida, USA).

Challenges and opportunities in computational science and engineering: Perspectives from data-driven learning and model reduction
Organizers: Ionut Farcas, Marco Tezzele & Aniketh Kalur p97
Location: CBB 120

(a) *Discovering Model Error with interpretability and Data-Assimilation: Sparse observations of multi-scale flows*.
Rambod Mojgani[1], Ashesh Chattopadhyay[1], Pedram Hassanzadeh[1] (1: Rice University).

(b) *Compiler-based Differentiable Programming for Accelerated Simulations*.
Ludger Paehler[1,2] and Jan Hueckelheim[2] and Johannes Doerfert[3] (1: Technical University of Munich, 2: Argonne National Laboratory, 3: Lawrence Livermore National Laboratory).

(c) *Advances in parameter space reduction with applications in naval engineering*.
M. Tezzele[1] and G. Rozza[2] (1: University of Texas at Austin, 2: International School for Advanced Studies).

Scientific Deep Learning
Organizers: Hai Nguyen, Tan Bui-Thanh & C. G. Krishnanunni p93
Location: CBB 122

(a) *A Model-Constrained Tangent Manifold Learning Approach for Dynamical Systems*.
Hai Nguyen and Tan Bui-Thanh (University of Texas at Austin).

(b) *Exploiting the local parabolic landscapes of adversarial losses to accelerate black-box adversarial attack*.
Hoang Tran, Dan Lu and Guannan Zhang (1: Oak Ridge National Laboratory).

(c) *The approximation of the wave equation operator using deep learning*.
Ziad Aldirany[1], Marc Laforest[1], Régis Cottereau[2] and Serge Prudhomme[1] (1: Polytechnique Montréal, 2: Centrale Marseille).

(d) *Strengthening Gradient Descent by Sequential Motion Optimization for Deep Neural Networks*.
Thang Duc-Le[1], Quoc-Hung Nguyen[2], Jaehong Lee[1] and H. Nguyen-Xuan[3] (1: Deep Learning Architecture Research Center, Sejong University, 2: Department of Computational Engineering, Vietnamese-German University, 3: CIRTech Institute, HUTECH University).

Mathematics and Computation in Biomedicine
Organizers: Sebastian Acosta and Charles Puelz p62
Location: CBB 124

(a) *Optimal experimental design for quantitative MRI with MR fingerprinting*.
Bo Zhao, Evan Scope Crafts, and Hengfa Lu (University of Texas at Austin).

(b) *Registering MRA images to 4D flow MRI images*.
Dan Lior (Baylor College of Medicine).

(c) *Early detection of cardiac arrest in infant with congenital heart defects using convolutional denoising autoencoders*.
Arko Barman, Kunal Rai, Chiraag Kaushik, Frank Yang, Tucker Reinhardt, Andrew Pham, Aneel Damaraju, Mubbasheer Ahmed, Sebastian Acosta, Parag Jain (Rice University and Baylor College of Medicine).

(d) *Generalized broken ray transforms in tomography*.
Gaik Ambartsoumian[1] and Mohammad J. Latifi[2] (1: University of Texas at Arlington, 2: Dartmouth College).

High Order Methods for Computational Hydrodynamics
Organizers: Madison Sheridan & Bennett Clayton p89
Location: CBB 214

(a) *A high-order explicit Runge-Kutta method for approximating the Shallow Water Equations with sources*.
Eric J. Tovar (Los Alamos National Laboratory).

(b) *Modeling Shallow Water Flows through Obstacles with Windows*.
Suncica Canic[1], Alina Chertock[2], Shumo Cui[3], Alexander Kurganov[3], Xin Liu[4], Abdolmajid Mohammadian[4] and Tong Wu[5] (1: University of California, Berkeley, and University of Houston, 2: North Carolina State University, 3: Southern University of Science and Technology, 4: University of Ottawa, and 5: The University of Texas at San Antonio).

(c) *A positivity-preserving and conservative high-order flux reconstruction method for the polyatomic Boltzmann–BGK equation*.
Tarik Dzanic[1] (1: Texas A&M University).

(d) *Greedy invariant-domain preserving approximation for hyperbolic system*.
J.-L. Guermond[1], M. Maier[1], B. Popov[1], L. Saavedra[2], I. Tomas[3] (1: Department of Mathematics, Texas A&M University, 3368 TAMU, College Station, TX 77843, USA. 2: Departamento de Matemática Aplicada a la Ingeniería Aeroespacial, E.T.S.I. Aeronáutica y del Espacio, Universidad Politécnica de Madrid, 28040 Madrid, Spain. 3: Department of Mathematics and Statistics, Texas Tech University, 2500 Broadway Lubbock, TX 79409, USA.).

Recent advances in large-scale inverse problems: Numerics, theory, and applications
Organizer: Alexander Mamonov, Andreas Mang & Daniel Onofrei p33
Location: CEMO 101

(a) ~~*Some results on inverse problems to elliptic PDEs with solution data and their implications in operator learning*~~.
~~Kui Ren~~ (~~Department of Applied Physics and Applied Mathematics and Data Science Institute, Columbia University~~; Talk Cancelled).

(b) ~~*Estimating the noise level in seismic data while overcoming cycle skipping*~~.
~~Susan Minkoff[1], Huiyi Chen[1] & William Symes[2]~~ (~~1: Department of Mathematical Sciences, University of Texas at Dallas, 2: Department of Computational and Applied Mathematics, Rice University~~; Talk Cancelled).

(c) *Fast approximations of high-rank Hessians: Applications to seismic inversion and uncertainty quantification*.
Mathew Hu[1,*], Nick Alger[1], Longfei Gao[1], Omar Ghattas[1] & Rami Nammour[2] (1: Oden Institute, The University of Texas at Austin; 2: Total E&P Research and Technology; Updated).

(d) *Matrix-free PSF approximation of ice-sheet Hessians*.
Nick Alger[1,*], Tucker Hartland[2], Noemi Petra[2], Omar Ghattas[1] (1: Oden Institute, The University of Texas at Austin; 2: Applied Mathematics, University of California, Merced; Updated).

(e) *Conductivity imaging from thermal noise*.
Trent DeGiovanni & Fernando Guevara Vasquez (University of Utah).

(f) *Lippmann–Schwinger–Lanczos algorithm for inverse scattering problems*.
V. Druskin[1], S. Moskow[2] & M. Zaslavsky[3] (1: Department of Mathematical Sciences, Worcester Polytechnic Institute, 2: Department of Mathematics, Drexel University, 3: Schlumberger-Doll Research Center).

Applications and Computation in Algebraic Geometry
Organizers: Jordy Lopez Garcia, Josué Tonelli-Cueto & Thomas Yahl p102
Location: CEMO 105

(a) *On the geometry of geometric rank*.
Runshi Geng[1] (1: Texas A&M University).

(b) *Approximate Rank for Real Symmetric Tensors*.
Alperen Ergur[1] (1: University of Texas at San Antonio).

(c) *Computing Galois groups of Fano problems*.
Thomas Yahl[1] (1: Texas A&M University).

(d) *The Point Scheme and Line Scheme of a Certain Quadratic Quantum* $\mathbb{P}^3$.
José Lozano[1] (1: University of Texas at Arlington).

Numerical methods and applications for geosciences
Organizers: G. Sosa Jones & L. Cappanera p60
Location: CEMO 109

(a) *Coupling and decoupling two-phase flows in superposed free flow and porous media*.
Daozhi Han (University at Buffalo).

(b) *Finite element methods of porous media flows with low permeability faults/membranes*.
Jeonghun Lee (Baylor University).

(c) *Finite element methods for incompressible flows with variable density applied to thermodynamics.*.
An Vu (University of Houston).

(d) *Convergence Analysis of a Continuous Interior Penalty Method for the Modified Phase Field Crystal Equation*.
Natasha Sharma[1], Amanda E. Diegel[2], Daniel Bond[3] (1: University of Texas at El Paso, 2: Mississippi State University, 3: University of Tennessee).

Mini-symposia: Saturday 01:30–03:30

Mathematical physics and graph theory

Organizers: R. Han, J. Fillman & S. Shipman p53
Location: CBB 104

(a) *Inverse Uniqueness Result for Hamiltonian System with Measure Coefficients*.
Chunyi Wang (Rice University).

(b) *Hyponormal Toeplitz Operators Acting on the Bergman Space*.
Brian Simanek (Baylor University).

(c) *Fermi Isospectrality*.
Frank Sottile (Texas A&M University).

(d) *Quantum Complexity of Permutations*.
Andrew Yu (Phillips Academy - Andover).

Mathematical modeling for biological dynamics

Organizers: Zhuolin Qu, Lale Asik & Xiang-Sheng Wang p38
Location: CBB 106

(a) *Stochastic Avian Influenza Model*.
U. Bulut[1], T. Oraby[2], and E. Suazo[2] (1: University of the Incarnate Word, 2: The University of Texas Rio Grande Valley).

(b) *Multiscale Modeling of Infectious Disease: The Case of Malaria*.
Juan B. Gutiérrez[1] (1: University of Texas at San Antonio).

(c) *Reconciling contrasting effects of nitrogen on pathogen transmission and host immunity using stoichiometric models* .
Dedmer B. Van de Waal [1,2], Lauren A. White [3], Rebecca Everett[4], Lale Asik[5,6], Elizabeth T. Borer[7], Thijs Frenken [1,8], Angélica L. González[9], Rachel Paseka[7], Eric W. Seabloom[7], Alexander T. Strauss [7,10], and Angela Peace [6] (1: Department of Aquatic Ecology, Netherlands Institute of Ecology (NIOO-KNAW), Wageningen, The Netherlands, 2: Department of Freshwater and Marine Ecology, Institute for Biodiversity and Ecosystem Dynamics, University of Amsterdam, Amsterdam, The Netherlands, 3: National Socio-Environmental Synthesis Center (SESYNC), University of Maryland, Annapolis, MD, US, 4:Department of Mathematics and Statistics, Haverford College, Haverford, PA, USA, 5: Department of Mathematics and Statistics, University of the Incarnate Word, San Antonio, TX, USA, 6: Department of Mathematics and Statistics, Texas Tech University, Lubbock, TX, USA, 7: Department of Ecology, Evolution, and Behavior, University of Minnesota, St. Paul, MN, USA, 8: Great Lakes Institute for Environmental Research (GLIER), University of Windsor, Windsor, ON, Canada, 9: Department of Biology and Center for Computational and Integrative Biology, Rutgers University, Camden, NJ, US, 10: Odum School of Ecology. University of Georgia, Athens, GA, USA).

(d) *Modeling Immunity to Malaria with an Age-Structured PDE Framework*.
Zhuolin Qu[1], Denis Patterson[2], Lauren Childs[3], Christina Edholm[4], Joan Ponce[5], Olivia Prosper[6], and Lihong Zhao[7] (1: University of Texas at San Antonio, 2: Princeton University, 3: Virginia Tech, 4: Scripps College, 5: University of California, Los Angeles, 6: University of Tennessee, Knoxville, 7: University of California, Merced).

Recent Advances in Reduced Order Models
Organizers: Matthias Heinkenschloss p68
Location: CBB 108

(a) *Waveform inversion via reduced order modeling*.
Alexander V. Mamonov[1] and Liliana Borcea[2] and Josselin Garnier[3] and Jörn Zimmerling[4] (1: University of Houston, 2: University of Michigan, 3: Ecole Polytechnique, 4: Uppsala University).

(b) *Line-search methods for unconstrained optimization with inexactness arising from reduced order models*.
Dane Grundvig and Matthias Heinkenschloss (Rice University).

(c) *Filtering in non-intrusive data-driven reduced-order modeling of large-scale systems*.
Ionut-Gabriel Farcas[1], Rayomand P. Gundevia[2], Ramakanth Munipalli[3], and Karen E. Willcox[1] (1: The University of Texas at Austin 2: Jacobs Engineering Group, Inc., 3: Air Force Research Laboratory).

(d) *Gaussian process subspace prediction for model reduction*.
Ruda Zhang[1], Simon Mak[2], and David Dunson[2] (1: University of Houston, 2: Duke University).

Modeling, analysis and numerical simulations involving thin structures
Organizers: F. Marazzato, A. Bonito, A. Quaini, M. Olshanskii & F. Marazzato p41
Location: CBB 110

(a) *Convergence of TraceFEM to minimum regularity solutions*.
Lucas Bouck, Ricardo H. Nochetto, Mansur Shakipov[1] and Vladimir Yushutin[2] (1: University of Maryland, 2: Clemson University).

(b) *FEM for surface Navier-Stokes-Cahn-Hilliard equations*.
Yerbol Palzhanov (University of Houston).

(c) *Interpolation based immersogeometric analysis with application to Kirchhoff–Love shells*.
Jennifer Fromm[1], Nils Wunsch[2], Ru Xiang [1], Han Zhao[1], Kurt Maute[2], John A. Evans[2],and David Kamensky[1] (1: University of California San Diego, 2: University of Colorado Boulder).

(d) *Navier-Stokes equations on evolving surfaces*.
A. Reusken, P. Brandner, P. Schwering[1] and M. Olshanskii[2] (1: RWTH Aachen University, 2: University of Houston).

Modeling of air flow and droplet transport for biomedical applications
Organizers: Vladimir Ajaev & Andrea Barreiro p99
Location: CBB 118

(a) *Building the Next-Generation Physiologically Realistic Human Respiratory Digital Twin System for Pulmonary Healthcare*.
Yu Feng (Oklahoma State University).

(b) *Computational Prediction of Transport, Deposition, and Resultant Immune Response of Nasal Spray Vaccine Droplets to Potentially Prevent COVID-19*.
Hamideh Hayati[1], Yu Feng[1], Xiaole Chen[2], Emily Kolewe[3], Catherine Fromen[3] (1:Oklahoma State University2:Nanjing Normal University, China, 3:University of Delaware).

(c) *Analytical Solutions for Fluid Flow and Diffusion around a Slowly Condensing Levitating Liquid Droplet*.
Jacob E. Davis, Vladimir S. Ajaev (Southern Methodist University).

Nonlinear Physics Models and Mathematical Structures
Organizers: Vesselin Vatchev, Zhijun Qiao, Wilson Zuniga Galindo & Erwin Suazo p87
Location: CBB 120

(a) *5th-order CH equation with pseudo-peakons*.
Zhijun Qiao (UT Rio Grande Valley).

(b) *Self-similar transformation and chirped nonlinear waves for the Davey-Stewartson I equation*.
Jiefang Zhang (Communication University of Zhejiang,Hangzhou 310018,China).

(c) *Interactions of Traveling Waves in Low Order Approximations for the Two-Dimensional Euler Equations* .
Julio Paez (UT Rio Grande Valley).

(d) *Engineered Approximate Solutions to the Two-Dimensional Euler Equations*.
Vesselin Vatchev (UT Rio Grande Valley).

Scientific Deep Learning
Organizers: Hai Nguyen, Tan Bui-Thanh & C. G. Krishnanunni p93
Location: CBB 122

(a) *Leveraging Data-driven Surrogates to Enable Efficient Density Estimation of Sparse Observable Data on Low-dimensional Manifolds*.
Tian Yu Yen and Tim Wildey (Sandia National Laboratories).

(b) *Layerwise Sparsifying Training and Sequential Learning Strategy for Neural Architecture Adaptation*.
C G Krishnanunni and Tan Bui-Thanh (University of Texas at Austin).

(c) *Scalable neural network approximation for high-dimensional inverse problems*.
Jinwoo Go and Peng Chen (Georgia Institute of Technology).

(d) *Finite Expression Method for Solving High-Dimensional PDEs*.
Haizhao Yang (University of Maryland, College Park).

Mathematics and Computation in Biomedicine
Organizers: Sebastian Acosta and Charles Puelz p62
Location: CBB 124

(a) *Estimation of aortic valve interstitial contractile behaviors using an inverse finite element approach*.
Alex Khang and Michael S. Sacks (University of Texas at Austin).

(b) *Control of stochastic signaling pathways in esophageal cancer*.
Souvik Roy, Zui Pan and Zain Khan (University of Texas at Arlington).

(c) *Modeling supraventricular tachycardia using dynamic computer-generated left atrium*.
Bryant Wyatt, Avery Campbell, Gavin McIntosh, and Melanie Little (Tarleton State University).

(d) *A hemodynamic comparison of single ventricle patients*.
Alyssa M. Taylor-LaPole[1], Mitchel J. Colebank[2], Justin D. Weigand[3,4], Mette S. Olufsen[1], Charles Puelz[3,4] (1: NC State University, 2: University of California, Irvine, 3: Baylor College of Medicine, 4: Texas Children's Hospital).

Advances in theory and computation of functional optical materials
Organizers: Matthias Maier & Daniel Massatt p74
Location: CBB 214

(a) *Dirac points for the honeycomb lattice with impenetrable obstacles*.
Junshan Lin[1], Wei Li[2], Hai Zhang[3] (1: Auburn University, 2: DePaul University, 3: Hong Kong University of Science and Technology).

(b) *Optimal control of the Landau–de Gennes model of nematic liquid crystals*.
Shawn Walker[1] and Thomas Surowiec[2] (1: LSU, 2: Philipps University of Marburg).

(c) *Embedded eigenvalues for discrete magnetic Schrödinger operators*.
Jorge Villalobos[1] and Stephen Shipman[1] (1: LSU).

(d) *Effective Impedance Condition for Thin Metasurfaces*.
Zachary Jermain[1], Robert Lipton[1] (1: LSU).

Recent advances in large-scale inverse problems: Numerics, theory, and applications
Organizer: Alexander Mamonov, Andreas Mang & Daniel Onofrei p33
Location: CEMO 101

(a) *Carleman Weighted Hilbert Spaces for Coefficient Inverse Problems*.
Michael V. Klibanov (Department of Mathematics, University of North Carolina at Charlotte).

(b) *New sampling indicator functions for stable imaging of photonic crystals*.
Dinh-Liem Nguyen (Kansas State University).

(c) *Reconstructing a space-dependent source term of the Helmholtz equation via the quasi-reversibility method*.
Loc Hoang Nguyen (Department of Mathematics and Statistics, University of North Carolina at Charlotte).

(d) *Active control of electromagnetic fields in layered media*.
Chaoxian Qi[1,*], Neil Jerome A. Egarguin[2], Daniel Onofrei[3], Jiefu Chen[1] (1: Department of Electrical and Computer Engineering, University of Houston, 2: Institute of Mathematical Sciences and Physics, University of the Philippines Los Baños, 3: Department of Mathematics, University of Houston).

Applications and Computation in Algebraic Geometry
Organizers: Jordy Lopez Garcia, Josué Tonelli-Cueto & Thomas Yahl p102
Location: CEMO 105

(a) *The dimension of the semirings of polynomials and convergent power series.*.
Kalina Mincheva[1], Netanel Friedenberg[2] (1: Tulane University, 2: Tulane University).

(b) *Generating random points uniformly distributed on a parametric curve*.
Josué Tonelli-Cueto[1], Apostolos Chalkis[2], and Christina Katsamaki[3] (1: The University of Texas at San Antonio 2: Quantagonia, 3: Inria Paris & IMJ-PRG).

(c) *Algebraic, Geometric, and Combinatorial Aspects of Unique Model Identification*.
Brandilyn Stigler[1] (1: Southern Methodist University).

(d) *Identifiability of Cycle Compartmental Models With Two Leaks and Identifiability of Submodels*.
Dessauer, Paul R[1], Tanisha Grimsley[2], Jose Lopez[3] (1. Department of Mathematics, University of Texas El Paso, El Paso, Texas 2. Department of Mathematics, Juniata College, Huntingdon, Pennsylvania 3. Department of Mathematics, California State University - Fresno, Fresno, California).

Numerical methods and applications for geosciences
Organizers: G. Sosa Jones & L. Cappanera p60
Location: CEMO 109

(a) *A sequential discontinuous Galerkin method for three-phase flows in porous media*.
Giselle Sosa Jones[1], Loic Cappanera[2], and Beatrice Riviere[3] (1: Oakland University, 2: University of Houston, 3: Rice University).

(b) *Implicit dynamical low rank discontinuous Galerkin methods for space homogeneous neutrino transport equations*.
Peimeng Yin, Eirik Endeve, Cory Hauck, and Stefan Schnake (Oak Ridge National Laboratory).

(c) *Numerical solution of two-phase poroelasticity equations*.
Beatrice Riviere[1] and Boqian Shen[2] (1: Rice University, 2: KAUST).

(d) *Applications of Space-Time Methods to Multiphase Flow in Porous Media : Channel Flow and Snap Shot Selection for Deep-Learning Reduced-Order Models* .
Mary Wheeler[1], Thamer Abbas Alsulaimani[2] and Hanyu Li[3] (1: University of Texas at Austin, 2: Aramco, 3: Lawrence Livermore National Laboratory).

Mini-symposia: Saturday 04:30–06:30

Recent advances of scientific computing and applications

Organizers: Ying Wang p67
Location: CBB 104

(a) *Efficient numerical solutions of Laplace equations with mixed boundary conditions using Steklov eigenfunctions* .
Manki Cho (University of Houston at Clear Lake).

(b) *Exterior Finite Energy Harmonic Functions*.
Giles Auchmuty[1] and Qi Han[2] (1: University of Houston, 2: Texas A&M University-San Antonio).

(c) *Numerical studies to the Chaplygin gas equation*.
Ling Jin[1] and Ying Wang[2] (1: University of Oklahoma, 2: University of Oklahoma).

(d) *Optimal control of Pentadesma fruit harvesting under habitat reduction*.
Benito Chen-Charpentier (University of Texas at Arlington).

Tensor modeling and applications

Organizers: Y. Lou & S. Minkoff p59
Location: CBB 106

(a) *Tensor regularization and reconstruction workflow for time-lapse seismic data*.
Jonathan Popa, Susan E. Minkoff, and Yifei Lou (The University of Texas at Dallas).

(b) *Tensor-tensor algebra for optimal representations and compression of multiway data*.
Misha Kilmer[1] and Lior Horesh[2] and Haim Avron[3] and Elizabeth Newman[4] (1: Tufts University, 2: IBM Research, 3: Tel Aviv University, 4: Emory University).

(c) *Modewise tensor decompositions and applications*.
HanQin Cai[1], Keaton Hamm[2], Longxiu Huang[3], and Deanna Needell[4] (1: University of Central Florida, 2: University of Texas at Arlington, 3: Michigan State University, 4: University of California, Los Angeles).

(d) *Moment Estimation for Nonparametric Mixture Models through Implicit Tensor Decomposition*.
Yifan Zhang, Joe Kileel (University of Texas at Austin).

Deep learning methods for biomedical image analysis & modeling

Organizers: E. Castillo p45
Location: CBB 108

(a) *Respecting Variation in Physician Clinical Practice* .
Steve Jiang (University of Texas Southwestern Medical Center).

(b) *Application of Deep Learning for real-time non-invasive continuous monitoring for enhanced peripheral oxygen saturation in intensive care unit (ICU) and Operating Room (OR)*.
Sungsoo Kim[1,2], Sohee Kwon[1], Alan Bovik[2], Mia Markey[2], and Maxime Cannesson[1] (1: The University of California Los Angeles, 2: The University of Texas at Austin).

(c) *Imaging based estimation of pathology in a large adult glioma population*.
D. Fuentes, E. Gates, A. Celaya, D. Suki, J. Weinberg, S. Prabhu, D. Schellingerhout (The University of Texas MD Anderson Cancer Center).

(d) *Neural Network 'Finite Element' Based Models for Cardiac Simulations*.
Michael Sacks, Shruti Motiwale, and Christian Goodbrake (The University of Texas at Austin).

Modeling, analysis and numerical simulations involving thin structures
Organizers: F. Marazzato, A. Bonito, A. Quaini, M. Olshanskii & F. Marazzato p41
Location: CBB 110

(a) *Continuum field theory for the deformations of planar kirigami*.
Paul Plucinsky[1], Ian Tobasco[2], Yue Zheng[3], and Paolo Celli[4] (1: University of Southern California, 2: University of Illinois Chicago, 3: University of Massachusetts Amherst, 4: Stony Brook University).

(b) *Numerical Approximations of Origami with Curved Creases*.
Andrea Bonito (Texas A&M University).

(c) *The Poisson coefficient of zigzag sums*.
Hussein Nassar[1] and Arthur Lebée[2] (1: University of Missouri, 2: École des Ponts).

(d) *Computation of Miura Surfaces*.
Frederic Marazzato (Louisiana State university).

Modeling of air flow and droplet transport for biomedical applications
Organizers: Vladimir Ajaev & Andrea Barreiro p99
Location: CBB 118

(a) *Predicting Transport and Deposition of Multicomponent E-cigarette Aerosols in a Subject-specific Airway Model with Different Nicotine Forms: An in silico Study*.
Ted Sperry, Yu Feng (Oklahoma State University).

(b) *Mathematical Modeling of Phase Change in Respiratory Droplets*.
Vladimir S. Ajaev, Art Taychameekiatchai, James Barrett (Southern Methodist University).

(c) *Investigating the Impact of Mechanosensation on Retronasal Olfaction*.
Abdullah Saifee[1], Andrea Barreiro[1],Cheng Ly[2],Woodrow Shew[3] (1:Southern Methodist University, 2:Virginia Commonwealth University, 3:University of Arkansas).

Nonlinear Physics Models and Mathematical Structures
Organizers: Vesselin Vatchev, Zhijun Qiao, Wilson Zuniga Galindo & Erwin Suazo p87
Location: CBB 120

(a) *p-Adic Statistical Field Theory and Deep Belief Networks*.
W. A. Zúñiga-Galindo (UT Rio Grande Valley).

(b) *Quantum Control of Qubits and Qutrits*.
Baboucarr Dibba (UT Rio Grande Valley).

(c) *p-adic Cellular Neural Networks: Applications to Image Processing*.
Brian Zambrano (UT Rio Grande Valley).

(d) *Probabilistic solutions of fractional differential and partial differential equations and their Monte Carlo simulations*.
Erwin Suazo (UT Rio Grande Valley).

Physics-based and data-driven models for engineering applications
Organizers: M. Tyagi & Y. Akkutlu p46
Location: CBB 122

(a) *Pseudo-spectral methods for the incompressible magnetohydrodynamics equations with variable density*.
Loic Cappanera (University of Houston).

(b) *Numerical Investigation of Wave Scour Around Group of Vertical Cylinders* .
Haq Murad Nazari and Celalettin Ozdemir (Louisiana State University).

(c) *Data driven modeling of shear-thinning polymer flooding*.
Prabir Daripa (Texas A&M University).

(d) *Physics-Informed Neural Networks for Capacitance-Resistance Models of Reservoir*.
Mayank Tyagi (Louisiana State University).

Mathematics and Computation in Biomedicine
Organizers: Sebastian Acosta and Charles Puelz p62
Location: CBB 124

(a) *Fast algorithms for diffeomorphic image registration*.
Andreas Mang (Department of Mathematics, University of Houston).

(b) *PocketNet: A smaller neural network for medical image analysis*.
Adrian Celaya, Jonas A. Actor, Rajarajeswari Muthusivarajan, Evan Gates, Caroline Chung, Dawid Schellingerhout, Beatrice Riviere, and David Fuentes (Rice University and MD Anderson Cancer Center).

(c) *Optimal transport-based segmentation and classification of ECG signals: Preliminary results and challenges*.
Cesar A Uribe[1], Edward Nguyen[1], Sebastian Acosta[2], Emily Zhang[3], Jelena Lazic[1] (1: Rice University, 2: Baylor College of Medicine, 3: Wellesley College).

(d) *Using deep learning and macroscopic imaging of porcine heart valve leaflets to predict uniaxial stress-strain responses*.
Luis Hector Victor, CJ Barberan, Richard G. Baranuik, and Jane Grande-Allen (Rice University).

Recent Advances of Numerical Simulations for Fluid Flows and Applications
Organizers: Yong Yang & Yonghua Yan p83
Location: CBB 214

(a) *Study on the asymmetrical structure in late transitional boundary layer using DNS and Rortex*.
Yong Yang[1], Yonghua Yan[2], and Caixia Chen[3] (1: West Texas A&M University, 2: Jackson State University, 3: Tougaloo College).

(b) *Numerical study of the vortical structures in MVG controlled supersonic flow under different Mach numbers*.
Yonghua Yan[1], Yong Yang[2], and Shiming Yuan[1] (1: Jackson State University, 2: West Texas A&M University).

(c) *LBM simulation of swallowing process with dysphagia*.
Caixia Chen[1], Yonghua Yan[2], Yong Yang[3], and Demetric L. Barnes[2] (1: Tougaloo College, 2: Jackson State University, 3: West Texas A&M University).

(d) *Power spectrum analysis of the interaction between large vortices and ramp shock waves in MVG controlled supersonic ramp flow*.
Demetric I Banines[1], Yong Yang[2], Shiming Yuan[1], and Yonghua Yan[1] (1: Jackson State University, 2: West Texas A&M University).

Modeling the heart-brain axis and age-related pathology

Organizers: Travis Thompson p76

Location: CEMO 101

(a) *Senescence, Sangre, Senility and Simulation: Mathematics at the intersection of the heart and the brain*.
Travis B. Thompson[1] (1: Department of Mathematics and Statistics, Texas Tech University).

(b) *Multi-scale computational models of cardiac and brain tissues*.
Michael S. Sacks[1] and David S. Li[1] (1:Willerson Center for Cardiovascular Modeling and Simulation, Oden Institute and the Department of Biomedical Engineering, University of Texas at Austin).

(c) *Oscillopathies of Brain and Heart: Lessons From the Computational Medicine Clinic*.
David Paydarfar[1,2] (1: Dell Medical School, Mulva Clinic for the Neurosciences 2: Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin).

Spectral theory of Schrodinger operators and related topics

Organizers: W. Liu, R. Matos & F. Yang p49

Location: CEMO 105

(a) *Some spectral inequality for Schrödinger equations with power growth potentials.*.
Jiuyi Zhu (Louisiana State University).

(b) *1-Dim Half-line Schrödinger Operators with H^{-1} Potentials*.
Xingya Wang (Rice University).

(c) *Continuity of the Lyapunov exponent for analytic multi-frequency quasi-periodic cocycles*.
Matthew Taylor Powell (UC Irvine).

(d) *On the Irreducibility of Bloch and Fermi Varieties*.
Matthew Faust (Texas A&M University).

Hamiltonian and integrable systems

Organizers: B. Feng & T. Ohsawa p58

Location: CEMO 109

(a) *Regularity and Lipschitz optimal transport metric for scalar integrable systems with cusp singularity*.
Geng Chen (University of Kansas).

(b) *Semi-discrete Camassa-Holm and modified Camassa-Holm equations and their connection with the discrete KP equation*.
Baofeng Feng (University of Texas Rio Grande Valley).

(c) *Crack Problem Under Strain Gradient Elasticity Of Bi-Helmholtz Type*.
Youn-Sha Chan (University of Houston-Downtown).

Mini-symposia: Sunday 08:30–10:30

Nonlocal models in mathematics and computation

Organizers: Patrick Diehl, Debdeep Bhattacharya, Burak Aksoylu & Robert P. Lipton p37
Location: CBB 104

(a) *Four Mutual Properties of Classical and Nonlocal Wave Equations*.
Burak Aksoylu (Texas A&M University-San Antonio).

(b) *Macroscopic effects of inter and intra particle dynamics on vehicle dynamics using nonlocal particle based modeling*.
Debdeep Bhattacharya & Robert P. Lipton (Louisiana State University).

(c) *Challenges for coupling approaches for classical linear elasticity and bond-based peridynamic models for non-uniform meshes and damage*.
Patrick Diehl, Serge Prudhomme, Emily Downing & Autumn Edwards (Louisiana State University).

Mathematical modeling for biological dynamics

Organizers: Zhuolin Qu, Lale Asik & Xiang-Sheng Wang p38
Location: CBB 106

(a) *Global Dynamics of Discrete Mathematical Models of Tuberculosis*.
Saber Elaydi[1] and Rene Lozi[2] (1: Trinity University, 2: Universite de Provence Côte d'Azur).

(b) *Population Persistence in Stream Networks: Growth Rate and Biomass*.
T. D. Nguyen[1*], Y. Wu[2], A. Veprauskas[3], T. Tang[4], Y. Zhou[5], C. Beckford[6], B. Chau[7], X. Chen[8], B. D. Rouhani[9], A. Imadh[10], Y. Wu[11], Y. Yang[12], and Z. Shuai[13] (1: Texas A&M University, 2: Middle Tennessee State University, 3: University of Louisiana at Lafayette, 4: San Diego State University, 5: Lafayette College, 6: University of Tennessee, 7: University of Alberta, 8: University of North Carolina at Charlotte, 9: University of Texas at El Paso, 10: University of Central Florida, 11: Georgia State University, 12: The Ohio State University, 13: University of Central Florida).

(c) *Assessing Southern Pine Beetle Infestation Risks Using Agent-Based Modeling*.
John G. Alford[1], William I. Lutterschmidt[1], and Abigail Miller[2] (1: Sam Houston State University, 2: American Institutes for Research).

(d) *Global dynamics of a cholera model with two nonlocal and delayed transmission mechanisms*.
Xiang-Sheng Wang[1] (1: University of Louisiana at Lafayette).

Data-driven and Nonlinear Model Reduction Methods for Physical Sciences and Engineering

Organizers: Rudy Geelen & Shane McQuarrie p104
Location: CBB 108

(a) *A mixture of experts approach for efficient representation of combustion manifolds*.
Ope Owoyele[1,2] Pinaki Pal[2] (1: Argonne National Laboratory, 2: Louisiana State University).

(b) *Neural Ordinary Differential Equations with Physics-Informed Architectures and Constraints for Dynamical Systems Modeling*.
Cyrus Neary[1], Franck Djeumou[1], Eric Goubault[2], Sylvie Putot[2] and Ufuk Topcu[1] (1: University of Texas at Austin, 2: LIX, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, France).

(c) *Derivative informed neural operators for PDE-constrained optimization under uncertainty*.
Dingcheng Luo[1], Thomas O'Leary-Roseberry[1], Peng Chen[2] and Omar Ghattas[1] (1: University of Texas at Austin, 2: Georgia Institute of Technology).

(d) *Prediction of numerical homogenization using deep learning for the Richards equation*.
Sergei Stepanov[1], Denis Spiridonov[1] and Tina Mai[2] (1: North-Eastern Federal University, 2: Duy Tan University and Texas A&M University).

Recent Advances in Learning
Organizers: Andrea Bonito & Ming Zhong p71
Location: CBB 110

(a) *Residual-based error correction for neural operator accelerated infinite-dimensional Bayesian inverse problem*.
Lianghao Cao[1], Thomas O'Leary-Roseberry[1], Prashant K. Jha[1], J. Tinsley Oden[1], Omar Ghattas[1] (1: Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin).

(b) *Scalable Model Selection of Interacting Particle Models with Gaussian processes*.
Jinchao Feng[1], Charles Kulick[2], Sui Tang[2] (1: Deparment of Applied Mathematics and Statistics, Johns Hopkins University; 2: Department of Mathematics, University of California, Santa Barbara).

(c) *Data-Driven Learning Based Algorithms for Multiscale Problems*.
Sai Mang Pun (Deparment of Mathematics, Texas A&M University).

(d) *Efficient Computation of Multiscale Hamiltonian Systems Aided by Machine Learning*.
Rui Fang[1], Richard Tsai[1] (1: Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin).

Sparse representation and model reduction for scientific problems
Organizers: Y. Lou, J. Hu & Y. Yang p51
Location: CBB 118

(a) *Blind image inpainting: from sparse multiscale representations to CNNs*.
Demetrio Labate (University of Houston).

(b) *Riemannian Optimization for Projection Robust Optimal Transport*.
Shiqian Ma (Rice University).

(c) *Quantifying uncertainty at scale via structure-exploiting sparse grid approximation*.
Ionut-Gabriel Farcas[1], Gabriele Merlo[1] and Frank Jenko[2] (1:The University of Texas at Austin, 2: Max Planck Institute for Plasma Physics).

(d) *A general framework of rotational sparse approximation in uncertainty quantification*.
Mengqi Hu, Yifei Lou, and Xiu Yang (1: Lehigh University, 2: University of Texas at Dallas).

Recent Developments in Model Reduction and Low Rank Algorithms
Organizers: Zhichao Peng & Min Wang p80
Location: CBB 120

(a) *Achieving Stable Long-Term Predictions in Machine Learning Architectures with Parameterization*.
Daniel Serino[1], Qi Tang[1], Joshua Burby[1] (1: Los Alamos National Labotary).

(b) *Contrast-independent partially explicit time discretizations for multiscale problems*.
Wenyuan Li[1],Yalchin Efendiev[1], Wing Tat Leung[2] (1: Texas A&M University, 2: City University of Hong Kong).

(c) *A symplectic deep autoencoder for Hamiltonian systems*.
Wei Guo[1], Qi Tang[2], Joshua Burby[2] (1: Texas Tech University, 2: Los Alamos National Labotary).

(d) *Bayesian operator inference for data-driven reduced-order modeling*.
Shane A. McQuarrie[1], Mengwu Guo[2], and Karen Willcox[1] (1: The University of Texas at Austin, 2: University of Twente).

Physics-based and data-driven models for engineering applications
Organizers: M. Tyagi & Y. Akkutlu p46
Location: CBB 122

(a) *Physics-based Data-driven Modeling on Multi-phase Flow in Converging-Diverging Annulus*.
Yitong Hao, Yingjie Tang, Matthew Franchek, Karolos Grigoriadis (University of Houston).

(b) *LES of Tropical Cyclone Winds and Application in Energy Infrastructure Systems*.
Chao Sun (Louisiana State University).

(c) *Multiscale Modeling for Clean Energy Transition*.
Kyung Jae Lee and Jiahui You (University of Houston).

(d) *Spectral Element Simulation of Particulate Flow and Convective Heat Transfer*.
Don Liu (Louisiana Tech University).

High-order numerical methods for partial differential equations
Organizers: J. Huang & Z. Sun p55
Location: CBB 124

(a) *Hermite Methods for Wave Equations*.
Tom Hagstrom[1] and Yann-Meing Law-Kam-Cio[2] and Daniel Appelo[2] (1: Southern Methodist University, 2: Michigan State University).

(b) *An energy-based discontinuous Galerkin method for a nonlinear variational wave equation*.
Lu Zhang (Columbia University).

(c) *Build Frequency Domain Maxwell/Helmholtz Solver form Time Domain Solvers with WaveHoltz Method and Its Preconditioning*.
Zhichao Peng (Michigan State University).

(d) *On a numerical artifact of solving shallow water equations with a discontinuous bottom: Analysis and a nontransonic fix*.
Zheng Sun[1] and Yulong Xing[2] (1: The University of Alabama, 2: The Ohio State University).

High Order Methods for Computational Hydrodynamics
Organizers: Madison Sheridan & Bennett Clayton p89
Location: CBB 214

(a) *The immersed interface method for simulating flows around rigid objects represented by triangular meshes*.
Sheng Xu (Southern Methodist University).

(b) *A parallel high-order overset framework for compressible turbulent flows*.
Amir Akbarzadeh[1], Lai Wang[1], Freddie Witherden[2], Antony Jameson[1,2] (1: Texas A&M University, Department of Aerospace Engineering, 1: Texas A&M University, Department of Ocean Engineering).

(c) *Guaranteed upper bound for the maximum speed of propagation in the Riemann problem*.
Bennet Clayton[1], Jean-Luc Guermond[1], Bojan Popov[1] (1: Department of Mathematics, Texas A&M University, 3368 TAMU, College Station, TX 77843, USA.).

(d) *Higher-order methods for phase-resolving wave/structure interaction*.
Chris Kees and Wen-Huai Tsao and Rebecca Schurr (Louisiana State University).

Modeling the heart-brain axis and age-related pathology
Organizers: Travis Thompson p76
Location: CEMO 101

(a) *Reduced models for solute transport and numerical convergence of solutions of PDEs with line source*.
Beatrice Riviere[1] and Charles Puelz[2] (1: Dept. of Comp. and Appl. Mathematics, Rice University 2: Dept. of Pediatrics, Baylor College of Medicine).

(b) *Hierarchical Modular Structure of the Drosophila Connectome*.
Alexander B. Kunin[1,2], Jiahao Guo[1], Kevin E. Bassler[1], Xaq Pitkow[2,3] and Krešimir Josić[1] (1: University of Houston 2: Baylor College of Medicine 3: Rice University).

(c) *A deep learning framework for the automated detection and morphological analysis of GFAP-labeled astrocytes in micrographs*.
Demetrio Labate[1], Yewen Huang[1], Anna Kruyer[2], Sarah Syed[1], Cihan Kayasandik[3], Manos Papadakis[1] (1: Department of Mathematics, University of Houston 2:Medical University of South Carolina 3:Istanbul Medipol University).

(d) *Robust Incorporation of DTMRI Data in Soft Tissue Modeling*.
Christian Goodbrake[1], Kenneth Meyer[1], Jack Hale[2] and Michael S. Sacks[1] (1: Oden Institute for Computational Engineering and Sciences and the Department of Biomedical Engineering, The University of Texas at Austin 2: The University of Luxembourg).

Spectral theory of Schrodinger operators and related topics
Organizers: W. Liu, R. Matos & F. Yang p49
Location: CEMO 105

(a) *Nonlinear Schrodinger Equation with Growing Potential*.
Setenay Akduman (Texas A&M University and Izmir Democracy University).

(b) *On Pleijel's nodal domain theorem for quantum graphs*.
Matthias Hofmann (Texas A&M University).

(c) *Electrostatic partners (Stieltjes meets Hermite and Padé)*.
Andrei Martinez-Finkelshtein (Baylor University).

(d) *Complete Non-Selfadjointness for Schrödinger Operators on the Half-Line*.
Christoph Fischbacher (Baylor University).

Hamiltonian and integrable systems
Organizers: B. Feng & T. Ohsawa p58
Location: CEMO 109

(a) *Alchemy as a quantum control problem: Mathematical prospective*.
Denys I. Bondar (Tulane University).

(b) *On metriplectic dynamics: joint Hamiltonian and dissipative dynamics*.
Philip J. Morrison (University of Texas at Austin).

(c) *Approximation of semiclassical expectation values by symplectic Gaussian wave packet dynamics*.
Tomoki Ohsawa (University of Texas at Dallas).

Mini-symposia: Sunday 01:00–03:00

Mathematical modeling and robust numerical algorithmsin various biological processes
Organizers: Shuang Liu p107
Location: CBB 104

(a) *Pattern formation and bistability in a synthetic intercellular genetic toggle*.
Bárbara de Freitas Magalhães[1], Gaoyang Fan[2], Eduardo Sontag[3], Krešimir Josić[2], and Matthew R. Bennett[1] (1:Rice University, 2: University of Houston, 3: Northeastern University).

(b) *Cell Polarity and Movement with Reaction-Diffusion and Moving Boundary*.
Shuang Liu[1], Li-Tien Cheng[1], and Bo Li[1] (1:University of California, San Diego).

(c) *Computational Modeling of Cell Migration in Microfluidic Channel*.
Zengyan Zhang[1], Yanxiang Zhao[2], and Jia Zhao[1] (1: Utah State University, 2: George Washington University).

(d) *Parameter Inference in Diffusion-Reaction Models of Glioblastoma Using Physics-Informed Neural Networks*.
Zirui Zhang[1], Andy Zhu[2], John Lowengrub[1] (1: University of California, Irvine, 2: Carnegie Mellon University).

Data-driven and Nonlinear Model Reduction Methods for Physical Sciences and Engineering
Organizers: Rudy Geelen & Shane McQuarrie p104
Location: CBB 108

(a) *Why are deep learning-based models of geophysical turbulence long-term unstable?*.
Ashesh Chattopadhyay[1] and Pedram Hassanzadeh[1] (1: Rice University).

(b) *Smoothness and Sensitivity of Principal Subspace-valued Map*.
Ruda Zhang[1] (1: University of Houston).

(c) *Adaptive planning for digital twins*.
Marco Tezzele[1] and Karen Willcox[1] (1: University of Texas at Austin).

Recent Advances in Learning
Organizers: Andrea Bonito & Ming Zhong p71
Location: CBB 110

(a) *TNet: A Model-Constrained Tikhonov Network Approach for Inverse Problems*.
Hai Van Nguyen[1], Tan Bui Thanh[1] (1: Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin).

(b) *Approximation with Neural Networks: advantages and limitations*.
Guergana Petrova (Deparment of Mathematics, Texas A&M University).

(c) *Optimal Recovery from Inaccurate Data in Hilbert Spaces: Regularize, but what of the parameter?*.
Simon Foucart[1], Chunyang Liao[1] (1: Deparment of Mathematics, Texas A&M University).

(d) *Learning of Transition Operators From Sparse Space-Time Samples*.
Christian Kuemmerle[1], Mauro Maggioni[2], Sui Tang[3] (1: Department of Computer Science, University of North Carolina, Charlotte; 2: Department of Mathematics and Department of Applied Mathematics and Statistics, Johns Hopkins University; Department of Mathematics, University of California Santa Barbara).

Sparse representation and model reduction for scientific problems
Organizers: Y. Lou, J. Hu & Y. Yang p51
Location: CBB 118

(a) *Low-rank methods for solving high-dimensional collisional kinetic equations*.
Jingwei Hu (University of Washington).

(b) *An Inverse Problem in Mean Field Games from Partial Boundary Measurement*.
Yat Tin Chow[1], Samy Wu Fung[2], Siting Liu[3], Levon Nurbekyan[3] and Stanley J. Osher[3] (1: University of California Riverside, 2: Colorado School of Mines, 3: University of California Los Angeles).

(c) *Adaptive deep density approximation for Fokker-Planck equations*.
Xiaoliang Wan (Department of Mathematics and Center for Computation and Technology, Louisiana State University, USA).

(d) *Sparse representation of seismic data using chains of destructors*.
Sergey Fomel (Jackson School of Geosciences, the University of Texas at Austin).

Recent Developments in Model Reduction and Low Rank Algorithms
Organizers: Zhichao Peng & Min Wang p80
Location: CBB 120

(a) *Least-squares Parametric Reduced-order Modeling*.
Petar Mlinarić and Serkan Güğercin (Virginia Tech).

(b) *Structure-preserving machine learning moment closures for the radiative transfer equation*.
Juntao Huang[1], Yingda Cheng[2], Andrew J. Christlieb[2], Luke F. Roberts[3] and Wen-An Yong[4] (1: Texas Tech University, 2: Michigan State University, 3: Los Alamos National Lab, 4: Tsinghua University).

(c) *Fast Online Adaptive Enrichment for Poroelasticity with High Contrast*.
Xin Su[1], Sai-Mang Pun[1] (1: Texas A&M University).

(d) *A new reduced order model of linear parabolic PDEs*.
Yangwen Zhang[1], Noel Walkington[1], Franziska Weber[2] (1: Carnegie Mellon University, 2: University of California Berkeley).

High-order numerical methods for partial differential equations
Organizers: J. Huang & Z. Sun p55
Location: CBB 124

(a) *Structure preserving methods for the Euler-Poisson system*.
Ignacio Tomas[1] and Matthias Maier[2] and John Shadid[3] (1: Texas Tech University, 2: Texas A&M University, 3: Sandia National Laboratories).

(b) *A positivity preserving strategy for entropy stable discontinuous Galerkin discretizations of the compressible Euler and Navier-Stokes equations*.
Yimin Lin[1], Jesse Chan[1], Ignacio Tomas[2] (1: Rice University, 2: Sandia National Laboratories).

(c) *A structure preserving, conservative, low-rank tensor scheme for solving the 1D2V Vlasov-Fokker-Planck equation*.
Joseph H. Nakao (University of Delaware).

(d) *Uniform accuracy of implicit-explicit methods for stiff hyperbolic relaxation systems and kinetic equations*.
Ruiwen Shu[1] and Jingwei Hu[2] (1: University of Georgia, 2: University of Washington).

Advances in theory and computation of functional optical materials
Organizers: Matthias Maier & Daniel Massatt p74
Location: CBB 214

(a) *Domain wall junctions and networks in Dirac topological materials*.
P. Cazeaux[1], D. Massatt[2], G. Bal[3], and S. Quinn[3] (1: Virginia Tech, 2: LSU, 3: University of Chicago).

(b) *Shape Optimization of Microstructures Governed by Maxwell's Equations*.
Manaswinee Bezbaruah[1], Matthias Maier[1], Winnifried Wollner[2] (1: Texas A&M University, 2: Universitaet Hamburg, Germany).

(c) *Two new finite element schemes for a time-domain carpet cloak model with metamaterials*.
Jichun Li[1], Chi-Wang Shu[2] and Wei Yang[3] (1: University of Nevada Las Vegas, 2: Brown University, 3. Xiangtan University).

(d) *Bloch Waves for Maxwell's Equations in High-Contrast Electromagnetic Crystals*.
Robert Viator (Swarthmore College).

Modeling the heart-brain axis and age-related pathology
Organizers: Travis Thompson p76
Location: CEMO 101

(a) *Computer modeling and simulation of blood flow and tissue deformation in congenital heart defects*.
Charles Puelz[1], Dan Lior[1], Craig Rusin[1], Colin Edwards[2] and Silvana Molossi[1] (1: Department of Pediatrics, Division of Cardiology, Baylor College of Medicine and Texas Children's Hospital 2: Department of Mechanical Engineering, Rice University).

(b) *Mathematical models and methods in computational neurology*.
Pedro D. Maia[1] (1: Department of Mathematics, The University of Texas at Arlington).

(c) *Telomerase Therapy Reverses Vascular Senescence*.
Anahita Mojiri[1], Xu Qiu[1], Elisa Morales[1], Luay Boulahouache[1], Chiara Mancino[1], Rhonda Holgate[1], Chongming Jiang[1], Abbie Johnson[1], Brandon K. Walther[1], Guangyu Wang[1], John P. Cooke[1] MD PhD (1: Houston Methodist Research Institute).

Recent advances in large-scale inverse problems: Numerics, theory, and applications
Organizer: Alexander Mamonov, Andreas Mang & Daniel Onofrei p33
Location: CEMO 105

(a) ~~*Fast approximations of high rank Hessians: Applications to seismic inversion and uncertainty quantification*~~.
~~Mathew Hu[1,*], Nick Alger[1], Longfei Gao[1], Omar Ghattas[1] & Rami Nammour[2]~~ (~~1: Oden Institute, The University of Texas at Austin; 2: Total E&P Research and Technology~~ Talk moved to Saturday, 8:30 AM).

(b) ~~*Matrix-free PSF approximation of ice sheet Hessians*~~.
~~Nick Alger[1,*], Tucker Hartland[2], Noemi Petra[2], Omar Ghattas[1]~~ (~~1: Oden Institute, The University of Texas at Austin; 2: Applied Mathematics, University of California, Merced~~ Talk moved to Saturday, 9:00 AM).

(c) *TBA*.
TBA (TBA).

(d) *TBA*.
TBA (TBA).

Mini-symposia Program Overview

		CBB104	CBB106	CBB108	CBB110	CBB118	CBB120	CBB122	CBB124	CBB214	CEMO101	CEMO105	CEMO109
Fr	3:00PM					MS23a	MS27a	MS26a	MS14a	MS25a	MS01a		
Sa	8:30AM	MS09a	MS22a	MS16a	MS04a	MS23b	MS27b	MS26b	MS14b	MS25b	MS01b	MS29a	MS13a
Sa	1:00PM	MS09b	MS03a	MS16b	MS04b	MS28a	MS24a	MS26c	MS14c	MS18a	MS01c	MS29b	MS13b
Sa	4:30PM	MS15a	MS12a	MS05a	MS04c	MS28b	MS24b	MS06a	MS14d	MS21a	MS19a	MS07a	MS11a
Su	8:30AM	MS02a	MS03b	MS30a	MS17a	MS08a	MS20a	MS06b	MS10a	MS25c	MS19b	MS07b	MS11b
Su	1:00PM	MS31a		MS30b	MS17b	MS08b	MS20b		MS10b	MS18b	MS19c	MS01d	

#	Title	Organizers
MS01	Recent advances in large-scale inverse problems: Numerics, theory, and applications	Mamonov, Mang & Onofrei
MS02	Nonlocal Models in Mathematics and Computation	Diehl, Bhattacharya, Aksoylu & Lipton
MS03	Mathematical Modeling for Biological Dynamics	Qu, Asik & Wang
MS04	Modeling, analysis and numerical simulations involving thin structures	Bonito, Quaini, Olshanskii & Marazzato
MS05	Deep Learning Methods for Biomedical Image Analysis & Modeling	Castillo
MS06	Physics-based and Data-driven models for Engineering Applications	Tyagi & Akkutlu
MS07	Spectral theory of Schrodinger operators and related topics	Liu, Matos & Yang
MS08	Sparse representation and model reduction for scientific problems	Lou, Hu & Yang
MS09	Mathematical Physics and Graph Theory	Fillman, Han & Shipman
MS10	High-Order Numerical Methods for Partial Differential Equations	Huang & Sun
MS11	Hamiltonian and Integrable Systems	Feng & Ohsawa
MS12	Tensor Modeling and Applications	Lou & Minkoff
MS13	Numerical methods and applications for geosciences	Jones & Cappanera
MS14	Mathematics and Computation in Biomedicine	Acosta & Puelz
MS15	Recent advances of scientific computing and applications	Wang
MS16	Recent Advances in Reduced Order Models	Heinkenschloss
MS17	Recent Advances in Learning	Bonito & Zhong
MS18	Advances in theory and computation of functional optical materials	Maier & Massatt
MS19	Modeling the heart-brain axis and age-related pathology	Thompson
MS20	Recent Developments in Model Reduction and Low Rank Algorithms	Peng & Wang
MS21	Recent Advances of Numerical Simulations for Fluid Flows and Applications	Yang & Yan
MS22	Stability of Solitary Waves with applications to Optics and Fluids	Choi & Parker
MS23	Special Topics in Mathematical Biology	Atkins & Gulbudak
MS24	Nonlinear Physics Models and Mathematical Structures	Vatchev, Qiao, Galindo & Suazo
MS25	High Order Methods for Computational Hydrodynamics	Madison Sheridan & Bennett Clayton
MS26	Scientific Deep Learning	Nguyen, Bui-Thanh & Krishnanunni
MS27	Challenges and opportunities in computational science and engineering: perspectives from data-driven learning and model reduction	Farcas, Tezzele & Kalur
MS28	Modeling of air flow and droplet transport for biomedical applications	Ajaev & Barreiro
MS29	Applications and Computation in Algebraic Geometry	Garcia, Tonelli-Cueto & Yahl
MS30	Data-driven and Nonlinear Model Reduction Methods for Physical Sciences and Engineering	Geelen & McQuarrie
MS31	Mathematical modeling and robust numerical algorithmsin various biological processes	Liu

Abstracts

Abstracts of Plenary Lectures

Dr. Detlef Hohl

Chief Scientist, Computation and Data Science, Shell

Title: Content-based image retrieval for industrial material with deep learning

Abstract: Industrial materials images are an important application domain for content-based image retrieval (CBIR). Users need to quickly search databases for images that exhibit similar appearance, properties and/or features to reduce analysis turnaround time and cost. The images in this study are 2D images of millimeter-scale rock samples acquired at micrometer resolution with light microscopy and micro-CT. Labeled rock images are expensive and time consuming to acquire and thus are typically only available in the tens of thousands. Training a high-capacity deep learning (DL) model from scratch is therefore not practicable due to data paucity. To overcome this "few shot learning" challenge, we propose leveraging pre-trained common DL models in conjunction with transfer learning. We present a novel DL architecture that combines Siamese networks with a loss function that integrates classification and regression terms. For efficient inference, we use a highly compressed image feature representation, computed offline, to search the database for images similar to a query image. Numerical experiments demonstrate superior retrieval performance of our new architecture compared with other DL and custom-feature based approaches.

Dr. Carol Woodward

Distinguished Member of the Technical Staff, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory

Title: Time integration methods and software for scientific simulations

Abstract: Time-dependent systems are at the heart of numerous scientific applications requiring simulation. While single rate, fixed step size time integration methods have been used for decades, adaptive step methods and schemes that can efficiently evolve problems with multiple time scales have not yet been fully engaged in many science applications. In this talk, I will overview current adaptive methods and discuss new multirate methods that address multiphysics problems. The SUNDIALS time integration software library will be presented as a vehicle for getting innovative numerical mathematics into applications. Lastly, I will present examples of use of SUNDIALS in scientific applications on state-of-the-art computers.
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC. LLNL-ABS-834136.

Dr. Karen E. Willcox

Director, Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin

Title: Beyond forward simulations: From reduced-order models to digital twins with computational science

Abstract: Digital twins represent the next frontier in the impact of computational science on grand challenges across science, technology and society. A digital twin is a computational model or set of coupled models that evolves over time to persistently represent the structure, behavior, and context of a unique physical system or process. A digital twin is characterized by a dynamic and continuous two-way flow of information between the computational models and the physical system. This talk will highlight the important roles of reduced-order modeling and uncertainty quantification in achieving robust, reliable digital twins at scale. The talk will present our recent work on developing cancer patient digital twins in collaboration with the Oden Institute Center for Computational Oncology.

Dr. Minh-Binh Tran

Assistant Professor, Department of Mathematics, Texas A&M

Title: Some recent results on wave turbulence theory

Abstract: Wave turbulence describes the dynamics of both classical and non-classical nonlinear waves out of thermal equilibrium. In this talk, I will present our recent results on the rigorous justification of wave turbulence theory, starting from the stochastic Zakharov-Kuznetsov (ZK) equation, a multidimensional KdV type equation, on a hypercubic lattice. To the best of our knowledge, the work provides the first rigorous derivation of nonlinear 3-wave kinetic equations, for both homogeneous and inhomogeneous cases. Moreover, this is the first derivation for wave kinetic equations in the lattice setting and out-of-equilibrium. This is joint work with Gigliola Staffilani (MIT).

Abstracts of Mini-symposium Presentations

MS 1: Recent advances in large-scale inverse problems: Numerics, theory, and applications

Organizer: Alexander Mamonov, Andreas Mang & Daniel Onofrei

Despite formidable advances in recent years, significant challenges remain. In inverse problems, parameters are typically related to indirect measurements by a mathematical model (for example, a PDE) in a highly nonlinear way, resulting in non-convex, non-linear optimization problems. These problems are challenging to solve in an efficient way. We will discuss recent advances in numerical methods and the theory of inverse problems to address these challenges. This minisymposium aims to attract researchers at the forefront of inverse problems, inference, and data science to present their latest work on fast algorithms and theory in inverse problems, and exciting applications.

MS 1–Talk 1: **Inverse problems of subsurface flows with low permeability fault structures**

Authors: Jeonghun (John) Lee (Department of Mathematics, Baylor University)

Abstract: In this work we consider inverse problems of subsurface flow models with low permeability fault structures. We first consider deterministic inversion of fault transmissibility parameters via constrained optimization approach with Newton conjugate gradient methods. We then consider efficient Bayesian inversion using the Laplace approximation of posterior at MAP point. This is a joint work with Umberto Villa, Tan Bui-Thanh, Omar Ghattas at the Oden Institute of Computational Engineering and Sciences in University of Texas Austin.

MS 1–Talk 2: **An inverse solver for a multispecies tumor growth model**

Authors: Ali Ghafouri & George Biros (Oden Institute, The University of Texas at Austin)

Abstract: Biophysical models of tumor growth at the tissue level can be used for patient stratification, preoperative planning, treatment planning, and prognosis. They also help bridge imaging phenotype with molecular drivers of cancer. Here we focus on the mathematical structure of a parameter estimation problem for multi-species model of tumor growth. This model is designed for glioblastomas but in principle it can be used to other solid tumors. We establish connections with classical inverse problem theory, and we discuss some unique challenges. It is a single-shot inversion (that is we using only one time snapshot), it has a large number of parameters, and involves nonlinear, non-differential operators. We propose an inversion methodology that attempts to address some of these challenges, and we present numerical results that illustrate the strengths and weaknesses of the proposed scheme.

MS 1–Talk 3: **Spatio-temporal quantification of pathological tau spreading in Alzheimer's disease**

Authors: Zheyu Wen, Ali Ghafouri & George Biros (Oden Institute, The University of Texas at Austin)

Abstract: Tau lesions (tau) are one of the main biomarkers of Alzheimer's disease (AD). Quantitatively describing how tau spreads in human brains can help with AD diagnosis and prognosis. Tau can be imaged spatially using positron emission tomography (tau-PET). Our goal is to use tau-PET images along with traditional magnetic resonance imaging to learn a spatio-temporal model of tau propagation. In this talk we will discuss the mathematical and computational challenges of the underlying methodology as well as a set of new algorithms that enable quantification and classification of tau spreading. We test our method on a cohort of subjects selected from publically available datasets.

MS 1–Talk 4: **Deep generative models and accelerated MRI**

Authors: Brett Levac, Alexandros G. Dimaki & Jon Tamir (Department of Electrical and Computer Engineering, The University of Texas at Austin)

Abstract: Recently, deep learning techniques have been used as powerful data-driven reconstruction methods for inverse problems, and in particular have led to reduced scan times in magnetic resonance imaging (MRI). Typically, these methods are implemented using end-to-end supervised learning based on idealized imaging conditions. While promising, reconstruction quality is known to degrade when applied to natural measurement and anatomy perturbations. In this talk we present an alternative approach to deep learning reconstruction based on distribution learning, in which we train a deep generative model to learn image priors without reference to the measurement process. We show that decoupling the measurement and statistical models provides a powerful framework for MRI reconstruction. We leverage recent advances in score-based generative modeling to learn the prior distribution and we pose the image reconstruction task as posterior sampling. We show that this approach is competitive with end-to-end methods when applied to in-distribution data, and we demonstrate theoretical and empirical robustness to various out-of-distribution shifts. In cases where the distribution shift is large, we empirically show a small amount of training data is sufficient to recover the performance. Finally, we demonstrate the utility of our framework for image reconstruction in the presence of subject motion.

MS 1–Talk 5: **Some results on inverse problems to elliptic PDEs with solution data and their implications in operator learning**

Authors: Kui Ren (Department of Applied Physics and Applied Mathematics and Data Science Institute, Columbia University)

Abstract: In recent years, there have been great interests in discovering structures of partial differential equations from given solution data. Very promising theory and computational algorithms have been proposed for such identification problems in different settings. We will try to review some recent understandings of such PDE learning problems from the perspective of inverse problems. In particularly, we will highlight a few computational and analytical understandings on learning a second-order elliptic PDE from single and multiple solutions.

MS 1–Talk 6: **Estimating the noise level in seismic data while overcoming cycle skipping**

Authors: Susan Minkoff[1], Huiyi Chen[1] & William Symes[2] (1: Department of Mathematical Sciences, University of Texas at Dallas, 2: Department of Computational and Applied Mathematics, Rice University)

Abstract: Full waveform inversion (FWI) suffers from the well-known cycle skipping problem in which local gradient-based optimization may fail to converge to geologically meaningful earth models if the initial guess for the optimization is not close enough to the true earth model. Extension methods attempt to overcome the cycle skipping problem by enlarging the space of acceptable models. In the case of source extension, the inverse problem is extended to allow for estimation of both the medium parameters (velocity) and the source wavelet via the addition of a penalty term. The extension does not require the source to be compactly supported in time. This extended objective function can be minimized efficiently via the discrepancy principle in which the source time function and velocity are estimated in a nested loop. While this approach has been shown to overcome cycle skipping, it does require use of a well-tuned penalty weight which depends on the data noise level, which is generally unknown. In this talk I will describe and illustrate an algorithm to simultaneously solve the inverse problem while accurately estimating the data noise level.

MS 1–Talk 7: **Conductivity imaging from thermal noise**

Authors: Trent DeGiovanni & Fernando Guevara Vasquez (University of Utah)

Abstract: We present a method for imaging the conductivity of a body from measurements of thermal noise currents between the body and the ground. Concretely we show that if the variances of the thermal noise currents are known, the inverse problem can be formulated as a deterministic internal functional inverse problem identical to the one occurring in ultrasound modulated electrical impedance tomography.

MS 1–Talk 8: **Lippmann–Schwinger–Lanczos algorithm for inverse scattering problems**

Authors: V. Druskin[1], S. Moskow[2] & M. Zaslavsky[3] (1: Department of Mathematical Sciences, Worcester Polytechnic Institute, 2: Department of Mathematics, Drexel University, 3: Schlumberger-Doll Research Center)

Abstract: Data-driven reduced order models (ROMs) are combined with the Lippmann[1]Schwinger integral equation to produce a direct nonlinear inversion method. The ROM is viewed as a Galerkin projection and is sparse due to Lanczos orthogonalization. Embedding into the continuous problem, a data-driven internal solution is produced. This internal solution is then used in the Lippmann-Schwinger equation, thus making further iterative updates unnecessary. We show numerical experiments for spectral domain data for which our inversion is far superior to the Born inversion and works as well as when the true internal solution is known.

MS 1–Talk 9: **Carleman Weighted Hilbert Spaces for Coefficient Inverse Problems**

Authors: Michael V. Klibanov (Department of Mathematics, University of North Carolina at Charlotte)

Abstract: Coefficient Inverse Problems (CIPs) are both ill-posed and highly nonlinear. These two factors cause the non-convexity of conventional least squares cost functionals, which are constructed for numerical solutions of CIPs. The speaker with coauthors has developed a new approach to numerical solutions of CIPs, called convexification. The convexification constructs globally strictly convex cost functionals for a broad class of CIPs. This functional is defined on a bounded convex set of an arbitrary but fixed diameter in an appropriate Hilbert space, which we call Carleman Weighted Hilbert Space. The weight is the Carleman Weight Function, which is used in the Carleman estimate for a corresponding PDE operator. Uniqueness and existence of the minimizer of such a functional on that set is established. Convergence of minimizers to the true solution of the CIP is proven, provided that the noise in the data tends to zero. Many numerical examples, including ones with experimentally collected data, confirm the theory.
Some of these results will be presented in my talk.
Main contributors are (in the alphabetical order): Vo Khoa, Thuy Le and Loc Nguyen.

MS 1–Talk 10: **New sampling indicator functions for stable imaging of photonic crystals**

Authors: Dinh-Liem Nguyen (Kansas State University)

Abstract: This talk is concerned with the inverse problem of determining the shape of penetrable periodic scatterers using electromagnetic waves. This inverse problem arises from the imaging of photonic crystals using electromagnetic inverse scattering. We develop a sampling method with a novel indicator function for solving this inverse problem. This indicator function is very simple to implement and robust against noise in the data. The resolution and stability analysis of the indicator function is analyzed. Our numerical study shows that the proposed sampling method is more stable than the factorization method and more efficient than the direct or orthogonality sampling method in reconstructing periodic scatterers. This is based on joint work with Kale Stahl and Trung Truong.

MS 1–Talk 11: **Reconstructing a space-dependent source term of the Helmholtz equation via the quasi-reversibility method**

Authors: Loc Hoang Nguyen (Department of Mathematics and Statistics, University of North Carolina at Charlotte)

Abstract: Our aim is to solve an important inverse source problem which is the linearization of the well-known inverse scattering problem. We propose to truncate the Fourier series of the solution to the governing equation with respect to a special basis of L^2. By this, we obtain a system of linear elliptic equations. Solutions to this system are the Fourier coefficients of the solution to the governing equation. After computing these Fourier coefficients, we can directly find the desired source function. Numerical examples are presented.

MS 1–Talk 12: **Active control of electromagnetic fields in layered media**

Authors: Chaoxian Qi[1,*], Neil Jerome A. Egarguin[2], Daniel Onofrei[3] & Jiefu Chen[1] (1: Department of Electrical and Computer Engineering, University of Houston, 2: Institute of Mathematical Sciences and Physics, University of the Philippines Los Baños, 3: Department of Mathematics, University of Houston)

Abstract: In this talk, we consider the problem of actively manipulating electromagnetic (EM) fields in layered media. We aim to characterize an EM source given some predetermined desired field patterns in prescribed disjoint exterior regions. The source characterization problem is treated as an inverse problem that requires solving an ill-posed optimization problem. The optimal current distribution is sought after such that the EM source can approximate the given EM fields in exterior regions. This study considers the case when the source and control regions are in a layered media, which can model various applications, such as enhanced subsurface sensing, radio communication through the water-air interface, etc.

MS 1–Talk 13: **Fast approximations of high-rank Hessians: Applications to seismic inversion and uncertainty quantification**

Authors: Mathew Hu[1,*], Nick Alger[1], Longfei Gao[1], Omar Ghattas[1] & Rami Nammour[2] (1: Oden Institute, The University of Texas at Austin; 2: Total E&P Research and Technology)

Abstract: We propose a high-rank, computationally efficient method to approximate the normal operator (Hessian) arising in the linearized seismic reflection inversion problem in two spatial dimensions. Computing the exact Hessian is intractable for large-scale problems. In fact, performing the Hessian vector product requires solving PDE problems. Moreover, slow decay of the Hessian's eigenvalues means that low-rank approximation of the Hessian is costly.

Our first approach is based on the locality of the Hessian impulses. The approximation includes two steps. First, apply Hessian on several particular vectors to draw information of impulses, and modify the impulses on boundaries if necessary. Second, build the operator with impulses and preset weight functions by a product-convolution scheme. Our second approach is based on the theory that the Hessian is a pseudodifferential operator under certain conditions. The approximation also includes two steps. First, apply the Hessian on a specific probing vector. Second, determine the symbol of the pseudodifferential operator by solving a smaller size optimization problem.

Both approaches approximate the Hessian operator within a small number of applications.

The approximation can be expressed as an H-matrix, which facilitates fast matrix computations, such as inversion, to obtain a preconditioner. We used the inverse of the approximation as a preconditioner in the second-order Newton-Krylov methods applied to full-waveform inversion (FWI). The preconditioner is highly desirable here because such preconditioners can reduce the required number of Krylov iterations within each Newton step, thereby reducing the computational cost.

We validate the method on the Marmousi model with constant density. Numerical experiments demonstrate that the preconditioner can reduce the computational costs substantially.

MS 1–Talk 14: **Matrix-free PSF approximation of ice-sheet Hessians**

Authors: Nick Alger[1,*], Tucker Hartland[2], Noemi Petra[2], Omar Ghattas[1] (1: Oden Institute, The University of Texas at Austin; 2: Applied Mathematics, University of California, Merced)

Abstract: We present an efficient matrix-free point spread function (PSF) method for approximating operators that have locally supported non-negative integral kernels. The method uses impulses of the operator (computed at a collection of scattered points) and interpolates translated and scaled versions of these impulses to approximate entries of the integral kernel. Impulse responses are computed by applying the operator to a small number of Dirac combs associated with "batches" of point sources. By solving an ellipsoid packing problem, we choose as many point sources as possible per batch, while ensuring that the supports of the impulses within each batch do not overlap. Support ellipsoids are estimated a-priori via a new procedure that involves applying the operator to a small number of polynomial functions. The ability to rapidly evaluate kernel entries allows us to construct a hierarchical matrix (H-matrix) approximation of the operator. Fast H-matrix methods are then used to perform further matrix computations in nearly linear complexity. We illustrate our approach by

applying the method to approximate the Hessian in an ice sheet flow PDE constrained inverse problem. Our results show that the method can accurately approximate the high rank ice sheet Hessian using only a small number of operator applies.

MS 2: Nonlocal models in mathematics and computation

Organizers: Patrick Diehl, Debdeep Bhattacharya, Burak Aksoylu & Robert P. Lipton

Nonlocal models have drawn increasing interest from both the mathematical and computational science communities in recent years. This is due to their ability to describe physical processes which lie outside classical local theories. Over the last fifteen years, mathematicians have begun to identify the mathematical theory behind these approaches. These efforts complement the advances in model development, computational methods and experiments necessary to validate nonlocal modeling. The objective of this mini-symposia is to bring together experts in nonlocal models from mathematics, computational science, and mechanics, in order to further the dialogue between these communities.

MS 2–Talk 1: **Four Mutual Properties of Classical and Nonlocal Wave Equations**

Authors: Burak Aksoylu (Texas A&M University-San Antonio)

Abstract: The main advantage that our nonlocal (NL) operators provide is the ability to enforce local boundary condition (BC) through the use of a forcing function only on the local boundary, not in the interior of the domain. The ability to incorporate such a widely accepted BC type into NL formulations is quite valuable.

We provide a comparative study on classical and NL wave equations. The NL operators employ local BCs, and this is why a comparison to the classical wave equation is relevant. We find out that the two equations are qualitatively identical in terms of the balance of linear momentum (BLM), conservation of energy, and the resonance and beating phenomena. For both equations, the BLM is satisfied for the Neumann and periodic BCs and fails for Dirichlet and antiperiodic BCs.

We also reveal a close connection between classical and NL wave equations. In d'Alembert's formula on a bounded domain, the BC is encoded in the solution using the extension artifice known as the method of images. Whereas in our integral formulation, since the only degree of freedom is the kernel function, it is encoded in the kernel of the operator. This is a striking difference from the local formulation. What is even more striking is the following similarity: we discovered that the same combination of the function piece (even or odd) and extension type (antiperiodic or periodic) is used in structuring the kernel function. We were able to discover such suitable kernel structures thanks to functional calculus.

MS 2–Talk 2: **Macroscopic effects of inter and intra particle dynamics on vehicle dynamics using nonlocal particle based modeling**

Authors: Debdeep Bhattacharya & Robert P. Lipton (Louisiana State University)

Abstract: We investigate vehicle mobility over dry gravel roads as a function of gravel shape, elastic deformation, topology, and damage at the particle level. We examine these effects on the dynamics at the particle length scale and their impact on the macroscopic properties of gravel aggregates that effect vehicle mobility. A shape-agnostic method is used to restrict the peridynamic interaction within gravel boundaries so that arbitrary gravel geometry, including nonconvex rock chips, can be accommodated. A history-dependent damage model is used to capture the breakage of the rock fragments. Motivated by the Discrete Element Method (DEM) framework, inter particle interactions are mediated by separate nonlocal particle boundary forces.Various types of gravel particle geometries and topologies are investigated. We apply numerical simulations to extract macroscopic properties of the gravel bed. We find that vehicle transit time and power consumption are affected by the shape and strength of particle grains. The driving torque to maintain a fixed wheel slip and the progressive damage due to the wheel weight is compared across aggregates consisting of gravels of different shapes.

MS 2–Talk 3: **Challenges for coupling approaches for classical linear elasticity and bond-based peridynamic models for non-uniform meshes and damage**

Authors: Patrick Diehl, Serge Prudhomme, Emily Downing & Autumn Edwards (Louisiana State University)

Abstract: Local-nonlocal coupling approaches provide a means to combine the computational efficiency of local models and the accuracy of nonlocal models. This paper studies the continuous and discrete formulations of three existing approaches for the coupling of classical linear elasticity and bond-based peridynamic models, namely 1) a method that enforces matching displacements in an overlap region, 2) a variant that enforces a constraint on the stresses instead, and 3) a method that considers a variable horizon in the vicinity of the interfaces. The performance of the three coupling approaches is compared on a series of one-dimensional numerical examples that involve cubic and quartic manufactured solutions. Accuracy of the proposed methods with respect to non-uniform meshes and damage is measured in terms of the difference between the solution to the coupling approach and the solution to the classical linear elasticity model, which can be viewed as a modeling error. The objective of the paper is to assess the quality and performance of the discrete formulation for this class of force-based coupling methods.

MS 3: Mathematical modeling for biological dynamics

Organizers: Zhuolin Qu, Lale Asik & Xiang-Sheng Wang

Mathematical models are powerful tools for understanding and informing complex biological phenomena. In recent years, there has been broad interest in applying mathematics to study a variety of biological fields, such as epidemiology, ecology, and neurology. Mathematical models at different spatial and temporal scales have been developed to focus on population-level dynamics, within-host processes, as well as multiscale dynamics that span several biological scales and capture the feedback between them. The utility of the proposed models requires a solid model formulation from realistic biological phenomena, rigorous analysis using mathematical theories, and accurately solved by numerical methods. This mini-symposium will highlight the new developments in these areas and bring together researchers who work on various models for biological systems from the perspectives of modeling, analysis, and computation. It will serve as a platform to present recent progress, exchange research ideas, extend academic networks, and seek future cooperation.

MS 3–Talk 1: **Stochastic Avian Influenza Model**

Authors: U. Bulut[1], T. Oraby[2], and E. Suazo[2] (1: University of the Incarnate Word, 2: The University of Texas Rio Grande Valley)

Abstract: Avian Influenza (AI) is a zootonic disease with a 53 % case fatality rate (H5N1 strain) since 2003. The number of human infectious with AI has increased in the recent epidemic wave during the period 2016-2017. In this paper, the stochastic diffusion advection equation is studied, with the time-dependent white noise, to model the spread of Avian Influenza (AI) through environmental contamination. Our goal is to see whether applying a random perturbation to the migration speed of the wild bird population can eradicate the disease. We prove that the disease-free equilibrium is exponentially asymptotically stable almost surely. Besides that, bird to human transmission model is constructed to understand the different dynamics of avian influenza among the human population.

MS 3–Talk 2: **Multiscale Modeling of Infectious Disease: The Case of Malaria**

Authors: Juan B. Gutiérrez[1] (1: University of Texas at San Antonio)

Abstract: Malaria is one of the most complex diseases known. It can be better understood through the systematic aggregation of the multiple scales at which its dynamics take place. Building a multiscale model of malaria that informs public health and clinical action requires pushing the boundary beyond traditional

multiscale modeling. In this presentation we will discuss the different aspects involved in creating quantitative models of malaria by passing through the realms of dynamical systems, molecular biology, PDEs, immunology, artificial intelligence, physiology, human-mosquito interactions, data science, and epidemiology. This discussion will demonstrate that quantitative areas that are not traditionally considered part of the mathematical corpus are needed to create realistic models.

MS 3–Talk 3: **Reconciling contrasting effects of nitrogen on pathogen transmission and host immunity using stoichiometric models**

Authors: Dedmer B. Van de Waal[1,2], Lauren A. White[3], Rebecca Everett[4], Lale Asik[5,6], Elizabeth T. Borer[7], Thijs Frenken[1,8], Angélica L. González[9], Rachel Paseka[7], Eric W. Seabloom[7], Alexander T. Strauss[7,10], and Angela Peace[6] (1: Department of Aquatic Ecology, Netherlands Institute of Ecology (NIOO-KNAW), Wageningen, The Netherlands, 2: Department of Freshwater and Marine Ecology, Institute for Biodiversity and Ecosystem Dynamics, University of Amsterdam, Amsterdam, The Netherlands, 3: National Socio-Environmental Synthesis Center (SESYNC), University of Maryland, Annapolis, MD, US, 4:Department of Mathematics and Statistics, Haverford College, Haverford, PA, USA, 5: Department of Mathematics and Statistics, University of the Incarnate Word, San Antonio, TX, USA, 6: Department of Mathematics and Statistics, Texas Tech University, Lubbock, TX, USA, 7: Department of Ecology, Evolution, and Behavior, University of Minnesota, St. Paul, MN, USA, 8: Great Lakes Institute for Environmental Research (GLIER), University of Windsor, Windsor, ON, Canada, 9: Department of Biology and Center for Computational and Integrative Biology, Rutgers University, Camden, NJ, US, 10: Odum School of Ecology. University of Georgia, Athens, GA, USA)

Abstract: Hosts rely on the availability of nutrients for growth, as well as for their defense against pathogens. At the same time, changes in primary producer nutrition can alter the dynamics of pathogens that rely on their host for reproduction. Enhanced nutrient loads may thus promote faster pathogen transmission through increased pathogen reproduction, as well as through higher host biomass that stimulates density-dependent transmission. However, this effect may be reduced if hosts allocate a growth-limiting nutrient to pathogen defense. In canonical disease models, transmission is not a function of nutrient availability, while this is required to mechanistically understand their response to changes in the environment. Here, we explored the implications of nutrient-mediated pathogen infectivity and host immunity on infection outcomes using a stoichiometric disease model that explicitly integrates the contrasting dependencies of pathogen infectivity and host immunity on nitrogen (N). Our findings reveal dynamic shifts in host biomass build-up, pathogen prevalence, and force of infection, along N supply gradients with N-mediated host infectivity and immunity, compared to a model where the transmission rate was fixed. We show contrasting responses in pathogen performance with increasing N supply between N-mediated infectivity and N-mediated immunity, revealing an optimum for pathogen transmission at intermediate N supply. This is caused by N limitation of the pathogen at low N supply and by pathogen suppression via enhanced host immunity at high N supply. By integrating both nutrient-mediated pathogen infectivity and host immunity into a stoichiometric model, we provide a theoretical framework that is a first step in reconciling the contrasting role nutrients can have on host-pathogen dynamics.

MS 3–Talk 4: **Modeling Immunity to Malaria with an Age-Structured PDE Framework**

Authors: Zhuolin Qu[1], Denis Patterson[2], Lauren Childs[3], Christina Edholm[4], Joan Ponce[5], Olivia Prosper[6], and Lihong Zhao[7] (1: University of Texas at San Antonio, 2: Princeton University, 3: Virginia Tech, 4: Scripps College, 5: University of California, Los Angeles, 6: University of Tennessee, Knoxville, 7: University of California, Merced)

Abstract: Malaria is one of the deadliest infectious diseases globally, causing hundreds of thousands of deaths each year. It disproportionately affects young children, with two-thirds of fatalities occurring in under-fives. Individuals acquire protection from disease through repeated exposure, and this immunity plays a crucial role in the dynamics of malaria spread. We develop a novel age-structured PDE malaria model, which couples

vector-host epidemiological dynamics with immunity dynamics. Our model tracks the acquisition and loss of anti-disease immunity during transmission and its corresponding nonlinear feedback onto the transmission parameters. We derive the basic reproduction number R_0 as the threshold condition for the stability of disease-free equilibrium; we also interpret R_0 probabilistically as a weighted sum of cases generated by infected individuals at different infectious stages and different ages. We parameterize our model using demographic and immunological data from sub-Saharan regions. Numerical bifurcation analysis demonstrates the existence of an endemic equilibrium, and we observe a forward bifurcation in R_0. Our numerical simulations reproduce the heterogeneity in the age distributions of immunity profiles and infection status created by frequent exposure. Motivated by the recently approved RTS,S vaccine, we also study the impact of vaccination; our results show a reduction in severe disease among young children but a small increase in severe malaria among older children due to lower acquired immunity from delayed exposure.

MS 3–Talk 5: **Global Dynamics of Discrete Mathematical Models of Tuberculosis**

Authors: Saber Elaydi[1] and Rene Lozi[2] (1: Trinity University, 2: Universite de Provence Côte d'Azur)

Abstract: We investigate the global stability and bifurcation of discrete-time mathematical models of Tuberculosis. First we study a mathematical model of TB with endogenous or exogenous infection without treatment. Then we extend our study to mathematical models with treatment wit endogenous or exogenous infection.

MS 3–Talk 6: **Population Persistence in Stream Networks: Growth Rate and Biomass**

Authors: T. D. Nguyen[1]*, Y. Wu[2], A. Veprauskas[3], T. Tang[4], Y. Zhou[5], C. Beckford[6], B. Chau[7], X. Chen[8], B. D. Rouhani[9], A. Imadh[10], Y. Wu[11], Y. Yang[12], and Z. Shuai[13] (1: Texas A&M University, 2: Middle Tennessee State University, 3: University of Louisiana at Lafayette, 4: San Diego State University, 5: Lafayette College, 6: University of Tennessee, 7: University of Alberta, 8: University of North Carolina at Charlotte, 9: University of Texas at El Paso, 10: University of Central Florida, 11: Georgia State University, 12: The Ohio State University, 13: University of Central Florida)

Abstract: We consider the logistic metapopulation model over a stream network and use the population growth rate and the total biomass (of the positive equilibrium) as measures for population persistence. Our objective is to find distributions of resources that maximize these persistence measures. We begin our study by considering stream networks consisting of three nodes and prove that the strategy to maximize the total biomass is to concentrate all the resources in the most upstream locations. In contrast, when the diffusion rates are sufficiently small, the population growth rate is maximized when all resources are concentrated in one of the most downstream locations. These two main results are generalized to stream networks with any number of patches.

MS 3–Talk 7: **Assessing Southern Pine Beetle Infestation Risks Using Agent-Based Modeling**

Authors: John G. Alford[1], William I. Lutterschmidt[1], and Abigail Miller[2] (1: Sam Houston State University, 2: American Institutes for Research)

Abstract: In Texas, the southern pine beetle (SPB) is recognized as the most destructive pest of commercial pine. In 1985 an outbreak killed over 50,000 acres. Over the last two decades the landscape of pine timberlands in Texas and across the southern United States has changed in dramatic ways that affect our current understanding of SPB outbreaks. For example, vast acreage has changed hands from pine timber managers to conservation managers. Conservation managers are expected to be less likely to cut-out beetle outbreaks or use chemical control, possibly increasing risk of outbreaks. Furthermore, conservation minded managers may be more likely to convert susceptible loblolly to more resistant longleaf pine. In this preliminary study, we discuss an agent-based model to simulate forest growth in a highly managed monoculture to be used to investigate various land management practices that may affect SPB infestation risk.

MS 3–Talk 8: **Global dynamics of a cholera model with two nonlocal and delayed transmission mechanisms**

Authors: Xiang-Sheng Wang[1] (1: University of Louisiana at Lafayette)

Abstract: A nonlocal and delayed cholera model with two transmission mechanisms in a spatially heterogeneous environment is derived. We introduce two basic reproduction numbers, one is for the bacterium in the environment and the other is for the cholera disease in the host population. If the basic reproduction number for the cholera bacterium in the environment is strictly less than one and the basic reproduction number of infection is no more than one, we prove globally asymptotically stability of the infection-free steady state. Otherwise, the infection will persist and there exists at least one endemic steady state. For the special homogeneous case, the endemic steady state is actually unique and globally asymptotically stable. Under some conditions, the basic reproduction number of infection is strictly decreasing with respect to the diffusion coefficients of cholera bacteria and infectious hosts. When these conditions are violated, numerical simulation suggests that spatial diffusion may not only spread the infection from high-risk region to low-risk region, but also increase the infection level in high-risk region.

MS 4: Modeling, analysis and numerical simulations involving thin structures

Organizers: F. Marazzato, A. Bonito, A. Quaini, M. Olshanskii & F. Marazzato

The last three decades have witnessed the development of powerful algorithms and corresponding numerical analysis leading to efficient approximations of the location and behavior of thin structures. Novel methods and modeling techniques have joined the more traditional front tracking techniques and in synergy with the development of ever more powerful and versatile computers, the simulation and understanding of rather complex phenomena are achievable.

This mini-symposium gathers experts in the numerical simulation of thin structures with a particular focus on geometric partial differential equations for their technical complexity and practical relevance.

MS 4–Talk 1: **A Descent Scheme for Thick Elastic Curves with Self-contact and Container Constraints**

Authors: Shawn Walker (Louisiana State university)

Abstract: We present a numerical method to simulate thick elastic curves that accounts for self-contact and container constraints under large deformations (the motivating model is DNA packing). The base model includes bending, torsion, and inextensibility. A minimizing movements, descent scheme is proposed for computing energy minimizers, under the non-convex inextensibility, self-contact, and container constraints (if the container is non-convex). At each pseudo time-step of the scheme, the constraints are linearized, which yields a convex minimization problem (at every time-step) with affine equality and inequality constraints. First order conditions are established for the descent scheme at each time-step, under reasonable assumptions on the admissible set. Furthermore, under a mild time-step restriction, we prove energy decrease for the descent scheme, and show that all constraints are satisfied to second order in the time-step, regardless of the total number of time-steps taken.

We also give a modification of the scheme that regularizes the inequality constraints, and establish convergence of the regularized solution. We then discretize the regularized problem with a finite element method using Hermite and Lagrange elements. Several numerical experiments are shown to illustrate the method, including an example that exhibits massive amounts of self-contact for a tightly packed curve inside a sphere. We also demonstrate the effect of parameter choices on packing configurations.

MS 4–Talk 2: **Finite Element Approximation of a Membrane Model for Liquid Crystal Polymeric Networks**

Authors: Lucas Bouck (University of Maryland)

Abstract: Liquid crystal polymeric networks are materials where a nematic liquid crystal is coupled with a rubbery material. When actuated with heat or light, the interaction of the liquid crystal with the rubber creates complex shapes. Starting from the classical 3D trace formula energy of Bladon, Warner and Terentjev (1994),

we derive a 2D membrane energy as the formal asymptotic limit of the 3D energy. We characterize the zero energy deformations and prove that the energy lacks certain convexity properties. We propose a finite element method to discretize the problem. To address the lack of convexity of the membrane energy, we regularize with a term that mimics a higher order bending energy. We prove that minimizers of the discrete energy converge to minimizers of the continuous energy. For minimizing the discrete problem, employ a nonlinear gradient flow scheme, which is energy stable. Additionally, we present computations showing the geometric effects that arise from liquid crystal defects. Computations of configurations from nonisometric origami are also presented.

MS 4–Talk 3: **The Preasymptotic Model of Prestrained Plates**

Authors: Angelique Morvant (Texas A&M University)

Abstract: A prestrained plate is a thin sheet of material that naturally deforms into some target configuration. Prestrained plates can be used to model various physical phenomena, from the closing of the Venus flytrap to the movement of microscopic medical devices. In this talk, we will discuss the preasymptotic model for the large bending of prestrained plates. This model assumes that the thickness of the plate is small and involves a bending and a stretching energy. After deriving this model, we will discuss an LDG-type discretization of the energy, its Gamma convergence and a discrete gradient flow for minimizing the energy. This discrete gradient flow will be compared to an alternate scheme involving a Nesterov acceleration. Finally, we present some simulations to demonstrate the applications of the model.

MS 4–Talk 4: **Mixed quasi-trace surface finite element methods**

Authors: Alan Demlow (Texas A&M University)

Abstract: In standard trace (or cut) finite element methods for surface PDE, a three-dimensional bulk mesh is approximately intersected with the given surface in order to obtain a highly unstructured anisotropic surface mesh. The surface finite element method is taken to be the restriction of a bulk finite element space to the surface mesh. This methodology works well for H1-conforming spaces, but it is not clear how to extend it to other fundamental finite element settings such as H(div)-conforming spaces. In this talk we explore the idea of using a trace mesh, but then defining a mixed finite element space directly on the trace mesh rather than as the trace of an bulk space. We prove basic error estimates and also discuss extension to higher-order trace surface approximations.

MS 4–Talk 5: **Convergence of TraceFEM to minimum regularity solutions**

Authors: Lucas Bouck, Ricardo H. Nochetto, Mansur Shakipov[1] and Vladimir Yushutin[2] (1: University of Maryland, 2: Clemson University)

Abstract: Existing convergence results for unfitted methods such as TraceFEM require sufficient regularity of solutions in order to show error-with-rate estimates. The difficulty of analysis stems from the stabilization form which ensures the well-posedness and robustness of discrete problems. To circumvent this issue, we study the strong convergence of continuous-in-time TraceFEM approximations for prototypical PDEs using compactness arguments and assuming no additional regularity above what is required by weak formulations. For example, to the best of our knowledge, we present the first convergence proof for solutions to Laplace–Beltrami problem on a surface Γ which belong to $H^1(\Gamma)$ only.
We show how the stabilization form can be modified for several prototypical problems so the resulting scheme becomes amenable to a proof by compactness. Moreover, we demonstrate in numerical experiments that the suggested modifications improve the robustness and effectiveness of time adaptive schemes when the time step size is forced to get arbitrarily small relative to the mesh size.
The developed analysis framework relies on an abstract structure, *T-Rex* FEM, and it involves notions of abstract *tr*ace and *ex*tension operators as well as of an abstract stabilization form. The framework can be of merit for other unfitted/non-conforming finite element methods.

MS 4–Talk 6: **FEM for surface Navier-Stokes-Cahn-Hilliard equations**

Authors: Yerbol Palzhanov (University of Houston)

Abstract: This talk addresses a thermodynamically consistent phase-field model of a two-phase flow of incompressible viscous fluids which allows for a non-linear dependence of fluid density on the phase-field order parameter. Driven by applications in biomembrane studies, the model is written for tangential flows of fluids constrained to a surface and consists of (surface) Navier–Stokes–Cahn–Hilliard type equations. We apply an unfitted finite element method to discretize the system and introduce a fully discrete time-stepping scheme with the following properties: (i) the scheme decouples the fluid and phase-field equation solvers at each time step, (ii) the resulting two algebraic systems are linear, and (iii) the numerical solution satisfies the same stability bound as the solution of the original system under some restrictions on the discretization parameters. Numerical examples are provided to demonstrate the stability, accuracy, and overall efficiency of the approach.

MS 4–Talk 7: **Interpolation based immersogeometric analysis with application to Kirchhoff–Love shells**

Authors: Jennifer Fromm[1], Nils Wunsch[2], Ru Xiang [1], Han Zhao[1], Kurt Maute[2], John A. Evans[2],and David Kamensky[1] (1: University of California San Diego, 2: University of Colorado Boulder)

Abstract: Thin shells appear in numerous engineering applications, including biological membranes, wind turbine blades, and aerospace structures, which can all be accurately modeled using the Kirchhoff–Love (KL) shell theory. However, this theory is rarely applied in classical finite element (FE) analysis because it involves 4^{th}-order derivatives of the displacement field, requiring C^1 continuity of the discrete solution space. The growth of isogeometric analysis (IGA) has led to increased interest in numerical analysis of KL shell theory because IGA's smooth spline spaces naturally accommodate KL theory's regularity requirements. IGA would ideally use spline spaces corresponding to design geometries from industrial computer aided design (CAD) software where structured rectangular B-spline or NURBS patches are often "trimmed", resulting in a need for immersed-boundary methods. We refer to the combination of isogeometric and immersed-boundary analysis as "immersogeometric" analysis. Most existing immersogeometric methods have been implemented in custom (often application-specific) research codes, which limits their accessibility. In this work, we introduce EXHUME (EXtraction for High-order Unfitted MEthods), which enables non-invasive implementation of immersed-boundary methods in existing FE solvers through a novel class of "interpolation-based" immersed-boundary discretizations. As its name implies, EXHUME employs a generalization of (Lagrange) extraction, which interpolates basis functions from an unfitted background mesh using Lagrangian nodal basis functions defined on a foreground mesh over which variational formulations are integrated. The foreground mesh is subject to fewer element quality or topological constraints than a standard FE mesh and is thus easier to generate. Interestingly, this approach remains highly effective even when the extraction is only approximate (and the discretization is no longer mathematically equivalent to existing CutFEM/CutIGA approaches). Approximate extraction permits significant improvements in both user convenience and computational efficiency. We demonstrate EXHUME's capabilities on benchmarks involving several different PDEs and on the application of immersogeometric KL shell analysis with trimmed geometries.

MS 4–Talk 8: **Navier-Stokes equations on evolving surfaces**

Authors: A. Reusken, P. Brandner, P. Schwering[1] and M. Olshanskii[2] (1: RWTH Aachen University, 2: University of Houston)

Abstract: In this presentation we briefly address several derivations of incompressible Navier-Stokes type equations that model the dynamics of an evolving fluidic surface. These derivations differ in the physical principles used in the modeling approach and in the coordinate systems in which the resulting equations are represented. The resulting surface Navier-Stokes equations have a natural splitting into equations for the normal and tangential velocity components. We present well-posedness results for the equations that describe the tangential motion of the fluid flow.

MS 4–Talk 9: **Continuum field theory for the deformations of planar kirigami**

Authors: Paul Plucinsky[1], Ian Tobasco[2], Yue Zheng[3], and Paolo Celli[4] (1: University of Southern California, 2: University of Illinois Chicago, 3: University of Massachusetts Amherst, 4: Stony Brook University)

Abstract: Mechanical metamaterials exhibit exotic properties that emerge from the interactions of many nearly rigid building blocks. Determining these properties theoretically has remained an open challenge outside a few select examples. Here, for a large class of periodic and planar kirigami, we provide a coarse-graining rule linking the design of the panels and slits to the kirigami's macroscale deformations. The procedure gives a system of nonlinear partial differential equations expressing geometric compatibility of angle functions related to the motion of individual slits. Leveraging known solutions of the partial differential equations, we present an illuminating agreement between theory and experiment across kirigami designs. The results reveal a dichotomy of designs that deform with persistent versus decaying slit actuation, which we explain using the Poisson's ratio of the unit cell.

MS 4–Talk 10: **Numerical Approximations of Origami with Curved Creases**

Authors: Andrea Bonito (Texas A&M University)

Abstract: The folding of thin elastic sheets along a prepared curved arc is considered. The resulting curved origamis find applications in many strategical areas. Telescopes, self-deployable structures, flapping and flytrap mechanisms, shields, airbags are a few examples.

We start from a thin three-dimensional hyper-elastic model and include a material defect favoring folding. We then justify the plate model obtained in the limit when the material thickness vanishes. In this reduced setting, the plate deformations satisfy a two-dimensional fourth order problem with interface along with a nonlinear constraint expressing the fact that the plate cannot sustain shear nor stretch. In passing, we offer a simple differential geometry argument explaining the rigidity (i.e. robustness) of isometric deformations in presence of curved creases.

We present a numerical algorithm based on local discontinuous Galerkin methods, where high order derivatives in the continuous models are replaced by weakly converging discrete reconstructions. We discuss its properties and conclude the talk by exploring numerically the features of this new model.

MS 4–Talk 11: **The Poisson coefficient of zigzag sums**

Authors: Hussein Nassar[1] and Arthur Lebée[2] (1: University of Missouri, 2: École des Ponts)

Abstract: We call "zigzag sums" periodic polyhedral surfaces whose period is composed of four parallelograms. These include notorious origami tessellations such as the "Miura ori" and have inspired designs of deployable structures useful in certain engineering applications. Indeed, zigzag sums can deform, isometrically, by folding along parallelogram edges so as to go from densely-packed states into states that "shadow" large areas. Throughout this folding motion, the ratio of the relative change in width to the relative change in length defines what is commonly referred to as a "Poisson coefficient". Zigzag sums can also deform isometrically by bending the parallelogram faces so as to go from apparently flat states to apparently doubly-curved states. Here, we demonstrate that, in the limit of infinitely small periods, the ratio of apparent normal curvatures due to bending is equal, but opposite, to the Poisson coefficient due to folding. This equality encodes a non-linear PDE whose solutions are the isometric deformations of the zigzag sums (again, in the limit of infinitely small periods). Interestingly, we find that the type of the PDE is function of the sign of the Poisson coefficient. This is important in applications, as it suggests the appropriate way of controlling the deformation path from the boundary, e.g., in terms of Dirichlet v.s. Cauchy boundary conditions. Last, for illustration purposes, we solve the PDE for axisymmetric states and explain certain origami forms that are aesthetically appealing. In particular, we show how to design an origami pseudosphere, almost.

MS 4–Talk 12: **Computation of Miura Surfaces**

Authors: Frederic Marazzato (Louisiana State university)

Abstract: Origami folds have found a large range of applications in engineering as, for instance, solar panels for satellites, or the folding of airbags for optimal deployment or metamaterials.
A homogenization process turning origami folds into smooth surfaces, developed in [Nassar et al, 2017], is first discussed. Then, its application to two specific folds is presented alongside the PDEs characterizing the associated smooth surfaces. The talk will then focus on the nonlinear elliptic equations describing Miura surfaces by studying existence and uniqueness of solutions and by proposing a numerical method to approximate them.
The numerical method is based on a least-squares formulation, $\mathbb{P}^1$–Lagrange finite elements and a Newton method to solve the nonlinear system. Finally, some numerical examples are presented.

MS 5: Deep learning methods for biomedical image analysis & modeling

Organizers: E. Castillo

Topics related to the use of deep learning, either as an ancillary method or as the primary mode of analysis, for biomedical applications will be presented. Discussion areas will include theoretical and computational approaches, as well as clinical translation considerations.

MS 5–Talk 1: **Respecting Variation in Physician Clinical Practice**

Authors: Steve Jiang (University of Texas Southwestern Medical Center)

Abstract: Ideally, deep learning models should be trained with large, representative, and high-quality annotated datasets. In reality, we often have to deal with small, biased, noisy, and sometimes scarcely or weakly annotated, or even completely unannotated, datasets. There are lot of research efforts addressing these problems. Here I would like to discuss about the noisy annotation problem due to expertise errors, i.e., the inconsistencies between different observers due to human subjectivity, using medical image segmentation as an example. The conventional wisdom considers this type of noisy annotations as a bad thing. To deal with it, we often try to achieve consensus from a group of expert observers during data annotation and try to use various strategies to mitigate its adverse effect during training. However, sometimes, or even many times, we may need to respect this type of noisy data annotation. This is because, medicine is still an art in many cases. Evidence based medicine and clinical guidelines only give physicians the floor not the ceiling. There is room for physicians to exercise their own judgements, leading to variation in physicians' clinical practice. There is often no ground truth to tell which one is the best. Additionally, variation among physicians could be inherent due to the variation in handling the tradeoffs between outcome and toxicity, cost and benefit, etc. We have to face this reality when we develop and deploy deep learning models to solve clinical problems. Some strategies will be discussed.

MS 5–Talk 2: **Application of Deep Learning for real-time non-invasive continuous monitoring for enhanced peripheral oxygen saturation in intensive care unit (ICU) and Operating Room (OR)**

Authors: Sungsoo Kim[1,2], Sohee Kwon[1], Alan Bovik[2], Mia Markey[2], and Maxime Cannesson[1] (1: The University of California Los Angeles, 2: The University of Texas at Austin)

Abstract: Non-invasive monitoring for peripheral oxygen saturation (SpO2) has been known as the fifth vital sign given its critical role in patient care in intensive care unit (ICU) or Operating Room (OR). However, a concern about the accuracy of pulse oximetry has been attained the public concerns recently, particularly with the possible racial bias or medical discrimination in this covid-pandemic. In this research, we propose an innovative approach applying Deep Neural Networks (DNNs) to develop an advanced monitoring approach for accurate oxygen saturation in real-time.

MS 5–Talk 3: **Imaging based estimation of pathology in a large adult glioma population**

Authors: D. Fuentes, E. Gates, A. Celaya, D. Suki, J. Weinberg, S. Prabhu, D. Schellingerhout (The University of Texas MD Anderson Cancer Center)

Abstract: Stereotactic biopsies were collected in an imaging trial targeting untreated patients with gliomas. The data included preoperative MR imaging and quantitative histopathology on biopsy samples. A random forest method was used to estimate pathology information density using local intensity information from the MR images and quantitative pathology measurements. We will present our evaluation of the prognostic ability of imaging-based estimates of pathoogy in 1181 glioma patients, with comparison to the gold standard reference of World Health Organization grading.

MS 5–Talk 4: **Neural Network 'Finite Element' Based Models for Cardiac Simulations**

Authors: Michael Sacks, Shruti Motiwale, and Christian Goodbrake (The University of Texas at Austin)

Abstract: All high-fidelity cardiac simulations require a comprehensive image-based finite element modeling pipeline. While quite accurate, such traditional approaches cannot be used in practical for time-sensitive clinical evaluations. In this work we developed a neural network surrogate modeling method to generate fast online predictions while frontload the computational cost to model training. Due to the complex geometry of the cardiac models, the finite element discretization is used and integrated with the neural network. To train the neural network model without the need to generate finite element solutions, we developed a physics-based training scheme using differentiable finite elements to backpropagate the gradients from residuals of partial differential equations (PDEs) to the neural network. We considered active contraction and spatially varying fiber structures, all incorporated into a prolate spheroidal model of the left ventricle (LV) as a first step scenario. We consider a prolate spheroidal model of the left ventricle. The domain is discretized using unstructured tetrahedron elements. The fiber geometry was based on a rules-based approach to approximagte the -60 to 60 degree transmural gradient, and a Fung-type material model with constants taken from the ovine heart used. The entire pipeline was then trained against a represented pressure-volume loop. To verify our differentiable implementation of finite elements, we utilized the same boundary conditions and use FEniCS for conventional FE model validation. The relative error of the displacements was $3.915\times10–7$. We then show how a NURBS-based approach can be directly integrated into the NNFE approach as a means to handle real cardiac geometries. While these and related approaches are in their early stages, they offer a method to perform complex organ-level simulations in clinically relevant time frames without compromising accuracy.

MS 6: Physics-based and data-driven models for engineering applications

Organizers: M. Tyagi & Y. Akkutlu

This mini-symposium will cover a wide range of engineering applications using physics-based simulations as well as data-driven machine learning models. Presentation examples would range from subsurface flow phenomena, fluid dynamics, and mathematical foundations of data-science. The proposed mini symposium would also bring together interdisciplinary researchers working on highly relevant societal challenges through their understanding of different aspects of underlying physics and data-driven models.

MS 6–Talk 1: **Pseudo-spectral methods for the incompressible magnetohydrodynamics equations with variable density**

Authors: Loic Cappanera (University of Houston)

Abstract: We introduce two numerical methods for the incompressible Navier-Stokes equations with variable density either based on projection methods or artificial compression techniques. These methods are made suitable for pseudo-spectral methods via the use of the momentum, equal to the density times the velocity, as primary unknown and an adequate treatment of the diffusion term. The stiffness matrix of both schemes are time-independent so they can be assembled and preconditioned at initialization. The convergence and

stability of both methods are investigated theoretically, and also numerically on various setups using large ratio of density. Applications to magnetohydrodynamics instabilities in liquid metal batteries and aluminum production cells will be presented.

MS 6–Talk 2: **Numerical Investigation of Wave Scour Around Group of Vertical Cylinders**

Authors: Haq Murad Nazari and Celalettin Ozdemir (Louisiana State University)

Abstract: In this study, numerical simulations of wave scouring around multiple configurations of vertical piles were performed using SedFOAM, a two-phase Eulerian-Eulerian solver built on OpenFOAM® framework. The kinetic theory of granular flows was used to predict sediment transport in scour configurations. The eddies in two-phase turbulence averaged formulations were resolved using the $k-\omega$ model. The results of the numerical simulations were validated using the experimental results reported in Sumer, B. M and Fredsøe, J. [Wave scour around a group of vertical piles. Journal of Waterway, Port, Coastal, and Ocean Engineering 1998]. The effect of the vortex field on sediment entrainment was rigorously examined. Bed shear stresses from numerical simulations were compared to the experimental results.

MS 6–Talk 3: **Data driven modeling of shear-thinning polymer flooding**

Authors: Prabir Daripa (Texas A&M University)

Abstract: Two distinct effects that polymers exhibit are shear thinning and viscoelasticity. The shear thinning effect is important as the polymers used in chemical enhanced oil recovery usually have this property. We propose a data driven approach to incorporate this shear thinning effect through an effective dynamic viscosity of the shear thinning polysolution. The procedure of viscosity calculation of the polysolution, although based on a very basic power law model, is data driven and uses the values of density, shear rates and power-law coefficients empirically guided by experimental data and local values of concentration of polymer which evolve in time. This method is very general and can be integrated with any method for a Newtonian physics based model of porous media flows. This is exemplified here using a hybrid numerical method developed by Daripa & Dutta [**?**, **?**, **?**]. This method solves a system of coupled elliptic and transport equations modelling Darcy's law based polymer flooding process using a discontinuous finite element method and a modified method of characteristics. Simulations show (i) competing effects of shear thinning and mobility ratio; (ii) injection conditions such as injection rate and injected polymer concentration influence the choice of polymers to optimise cumulative oil recovery; (iii) permeability affects the choice of polymer; (iii) dynamically evolving travelling viscosity waves; and (v) shallow mixing regions of small scale viscous fingers in homogeneous porous media. This work shows an effective yet easy data driven approach to make design choices of polymers in any given flooding condition. This is joint work with Rohit Mishra.

MS 6–Talk 4: **Physics-Informed Neural Networks for Capacitance-Resistance Models of Reservoir**

Authors: Mayank Tyagi (Louisiana State University)

Abstract: Reservoir simulators play an important role in the management and optimal production from oil and gas fields. However, the computational costs of detailed simulations can be prohibitively expensive and most certainly not useful for real time decision making. In this presentation, a reduced-order model (ROM) is built using the time-series production data from a real oil and gas field. The Capacitance-Resistance Model (CRM) is chosen here as a reduced-order representation for the reservoir simulator. With the increase in computational power and recent machine learning (ML) approaches, it is apparent that oil and gas industry will eventually adopt the useful models through proper validation. Physics-informed Neural Networks (PINNs) are the neural networks that can enforce the governing equations for the underlying dynamics as a part of building ML models. Results are compared against a detailed reservoir simulation to demonstrate the usefulness of ML models.

MS 6–Talk 5: **Physics-based Data-driven Modeling on Multi-phase Flow in Converging-Diverging Annulus**

Authors: Yitong Hao, Yingjie Tang, Matthew Franchek, Karolos Grigoriadis (University of Houston)

Abstract: Presented is the development and parameter identification of a multi-phase flow model in the converging-diverging annulus with potential applications of high-pressure-high-temperature (HPHT) annulus flow in subsea blowout preventer (BOP). This work is comprised of: (a) high-fidelity numerical simulations of multi-phase flow with cavitation phenomenon in annulus; (b) reduced order physics-based models of HPHT annulus flow derived from computational studies, targeting evaluation and forecast of the multi-phase flow profile and the cavitation critical status; and (c) experimental validation and calibration in the flow loop test facility using multi-phase flow. This research focuses on characterizing annulus flowing conditions under high pressure events where the potential for fluid cavitation exists. The multi-physics model will be developed using the Buckingham Pi theorem and data analytics processing simulation data, based on which the calculated non-dimensional parameters (Pi) are used as regressors, to develop parametric models estimating the time-based flow profile and the cavitation critical status. This family of parametric models produced from the regressors would be evaluated based on the metrics of mean squared estimation error and R-squared value, in comparison to the previous high-fidelity simulation database. In such process, the model orders will also be selected to balance the trade-offs between model complexities and estimation accuracy. As a result, the data-driven models are developed to describe the cavitation flow profiles in terms of downstream/upstream pressure conditions and non-dimensional geometric parameters of annulus. For industrial applications, the fluids considered in both modeling and experimental validation are currently comprised of water (in both liquid and vapor phases), air, and later with oil and solid particles thus closely emulate drilling fluid rheology. Using the obtained non-dimensional models, the multi-phase annulus flow profiles can be estimated under both choked and un-choked flow conditions across multi-scale flow channels. With experimental validation and model calibration, the study results can provide engineering guidance for designs of oil and gas drilling systems, the industrial offshore asset integrity analysis, extend the capability and reliability of the academic and industrial research on the subsea fluid system, and ultimately enhance future governing standards to prevent potential failures of subsea drilling systems.

MS 6–Talk 6: **LES of Tropical Cyclone Winds and Application in Energy Infrastructure Systems**

Authors: Chao Sun (Louisiana State University)

Abstract: Under climate changing conditions, extreme tropical cyclones have become more frequent and severe, causing extensive damages to critical civil infrastructure systems and residential communities. To estimate extreme wind loading on structures, spectral methods are widely used to generate neutral atmosphere boundary layer winds, which however are limited to describe extreme wind fields that are non-stationary and more turbulent. To overcome this limitation, a high-fidelity high-resolution computational model is developed to simulate hurricane wind field with detailed physics. A large eddy simulation (LES) solver is developed using a sub-grid-scale (SGS) model based on open-source program OpenFOAM. The simulated wind field is validated through comparison with observations. The proposed hurricane boundary layer (HBL) model and a neutral atmosphere boundary layer (ABL) model are compared in tropical storm and category-3 hurricane scenarios. Compared with the HBL model, the ABL model doesn't consider the mesoscale terms and overestimates the crosswind velocity and the turbulent kinetic energy (TKE) near the ground. As case studies, the HBL model is applied to simulate the performance of offshore wind turbines under different levels of tropical cyclones. An actuator model is used to represent the effect of wind turbines on the wind field. The results reveal the energy harvesting performance under representative wind conditions. Also, the dynamic response of a power transmission line system is modeled to assess its structural safety under high-level tropical cyclones. In summary, the developed LES-based HBL model can capture the main characteristics of tropical cyclone winds and is applicable for modeling critical infrastructure systems exposed to hurricanes at a large scale.

MS 6–Talk 7: **Multiscale Modeling for Clean Energy Transition**

Authors: Kyung Jae Lee and Jiahui You (University of Houston)

Abstract: Tackling climate change is one of the major challenges facing the U.S. today, and it has led to significant efforts to decarbonize energy use as a way to minimize greenhouse gas emissions. Major ways

to achieve this energy transition involve electrifying transportation and increasing renewable energy use in electricity generation. As both electric vehicles and renewable solar–and–wind electricity generation rely on lithium–ion energy storage (i.e., lithium–ion batteries), the demand for lithium has greatly increased during the past decade; it is predicted to escalate along the market growth of electric vehicles and renewable power generation. To enhance and diversify the supply of lithium, we investigate petroleum source rock brines as a sustainable new source of lithium, given that water produced from organic–rich petroleum and natural gas source rocks has been recently revealed as a potential source of substantial amounts of lithium. This opens new pathways to address the natural petroleum source rock systems at various scales. Micro (pore)–scale modeling with Finite Volume Method (FVM), which describes fluid–rock interactions, enables the understanding of mineralization and dissolution of lithium. Macro (basin)–scale modeling with Integrated Finite Discrete Method (IFDM), which describes the release, transport, and accumulation of lithium in petroleum source rock brines, enables the identification of high concentration zones of lithium. Throughout developing the multiscale modeling approach for the new and promising application area, the computational geoscience profession will be able to progress toward a solution to a complex and expensive problem.

MS 6–Talk 8: **Spectral Element Simulation of Particulate Flow and Convective Heat Transfer**

Authors: Don Liu (Louisiana Tech University)

Abstract: Particulate flows are ubiquitous in nature and engineering. Computational studies have provided some indispensable input and are complementary to lab experiments and theoretical analyses. This study presents a HPC algorithm and implementation in spectral element method for modeling viscous dominant particulate flows involving numerous particles using MPI on distributed memory platforms. In addition, convective and conductive heat transfer flows were simulated as well by adopting the additional energy equation with the thermal dissipation terms included. This will be beneficial to simulate phase-change heat transfer involving melting and solidification etc. Results were verified and validated with relevant discussions.

MS 7: Spectral theory of Schrodinger operators and related topics

Organizers: W. Liu, R. Matos & F. Yang

Spectral properties of Schrodinger operators have been intensely studied in the past decades due to their central relevance to quantum physics and also motivated many mathematical questions of independent interest. For instance, phase transitions in a physical system can often be detected through changes in the spectral types of the modeling operator. Schrodinger operators and techniques developed to understand their dynamics have also been key to the comprehension of transport properties of quasicrystals, crystals with random impurities, nonlinear Schrodinger equations, KDV equations, spin models in the presence of disorder, and many other math physics models.

MS 7–Talk 1: **Some spectral inequality for Schrödinger equations with power growth potentials.**

Authors: Jiuyi Zhu (Louisiana State University)

Abstract: We obtain a sharp spectral inequality for Schrödinger equations with power growth potentials. This sharp spectral inequality depends on the radius and thickness of the sensor sets, and the growth rate of the potentials. The proof relies on quantitative global and local Carleman estimates to obtain quantitative three-ball inequalities.

MS 7–Talk 2: **1-Dim Half-line Schrödinger Operators with H^{-1} Potentials**

Authors: Xingya Wang (Rice University)

Abstract: In this talk, I will present some spectral results of Schrödinger operators with locally H^{-1} potentials. In the first part, we will recover some general spectral theoretical results in the current setting, including Last-Simon-type criteria for the presence and absence of the absolutely continuous spectrum on the open half-line. In the second part, we will focus on potentials which are decaying in a locally H^{-1} sense and

present an analogue of short-range decay in the distributional setting. In particular, we will examine a class of Pearson-type distributional potentials and establish a spectral transition between short-range and long-range decay.

MS 7–Talk 3: **Continuity of the Lyapunov exponent for analytic multi-frequency quasi-periodic cocycles**

Authors: Matthew Taylor Powell (UC Irvine)

Abstract: The purpose of this talk is to discuss our recent work on multi-frequency quasi-periodic cocycles, establishing continuity (both in cocycle and jointly in cocycle and frequency) of the Lyapunov exponent for non-identically singular cocycles. Analogous results for one-frequency cocycles have been known for over a decade, but the multi-frequency results have been limited to either Diophantine frequencies (continuity in cocycle) or $SL(2,\mathbb{C})$ cocycles (joint continuity). We will discuss the main points of our argument, which extends earlier work of Bourgain.

MS 7–Talk 4: **On the Irreducibility of Bloch and Fermi Varieties**

Authors: Matthew Faust (Texas A&M University)

Abstract: Understanding the irreducibility of Bloch and Fermi varieties for discrete periodic operators is important in the study of the spectrum of periodic operators, providing insight into the structure of spectral edges, embedded eigenvalues, and other applications. In this talk we will present several new criteria for obtaining irreducibility of Bloch and Fermi varieties for infinite families of discrete periodic operators.

MS 7–Talk 5: **Nonlinear Schrodinger Equation with Growing Potential**

Authors: Setenay Akduman (Texas A&M University and Izmir Democracy University)

Abstract: This study deals with nonlinear Schrodinger (NLS) equations on infinite met-ric graphs. Motivation for the study of NLS equation comes from nonlinearoptics and fiber optics. If cables are branching, it is natural to look at quan-tum graphs. Assuming the linear potential is infinitely growing, we prove anexistence of solutions that covers both self-focusing and defocusing cases. Ourapproach is variational and based on generalized Nehari manifold. Thank Professor Alexander Pankov for his guidance, remarks and com-ments for the occurrence of this joint work.

MS 7–Talk 6: **On Pleijel's nodal domain theorem for quantum graphs**

Authors: Matthias Hofmann (Texas A&M University)

Abstract: We establish metric graph counterparts of Pleijel's theorem on the asymptotics of the number of nodal domains ν_n of the n-th eigenfunction(s) of a broad class of operators on compact metric graphs, including Schrödinger operators with L^1-potentials and a variety of vertex conditions as well as the p-Laplacian with natural vertex conditions, and without any assumptions on the lengths of the edges, the topology of the graph, or the behaviour of the eigenfunctions at the vertices. Among other things, these results characterise the accumulation points of the sequence $(\frac{\nu_n}{n})_{n\in\mathbb{N}}$, which are shown always to form a finite subset of $(0,1]$. This extends the previously known result that $\nu_n \sim n$ *generically*, for certain realisations of the Laplacian, in several directions. In particular, in the special cases of the Laplacian with natural conditions, we show that for graphs any graph with pairwise commensurable edge lengths and at least one cycle, one can find eigenfunctions thereon for which $\nu_n \not\sim n$; but in this case even the set of points of accumulation may depend on the choice of eigenbasis.
Joint work with James Kennedy, Delio Mugnolo, and Marvin Plümer.

MS 7–Talk 7: **Electrostatic partners (Stieltjes meets Hermite and Padé)**

Authors: Andrei Martinez-Finkelshtein (Baylor University)

Abstract: The well-known electrostatic interpretation of the zeros of classical orthogonal polynomials goes back to the 1885 work of Stieltjes. It has been extended to several contexts, such as orthogonal and quasi-orthogonal polynomials on the real line and the unit circle, for classical and semiclassical weights.

Multiple orthogonal (or Hermite-Padé) polynomials satisfy a system of orthogonality conditions with respect to a set of measures. They find applications in number theory, approximation theory, and stochastic processes, and their analytic theory, extremely rich, has been developing since the 1980s. However, no electrostatic interpretation of the zeros of such polynomials was known. In this talk, I will present such a model for the case of type II Hermite-Padé polynomials. It introduces the notion of an "electrostatic partner" that allows a unified description of all the known cases.

This is joint work with R. Orive (Universidad de La Laguna, Canary Islands, Spain) and J. Sanchez-Lara (Granada University, Spain).

MS 7–Talk 8: **Complete Non-Selfadjointness for Schrödinger Operators on the Half-Line**

Authors: Christoph Fischbacher (Baylor University)

Abstract: We investigate complete non-selfadjointness for all maximally dissipative extensions of a Schrödinger operator on a half-line with dissipative bounded potential and dissipative boundary condition. We show that all maximally dissipative extensions that preserve the differential expression are completely non-selfadjoint. However, it is possible for maximally dissipative extensions to have a one-dimensional reducing subspace on which the operator is selfadjoint. We give a characterization of these extensions and the corresponding subspaces and present a specific example.

(Joint work with Sergey Naboko and Ian Wood)

MS 8: Sparse representation and model reduction for scientific problems

Organizers: Y. Lou, J. Hu & Y. Yang

Many scientific problems involve predictive models of multi-scale and multi-physics systems, most of which are extremely complex and computationally expensive to simulate. Yet, a common feature of these problems is that there is often an underlying sparse or reduced representation which can greatly ease the heavy computation burden. This mini-symposium will bring researchers working on these relevant regimes to exchange ideas and encourage collaborations.

MS 8–Talk 1: **Blind image inpainting: from sparse multiscale representations to CNNs**

Authors: Demetrio Labate (University of Houston)

Abstract: Image inpainting is an image processing task aimed at recovering missing blocks of data in an image or a video. In the first part of the talk, I will show that sparse multiscale representations offer a well-justified theoretical setting to address the image inpainting problem. Since images found in most applications are dominated by edges, I will assume a simplified image model consisting of distributions supported on curvilinear singularities. I will prove that the theoretical performance of image inpainting depends on the microlocal properties of the representation system, namely exact image recovery is achieved if the size of the missing singularity is smaller than the size of the structure elements of the representation system. As a result, shearlet-based image inpainting algorithms significantly outperforms traditional multiscale methods due to the superiour microlocal properties of shearlets. In the second part of the talk, I will show how to apply this theoretical observation to improve a state-of-the-art algorithm for blind image inpainting based on Convolutional Neural Networks. This is a collaborative work with J. Schmalfuss, E. Scheurer, H. Zhao, N. Karantzas and A. Bruhn

MS 8–Talk 2: **Riemannian Optimization for Projection Robust Optimal Transport**

Authors: Shiqian Ma (Rice University)

Abstract: The optimal transport problem is known to suffer the curse of dimensionality. A recently proposed approach to mitigate the curse of dimensionality is to project the sampled data from the high dimensional probability distribution onto a lower-dimensional subspace, and then compute the optimal transport between the projected data. However, this approach requires to solve a max-min problem over the Stiefel manifold, which is very challenging in practice. In this talk, we propose a Riemannian block coordinate descent (RBCD) method to solve this problem. We analyze the complexity of arithmetic operations for RBCD to obtain an ϵ-stationary point, and show that it significantly improves the corresponding complexity of existing methods. Numerical results on both synthetic and real datasets demonstrate that our method is more efficient than existing methods, especially when the number of sampled data is very large.

MS 8–Talk 3: **Quantifying uncertainty at scale via structure-exploiting sparse grid approximation**

Authors: Ionut-Gabriel Farcas[1], Gabriele Merlo[1] and Frank Jenko[2] (1:The University of Texas at Austin, 2: Max Planck Institute for Plasma Physics)

Abstract: In many fields of science, remarkably comprehensive and realistic computational models are available nowadays.
Often, the respective numerical calculations call for the use of powerful supercomputers, and therefore only a limited number of cases can be investigated explicitly.
This prevents straightforward approaches to important tasks like uncertainty quantification and sensitivity analysis.
As it turns out, this challenge can be overcome via our recently developed sensitivity-driven dimension-adaptive sparse grid interpolation strategy.
The method exploits, via adaptivity, the structure of the underlying model (such as lower intrinsic dimensionality and anisotropic coupling of the uncertain inputs) to enable efficient and accurate uncertainty quantification and sensitivity analysis at scale.
We demonstrate the efficiency of our approach in the context of fusion research, in a realistic, computationally expensive scenario of turbulent transport in a magnetic confinement device with eight uncertain parameters and more than 264 million degrees of freedom in phase space, reducing the effort by at least two orders of magnitude.
In addition, we show that our method intrinsically provides an accurate surrogate model that is nine orders of magnitude cheaper than the high-fidelity model.

MS 8–Talk 4: **A general framework of rotational sparse approximation in uncertainty quantification**

Authors: Mengqi Hu, Yifei Lou, and Xiu Yang (1: Lehigh University, 2: University of Texas at Dallas)

Abstract: This paper proposes a general framework to estimate coefficients of generalized polynomial chaos (gPC) used in uncertainty quantification via rotational sparse approximation. In particular, we aim to identify a rotation matrix such that the gPC expansion of a set of random variables after the rotation has a sparser representation. However, this rotational approach alters the underlying linear system to be solved, which makes finding the sparse coefficients more difficult than the case without rotation.

MS 8–Talk 5: **Low-rank methods for solving high-dimensional collisional kinetic equations**

Authors: Jingwei Hu (University of Washington)

Abstract: Kinetic equations describe the nonlinear equilibrium dynamics of a complex system using a probability density function. Despite their important role in multiscale modeling to bridge microscopic and macroscopic scales, numerically solving kinetic equations is computationally demanding as they lie in the six-dimensional phase space. Dynamical low-rank method is a dimension-reduction technique that has been recently applied to kinetic theory, yet most of the endeavor is devoted to linear or collisionless problems. In this talk, we introduce efficient dynamical low-rank methods for BGK and Vlasov-Fokker-Planck equations, building on certain prior knowledge about the low-rank structure of the solution. This talk is based on the joint work with J. Coughlin, L. Einkemmer, and L. Ying.

MS 8–Talk 6: **An Inverse Problem in Mean Field Games from Partial Boundary Measurement**

Authors: Yat Tin Chow[1], Samy Wu Fung[2], Siting Liu[3], Levon Nurbekyan[3] and Stanley J. Osher[3] (1: University of California Riverside, 2: Colorado School of Mines, 3: University of California Los Angeles)

Abstract: In this talk, we consider a novel inverse problem in mean-field games (MFG). We aim to recover the MFG model parameters that govern the underlying interactions among the population based on a limited set of noisy partial observations of the population dynamics under the limited aperture. Due to its severe ill-posedness, obtaining a good quality reconstruction is very difficult. Nonetheless, it is vital to recovering the model parameters stably and efficiently to uncover the underlying causes of population dynamics for practical needs.

Our work focuses on the simultaneous recovery of running cost and interaction energy in the MFG equations from a finite number of boundary measurements of population profile and boundary movement. To achieve this goal, we formalize the inverse problem as a constrained optimization problem of a least squares residual functional under suitable norms. We then develop a fast and robust operator splitting algorithm to solve the optimization using techniques including harmonic extensions, three-operator splitting scheme, and primal-dual hybrid gradient method. Numerical experiments illustrate the effectiveness and robustness of the algorithm.

MS 8–Talk 7: **Adaptive deep density approximation for Fokker-Planck equations**

Authors: Xiaoliang Wan (Department of Mathematics and Center for Computation and Technology, Louisiana State University, USA)

Abstract: In this talk we present an adaptive deep density approximation strategy based on KRnet for solving Fokker-Planck (F-P) equations. F-P equations are usually high-dimensional and defined on an unbounded domain, which limits the application of traditional grid based numerical methods. With the Knothe-Rosenblatt rearrangement, KRnet improves the normalizing flow based on real NVP and provides an explicit PDF model as an effective solution candidate for the Fokker-Planck equations. KRnet has a weaker dependence on dimensionality than traditional computational approaches and can efficiently approximate general high-dimensional density functions. To obtain effective stochastic collocation points for the training set, we develop an adaptive sampling procedure, where samples are generated iteratively using the approximate PDF given by KRnet. Numerical experiments will be presented.

MS 8–Talk 8: **Sparse representation of seismic data using chains of destructors**

Authors: Sergey Fomel (Jackson School of Geosciences, the University of Texas at Austin)

Abstract: TBA

MS 9: Mathematical physics and graph theory

Organizers: R. Han, J. Fillman & S. Shipman

Quantum mechanics is a beautiful combination of mathematical elegance and descriptive insight into the physical world. Many different models have been proposed to understand phenomenons in quantum mechanic, but much of the literature was devoted to various models defined on the standard Zd lattice. Over the recent years, there have been an increasing interest in other lattice structures, which arise from different crystals, e.g. the hexagonal lattice in graphene. This has led to a beautiful combination of mathematical physics and graph theory. The aim of this mini-symposium intends to bring in experts in the TX-LA area to discuss and exchange insights over the recent developments. The proposed mini-symposium will be focused on the following areas of mathematical physics: • multi-layer graphene and other crystal, structures; • quantum graph models; • reducibility of Fermi surface and algebraic geometry; • critical points of periodic operators.

MS 9–Talk 1: **Eigenvalue statistics for the disordered Hubbard model within Hartree-Fock theory**

Authors: Rodrigo Matos (Texas A&M University)

Abstract: I will present recent progress on the spectral statistics conjecture for the Hubbard model within Hartree-Fock theory. Under weak interactions and for energies in the localization regime which are also Lebesgue points of the density of states, it is shown that a suitable local eigenvalue process converges in distribution to a Poisson process with intensity given by the density of states times Lebesgue measure. If time allows, proof ideas and further research directions will be discussed, including a Minami estimate and its applications.

MS 9–Talk 2: **A spectral statistic of quantum graphs without the semiclassical limit**

Authors: Jon Harrison (Baylor University)

Abstract: Energy level statistics of quantized chaotic systems are often evaluated in the semiclassical limit via their periodic orbits using the Gutzwiller or related trace formulae. Here, we evaluate a spectral statistic of 4-regular quantum graphs from their periodic orbits without the semiclassical limit. The variance of the n-th coefficient of the characteristic polynomial is determined by the sizes of the sets of distinct primitive periodic orbits with n bonds which have no self-intersections, and the sizes of the sets with a given number of self-intersections which all consist of two sections crossing at a single vertex. Using this we observe the mechanism that connects semiclassical results to the total number of orbits regardless of their structure. This is joint work with Tori Hudgins at the University of Kansas.

MS 9–Talk 3: **Limit-Periodic Dirac Operators with Thin Spectra**

Authors: Milivoje Lukić (Rice University)

Abstract: We prove that limit-periodic Dirac operators generically have spectra of zero Lebesgue measure and that a dense set of them have spectra of zero Hausdorff dimension. The proof combines ideas of Avila from a Schrödinger setting with a new commutation argument for generating open spectral gaps. This overcomes an obstacle previously observed in the literature; namely, in Schrödinger-type settings, translation of the spectral measure corresponds to uniformly small perturbations of the operator data, but this is not true for Dirac or CMV operators. The new argument is much more model-independent. To demonstrate this, we also apply the argument to prove generic zero-measure spectrum for CMV matrices with limit-periodic Verblunsky coefficients. This is joint work with Benjamin Eichinger, Jake Fillman, and Ethan Gwaltney.

MS 9–Talk 4: **Analytic tongue boundaries and Cantor spectrum**

Authors: Long Li (Rice University)

Abstract: We generalized an idea of Broer-Puig-Simo 2003, Puig-Simo 2004, that is, the analyticity of the tongue boundaries for continuous almost Mathieu operators. With this generalized result, we showed that adding a small quasi-periodic perturbation to periodic Verblunsky coefficients could lead to Cantor spectrum of the CMV matrices.

MS 9–Talk 5: **Inverse Uniqueness Result for Hamiltonian System with Measure Coefficients**

Authors: Chunyi Wang (Rice University)

Abstract: All self-adjoint differential operators of one variable can be written as a linear Hamiltonian system. To be more general, we can introduce Borel measures as coefficients of Hamiltonian systems in order to cover some singular cases, for example, δ and δ'-interactions in Schrödinger operators.
After building the direct spectral theory of Hamiltonian system with measure coefficients, including self-adjoint extension, Weyl-Titchmarsh theory and eigenfunction expansion, I will show the spectral uniqueness result of with the tool of canonical system and de Branges space.

MS 9–Talk 6: **Hyponormal Toeplitz Operators Acting on the Bergman Space**

Authors: Brian Simanek (Baylor University)

Abstract: We will consider Toeplitz operators with bounded symbol f acting on the Bergman space of the unit disk by multiplication followed by orthogonal projection. The goal is to understand those symbols f that make the resulting operator hyponormal. We will pay special attention to the case when the symbol is of the form $f + cg$, where the symbol f yields a hyponormal operator, the symbol g does not yield a hyponormal operator, and c is a complex constant. Our main results will consider specific choices of f and g that are algebraic functions of z and $\bar{z}$ and describe those constants c for which $f + cg$ yields a hyponormal operator. This is based on joint work with Trieu Le and Nicole Revilla.

MS 9–Talk 7: **Fermi Isospectrality**

Authors: Frank Sottile (Texas A&M University)

Abstract: Given a discrete operator L on a $\mathbb{Z}^d$-periodic graph with a periodic potential, Floquet theory refines the spectrum of L in terms of the unitary characters of $\mathbb{Z}^d$. This gives the Floquet Variety whose level sets at a fixed energy are Fermi varieties. A natural question is how much do the resulting Floquet and Fermi varieties determine the potential and parameters of the graph? Potentials with the same Floquet (Fermi) varieties are Floquet (Fermi) isospectral. For the Schrödiniger operator on the grid graph on $\mathbb{Z}^d$ acted on by the free abelian subgroup $q_1\mathbb{Z} + ... + q_d\mathbb{Z}$ (q_i are pairwise coprime), Kappeler showed that there are only finitely many potentials Floquet isospectral to a given potential. Liu introduced the term Fermi isospectrality and considered it for separable potentials when $d = 2$.
This talk will discuss this history and present continuing work with Faust and Liu studying Fermi isospectrality for the grid graph when $d = 2$.

MS 9–Talk 8: **Quantum Complexity of Permutations**

Authors: Andrew Yu (Phillips Academy - Andover)

Abstract: Quantum complexity of a unitary measures the runtime of quantum computers. In this talk, we discuss the complexity of a special type of unitaries, permutations. Let S_n be the symmetric group of all permutations of $\{1, \cdots, n\}$ with two generators: the transposition and the cyclic permutation (denoted by σ and τ). The permutations $\{\sigma, \tau, \tau^{-1}\}$ serve as logic gates. We give an explicit construction of permutations in S_n with quadratic quantum complexity lower bound $\frac{n^2-2n-7}{4}$. We also prove that all permutations in S_n have quadratic quantum complexity upper bound $3(n-1)^2$. Finally, we show that almost all permutations in S_n have quadratic quantum complexity lower bound when $n \to \infty$. The method described in this paper may shed light on the complexity problem for general unitaries in quantum computation.

MS 10: High-order numerical methods for partial differential equations

Organizers: J. Huang & Z. Sun

High order numerical methods have been continuously receiving intensive attentions for solving partial differential equations. They are typically able to better resolve solutions with overall fewer computational resources. The goal of the special session is to gather researchers in this area and to discuss the recent advances in the development of high order methods. Topics may cover but are not limited to numerical analysis of high order methods, techniques for enhancing robustness and efficiency of numerical schemes, and development of structure-preserving high order methods for physical models.

MS 10–Talk 1: **Hermite Methods for Wave Equations**

Authors: Tom Hagstrom[1] and Yann-Meing Law-Kam-Cio[2] and Daniel Appelo[2] (1: Southern Methodist University, 2: Michigan State University)

Abstract: An amazing property of Hermite interpolation is that it is a projection in a Sobolev seminorm. As a result, in contrast with the usual Lagrange interpolant, Hermite interpolation has a smoothing effect. We show how to exploit this projection property to develop Hermite-based solvers for differen- tial equations which, for hyperbolic pdes, admit order-independent time steps and highly localized evolution processes which can be

exploited on modern computer architectures. We highlight the application of Hermite methods to Maxwell's equations as well as recent developments related to the imposition of boundary conditions.

MS 10–Talk 2: **An energy-based discontinuous Galerkin method for a nonlinear variational wave equation**

Authors: Lu Zhang (Columbia University)

Abstract: We design and numerically validate an energy-based discontinuous Galerkin method for a nonlinear variational wave equation originally proposed to model liquid crystals. Energy-conserving or energy-dissipating methods follow from simple, mesh-independent choices of the interelement fluxes. Error estimates in an energy norm are established, and numerical experiments on structured grids display optimal convergence in the L2 norm for certain fluxes.

MS 10–Talk 3: **Build Frequency Domain Maxwell/Helmholtz Solver form Time Domain Solvers with WaveHoltz Method and Its Preconditioning**

Authors: Zhichao Peng (Michigan State University)

Abstract: Two main challenges to design efficient iterative solvers for the frequency-domain Maxwell/Helmholtz equations are the indefinite nature of the underlying system and the high resolution requirements. Scalable parallel solvers are highly desired. Recently, we develop a scalable iterative solver built on time-domain solvers called WaveHoltz to solve the Helmholtz equation and the time-harmonic Maxwell equations. Three main advantages of the proposed method are as follows. (1) It always results in a better conditioned linear system, and the resulting linear system is positive definite for energy conserving problems with PEC boundary conditions. The number of iterations for the convergence is independent of points per wavelength. (2) It is flexible and simple to convert available scalable time-domain solvers to an efficient frequency-domain solver. (3) It is possible to obtain solutions for multiple frequencies in one solve. In this talk, we would present the formulation of electromagnetic WaveHoltz for the time-harmonic Maxwell equations, and discuss deflation techniques to further accelerate the WaveHoltz iterative solver.

MS 10–Talk 4: **On a numerical artifact of solving shallow water equations with a discontinuous bottom: Analysis and a nontransonic fix**

Authors: Zheng Sun[1] and Yulong Xing[2] (1: The University of Alabama, 2: The Ohio State University)

Abstract: In this talk, we discuss a numerical artifact of solving the nonlinear shallow water equations with discontinuous bottom topography. For a few first-order schemes, the numerical solution will form a spurious spike in the momentum, which should not exist in the exact solution. The height of the spike cannot be reduced by the mesh refinement. In many problems, this numerical artifact may cause the wrong convergence, which means that the limit of the numerical solution is not a weak solution of the shallow water equations. To explain the formation of the spurious spike, we perform a convergence analysis of the numerical methods. It is shown that the spurious spike is caused by the numerical viscosity at the discontinuous bottom and its height is proportional to the viscosity constant in the numerical flux. Furthermore, by adopting appropriate modifications at the bottom discontinuity, we show that this numerical artifact can be removed in many cases. For various of numerical tests with nontransonic Riemann solutions, the modified scheme is able to retrieve the correct convergence.

MS 10–Talk 5: **Structure preserving methods for the Euler-Poisson system**

Authors: Ignacio Tomas[1] and Matthias Maier[2] and John Shadid[3] (1: Texas Tech University, 2: Texas A&M University, 3: Sandia National Laboratories)

Abstract: Depending on whether the forces are repulsive or attractive, the Euler-Poisson model may represent electrons subject to an electric field or a mass density subject to gravitational effects. This simple PDE model embodies one of the central themes of mathematical physics: the evolution of a density subject to its own self-consistent field. An exhaustive, but still incomplete, list of desirable properties for a numerical scheme solving the Euler-Poisson model is: (i) Preservation of positivity of density and internal energy, (ii) Satisfaction of discrete total energy-balance (kinetic + internal + potential), (iii) Asymptotically well-posed linear algebra (i.e. no artificial rank-deficiencies at asymptotic limits), (iv) Satisfaction of a discrete Gauss-law at the end of each time-step, (v) Numerical stability in the context of large plasma frequency regimes, (vi) Asymptotic preservation in the context of quasi-neutrality, (vii) Asymptotic preservation with respect to the drift-diffusion limit. All of these requirements are of great importance in practice, but in general, they will compete against each other and might not be attainable at the same time. In this talk, we advance numerical methods that can achieve properties (i)-(v).

MS 10–Talk 6: **A positivity preserving strategy for entropy stable discontinuous Galerkin discretizations of the compressible Euler and Navier-Stokes equations**

Authors: Yimin Lin[1], Jesse Chan[1], Ignacio Tomas[2] (1: Rice University, 2: Sandia National Laboratories)

Abstract: High-order entropy-stable discontinuous Galerkin methods for the compressible Euler and Navier-Stokes equations require the positivity of thermodynamic quantities in order to guarantee their well-posedness. In this work, we introduce a positivity limiting strategy for entropy-stable discontinuous Galerkin discretizations constructed by blending high order solutions with a low order positivity-preserving discretization. The proposed low order discretization is semi-discretely entropy stable, and the proposed limiting strategy is positivity preserving for the compressible Euler and Navier-Stokes equations. Numerical experiments confirm the high order accuracy and robustness of the proposed strategy.

MS 10–Talk 7: **A structure preserving, conservative, low-rank tensor scheme for solving the 1D2V Vlasov-Fokker-Planck equation**

Authors: Joseph H. Nakao (University of Delaware)

Abstract: We propose a hybrid low-rank tensor scheme for solving the 1D2V Vlasov-Fokker-Planck equation in Cartesian physical space and cylindrical velocity space. The solution is full rank in physical space and low rank in velocity space. By incorporating several robust methods into our proposed algorithm, we attain a scheme that is conservative, equilibrium preserving, relative entropy dissipative, and low-rank with low storage complexity. A kinetic ion – fluid electron model is assumed; the Leonard-Bernstein-Fokker-Planck operator is discretized using a structure preserving Chang-Cooper method; and the updated solution is truncated using a local macroscopic conservative low rank tensor method. Preliminary numerical results are presented to demonstrate these properties.

MS 10–Talk 8: **Uniform accuracy of implicit-explicit methods for stiff hyperbolic relaxation systems and kinetic equations**

Authors: Ruiwen Shu[1] and Jingwei Hu[2] (1: University of Georgia, 2: University of Washington)

Abstract: Many hyperbolic and kinetic equations contain a non-stiff convection/transport part and a stiff relaxation/collision part (characterized by the relaxation or mean free time ε). To solve this type of problems, implicit-explicit (IMEX) methods have been widely used and their performance is understood well in the non-stiff regime ($\varepsilon = O(1)$) and limiting regime ($\varepsilon \to 0$). However, in the intermediate regime (say, $\varepsilon = O(\Delta t)$), uniform accuracy has been reported numerically for most IMEX multistep methods, while complicated behavior of order reduction has been observed for IMEX Runge-Kutta (RK) methods. In this talk, I will take a linear hyperbolic systems with stiff relaxation as a model problem, and discuss how to use energy estimates with multiplier techniques to prove the uniform accuracy of IMEX methods. In particular, I will present my joint works with Jingwei Hu on the uniform accuracy of IMEX backward differentiation formulas (IMEX-BDF) up to fourth order, and that of IMEX-RK methods up to third order.

MS 11: Hamiltonian and integrable systems

Organizers: B. Feng & T. Ohsawa

Many mathematical models arising from physics and engineering are Hamiltonian systems, and in some special cases, also integrable systems as well. These systems can be studied by analytical, algebraic, and geometric approaches. The purpose of this minisymposium is to bring a group of researchers of Hamiltonian and integrable systems with diverse backgrounds to present their recent findings and exchange ideas for further developments.

MS 11–Talk 1: **Regularity and Lipschitz optimal transport metric for scalar integrable systems with cusp singularity**

Authors: Geng Chen (University of Kansas)

Abstract: The talk is concerned with some classes of scalar integrable systems with cusp singularity, such as the Camassa-Holm equation and Novikov equation. It is known that the equations determine a unique flow of conservative solutions within the natural energy space $H^1(R)$. However, the solution flow is not Lipschitz continuous w.r.t. the H^1 distance. We will discuss the regularity of solution and the optimal transport metric render Lipschitz continuous dependence.

MS 11–Talk 2: **Semi-discrete Camassa-Holm and modified Camassa-Holm equations and their connection with the discrete KP equation**

Authors: Baofeng Feng (University of Texas Rio Grande Valley)

Abstract: We will build up a deformed KP-Toda hierarchy from discrete KP equation via Miwa transformations. Then based on the set of bilinear equations and their Bäcklund transformations, we construct semi-discrete Camassa-Holm and modified Camassa-Holm equations.

MS 11–Talk 3: **Crack Problem Under Strain Gradient Elasticity Of Bi-Helmholtz Type**

Authors: Youn-Sha Chan (University of Houston-Downtown)

Abstract: A crack problem is solved under a higher order of strain gradient elasticity theory of bi-Helmholtz type, and it leads to a linear partial differential equation (PDE) of sixth order. The sixth order PDE can be viewed as a composition of two differential operators: a second order Navier operator coming from the classical linear elasticity theory, and a fourth order bi-Helmholtz operator due to the higher order strain gradient elasticity. The bi-Helmholtz operator consists of two length scales, l_1 and l_2. The sixth order PDE of the mode III crack problem is transformed to a hypersingular integral equation by the Fourier transform, and the corresponding integral equation is discretized by using the collocation method and a Chebyshev polynomial expansion. The numerical results include displacement profiles, strain, and stress fields under various combinations of l_1 and l_2.

MS 11–Talk 4: **Alchemy as a quantum control problem: Mathematical prospective**

Authors: Denys I. Bondar (Tulane University)

Abstract: Using the methods of quantum control, we theoretically unveiled an unexplored flexibility of optics that a shaped laser pulse can drive a quantum system to emit light as if it were an arbitrary different system. This realizes an aspect of the alchemist's dream to make different elements *look alike*, albeit for the duration of a laser pulse. I will review different unusual formulations of quantum control problems and outline some of their properties.

MS 11–Talk 5: **On metriplectic dynamics: joint Hamiltonian and dissipative dynamics**

Authors: Philip J. Morrison (University of Texas at Austin)

Abstract: Although an early generalization of Lagrangian mechanics to include dissipation was proposed by Rayleigh (1894) and subsequently various other frameworks for dissipation were given, e.g., for phase separation in Cahn-Hilliard (1958) and Ricci flows in Hamilton (1982), here we discuss, metriplectic dynamics (MD), a bracket formalism approach begun by the author (1982) for describing systems that have both Hamiltonian and dissipative parts, which places the laws of thermodynamics in a dynamical systems setting. The motivation of MD is to describe dissipation in a kind of bracket formalism that complements the nondissipative noncanonical Poisson bracket formalism (flows on Poisson manifolds). Recent thoughts on the topic will be presented.

MS 11–Talk 6: **Approximation of semiclassical expectation values by symplectic Gaussian wave packet dynamics**

Authors: Tomoki Ohsawa (University of Texas at Dallas)

Abstract: This talk concerns an approximation of the expectation values of the position and momentum of the solution to the semiclassical Schrödinger equation with a Gaussian as the initial condition. Of particular interest is the approximation obtained by our symplectic/Hamiltonian formulation of the Gaussian wave packet dynamics that introduces a correction term to the conventional formulation using the classical Hamiltonian system by Hagedorn and others. The main result is a proof that our formulation gives a higher-order approximation than the classical formulation does to the expectation value dynamics under certain conditions on the potential function. Specifically, as the semiclassical parameter ε approaches 0, our dynamics gives an $O(\varepsilon^{3/2})$ approximation of the expectation value dynamics whereas the classical one gives an $O(\varepsilon)$ approximation.

MS 12: Tensor modeling and applications

Organizers: Y. Lou & S. Minkoff

In many data-driven applications, high-dimensional data can be naturally represented by a tensor. Tensor-based methodologies ranging from modeling to optimization have received tremendous attention. This mini-symposium will feature talks on tensor algebra, representation theories, and optimization algorithms together with their applications. The aim is to provide a platform to exchange ideas across disciplines and encourage collaborations.

MS 12–Talk 1: **Tensor regularization and reconstruction workflow for time-lapse seismic data**

Authors: Jonathan Popa, Susan E. Minkoff, and Yifei Lou (The University of Texas at Dallas)

Abstract: Seismic surveys record data to image the Earth's subsurface. Time-lapse seismic data consists of multiple seismic surveys recorded over the same area. The time-lapse difference reveals changes in the subsurface over time. Inconsistencies in survey parameters, such as source and receiver locations, motivate the need for data processing to improve the repeatability between surveys. One such processing tool is regularization (or binning) that aligns multiple surveys with different source or receiver configurations onto a common grid. The binned data from each survey can be stored in a tensor. The presence of gaps and noise in data increases the rank of the tensor. By applying low rank based tensor completion seismic data can be reconstructed. The tensor nuclear norm (TNN) is defined by the tensor singular value decomposition (tSVD) which generalizes the matrix SVD. The tensor resulting from binning the time-lapse data can be completed using the alternating direction method of multipliers (or ADMM) to minimize the TNN. We apply this workflow of binning and reconstruction using TNN-ADMM to recover both synthetic and field time-lapse seismic data.

MS 12–Talk 2: **Tensor-tensor algebra for optimal representations and compression of multiway data**

Authors: Misha Kilmer[1] and Lior Horesh[2] and Haim Avron[3] and Elizabeth Newman[4] (1: Tufts University, 2: IBM Research, 3: Tel Aviv University, 4: Emory University)

Abstract: The explosion of data and data-driven approaches has demanded advancements in dimensionality reduction and feature extraction. Tensor-based approaches have gained significant traction in data compression by exploiting multilinear relationships in multiway data. In this talk, we will describe a matrix-mimetic tensor algebra that offers provably optimal compressed representations of high-dimensional data. We will compare this tensor-algebraic approach to other popular tensor decomposition techniques and show that our approach offers both theoretical and numerical advantages.

MS 12–Talk 3: **Modewise tensor decompositions and applications**

Authors: HanQin Cai[1], Keaton Hamm[2], Longxiu Huang[3], and Deanna Needell[4] (1: University of Central Florida, 2: University of Texas at Arlington, 3: Michigan State University, 4: University of California, Los Angeles)

Abstract: We discuss low-Tucker rank tensor decompositions obtained by subsampling along modes of a given tensor. These are tensor analogues of CUR decompositions for matrices (also called pseudoskeleton decompositions). We will characterize exact decompositions, low-rank approximations, and applications to image and video processing.

MS 12–Talk 4: **Moment Estimation for Nonparametric Mixture Models through Implicit Tensor Decomposition**

Authors: Yifan Zhang, Joe Kileel (University of Texas at Austin)

Abstract: Mixture models give reduced representations for complex data distributions. Despite the success of the Expectation-Maximization (EM) algorithm for fitting mixture models, recently Method of Moment (MoM) based algorithms have been receiving increased attention. In this talk, I will present a new nonparametric MoM algorithm on high dimensional conditionally independent mixture models (features are independent conditioning on the class label) that computes the mixture weights and moments of each class. It hinges on efficient computations with higher-order tensors and a certain coupled system of low-rank tensor problems. I will develop an alternating least-squares optimization scheme to solve this, with cost essentially independent of the tensor orders. I will compare this method to EM on a variety of simulated mixture models and also a real dataset. Time permitting, I will mention theoretical results on convergence and identifiability as well as a possible application to microscopy imaging. Joint work with Joe Kileel.

MS 13: Numerical methods and applications for geosciences

Organizers: G. Sosa Jones & L. Cappanera

Computational geosciences often involve complex nonlinear models that couple different physical processes. The study of such problems requires the development of robust and efficient numerical algorithms for high performance computing. In this mini symposium, we focus on numerical methods applied to phenomena arising in geosciences such as reservoir simulation, multiphase flow, water waves, etc. Speakers will present their recent research developments and applications in computational geosciences which includes numerical modeling, numerical analysis, and other computational aspects.

MS 13–Talk 1: **Coupling and decoupling two-phase flows in superposed free flow and porous media**

Authors: Daozhi Han (University at Buffalo)

Abstract: In this talk we introduce a Cahn-Hilliard-Navier-Stokes-Darcy model for two-phase flows in superposed free flow and porous media. The model satisfies an energy law. We then present an unconditionally stable numerical algorithm that preserves the energy law and decouples the computation of Cahn-Hilliard equation, Darcy equations, Navier-Stokes equations. Moreover, the velocity field and pressure are also decoupled in the Navier-Stokes solver that avoids the pressure interface boundary condition.

MS 13–Talk 2: **Finite element methods of porous media flows with low permeability faults/membranes**

Authors: Jeonghun Lee (Baylor University)

Abstract: In this work we consider porous media flow models with low permeability fault/membrane structures. Macroscopic models of such structures give fluid flow solutions with low regularities and pressure fields with jumps across the fault/membranes. We develop finite element methods for the models and analyze a priori and

a posteriori error estimates of solutions. We then consider extensions of the models for miscible displacement problems.

MS 13–Talk 3: **Finite element methods for incompressible flows with variable density applied to thermodynamics.**

Authors: An Vu (University of Houston)

Abstract: We introduce a semi-implicit time stepping scheme for the incompressible Navier-Stokes equations with variable density and viscosity. The scheme uses a projection method to enforce the incompressibility of the flow and the momentum, which equals the product of density and velocity, as dependent variable. We prove the stability and establish first order error estimates of this semi-implicit scheme. We also extend our study to thermodynamics setups by introducing a time stepping multiphase thermal solver and proving the stability estimates of this new method. A fully discretized algorithm is proposed using finite element and pseudo spectral methods, and its convergence properties are verified using numerical simulations.

MS 13–Talk 4: **Convergence Analysis of a Continuous Interior Penalty Method for the Modified Phase Field Crystal Equation**

Authors: Natasha Sharma[1], Amanda E. Diegel[2], Daniel Bond[3] (1: University of Texas at El Paso, 2: Mississippi State University, 3: University of Tennessee)

Abstract: The so-called phase-field crystal (PFC) approach proposed by Elder et al. has been employed as a continuum model to describe the microstructure of solid-liquid systems such as the crystal growth in a supercooled liquid and provides an accurate way to model crystal dynamics, especially defect dynamics in atomic-scale resolution. However, it fails to distinguish between elastic relaxation and diffusion time scales. To overcome this difficulty and to incorporate both the faster elastic relaxation (e.g., in a rapid quasi-phononic time scale) and the slower mass diffusion, the modified phase-field crystal (MPFC) equation has recently been proposed by P. Stefanovic and co-authors. The MPFC is a generalized damped wave equation characterized through the presence of a second-order time derivative weighted by a positive parameter. In this talk, we present a continuous interior penalty finite element method for the sixth-order modified phase field crystal equation and prove that the numerical scheme is uniquely solvable, unconditionally energy stable, and convergent. Finally, we close this talk with a numerical experiment demonstrating the performance of our proposed method.

MS 13–Talk 5: **A sequential discontinuous Galerkin method for three-phase flows in porous media**

Authors: Giselle Sosa Jones[1], Loic Cappanera[2], and Beatrice Riviere[3] (1: Oakland University, 2: University of Houston, 3: Rice University)

Abstract: In this talk, we first present and analyze a sequential discontinuous Galerkin method for the incompressible three-phase flow problem in porous media. We show existence and uniqueness of a discrete solution and obtain a priori error estimates. Then, we present a novel formulation for the black oil problem which uses as primary unknowns the liquid pressure and the aqueous and liquid saturations. This choice of primary variable produces a well-posed numerical scheme without any stringent restriction on the data, and without the introduction of nonphysical quantities. The equations are solved sequentially using an implicit time stepping scheme. We demonstrate the convergence properties of the method numerically, and present different realistic simulations such as injection problems in highly heterogeneous media.

MS 13–Talk 6: **Implicit dynamical low rank discontinuous Galerkin methods for space homogeneous neutrino transport equations**

Authors: Peimeng Yin, Eirik Endeve, Cory Hauck, and Stefan Schnake (Oak Ridge National Laboratory)

Abstract: Neutrino transport plays an important role in core-collapse supernova (CCSN) explosions. Due to the multiscale nature of neutrino transport in CCSN simulations, an implicit treatment is desired. The equations are high dimensional and their solutions can converge to isotropic equilibrium distributions, which are low dimensional, in regions of high Knudsen number. We propose implicit dynamical low rank discontinuous Galerkin (DLR-DG) methods for space homogeneous neutrino transport equations. Compared with the classical DG method, the DLR-DG solution here is a DG approximation with the corresponding coefficient matrix in a rank-r manifold. The proposed DLR-DG method is shown to be stable even for large time steps and has lower computational complexity compared with the classical DG method. Numerical test results are presented to justify the theoretical findings.

MS 13–Talk 7: **Numerical solution of two-phase poroelasticity equations**

Authors: Beatrice Riviere[1] and Boqian Shen[2] (1: Rice University, 2: KAUST)

Abstract: The two-phase Biot problem is discretized by a sequential scheme that utilizes the discontinuous Galerkin method in space. Because of appropriate stabilization terms, no iterations are required for stability. We study the effect of heterogeneities (different capillary pressures in different subdomains) and the effect of loading on the propagation of the fluid in three-dimensional domains.

MS 13–Talk 8: **Applications of Space-Time Methods to Multiphase Flow in Porous Media : Channel Flow and Snap Shot Selection for Deep-Learning Reduced-Order Models**

Authors: Mary Wheeler[1], Thamer Abbas Alsulaimani[2] and Hanyu Li[3] (1: University of Texas at Austin, 2: Aramco, 3: Lawrence Livermore National Laboratory)

Abstract: Numerical simulation of subsurface flow for applications such as carbon sequestration and nuclear waste deposit has always been a computational challenge. The main reason points to the strong nonlinearity inherited in the governing equations that describe the multiphysics phenomena. The enormous number of unknowns and small timesteps required for stable Newtonian convergence make this type of problems computationally exhaustive. To address this issue, we introduce adaptive finite element approaches guided by a posteriori error estimators to improve computational efficiency. A space-time discretization scheme with temporal and spatial mesh adaptivity is formulated for multiphase flow system. The solution algorithm adopts a geometric multigrid procedure that starts with solving the system in the coarsest resolution and locally refines the mesh in both space and time.

Error estimators that measure the spatial and temporal discretization error are employed to guide such an adaptivity. These estimators provide a global upper bound on the dual norm of the residual and the non-conformity of the numerical solution. Results from two-phase immiscible and three-phase miscible flow are presented to confirm solution accuracy and computational efficiency as compared to the uniformly fine timestep and fine spatial discretization solution. We also resolve the common issue of high frequency residuals in multigrid methods by local residual minimization and dynamic advection-diffusion coupling to achieve additional computational speedup and stability.

Here we introduce a novel approach based on space-time to select an optimal set of snapshots for training deep-learning ROM for two phase flow.. Snapshot selection is based on the jump in the number of local refinements between two consecutive snapshots provided by the space-time geometric multigrid solver. Results from the deep-learning reduced-order model show that we can achieve faster convergence to the solution using only 65% of the snapshots generated at fixed intervals. Computational time savings accrued while generating the snapshots and while using the optimized snapshots in the deep-learning model. Results generated using fixed time interval snapshots, and adaptively selected snapshots show similar accuracy.

MS 14: Mathematics and Computation in Biomedicine

Organizers: Sebastian Acosta and Charles Puelz

This mini-symposium is concerned with new developments in mathematical modeling, numerical methods, and computational science for applications in biomedicine in the broadest possible sense. Topics include biomechanics, cardiovascular simulations, inverse problems, imaging, computational oncology, epidemiology and machine learning.

MS 14–Talk 1: **Stochastics epidemic models with infection-age dependent infectivity in large populations**

Authors: Guodong (Gordon) Pang (Rice University)

Abstract: In this talk we will discuss several stochastic epidemic models recently developed to account for general infectious durations, infection-age dependent infectivity and/or progress loss of immunity/varying susceptibility, extending the standard epidemic models (including SIR, SEIR, SIRS, SEIRS). Each individual in the population is attached with a random function/process that represents the infectivity force to exert on other individuals. This approach models infection-age dependent infectivity, and is also extended to include a random function that represents the immunity/susceptibility attached to each individual. A typical infectivity function first increases and then decreases from the epoch of becoming infected to the time of recovery, while a typical susceptibility function gradually increases from the time of recovery to the time of losing immunity and becoming fully susceptible. We analyze the population dynamics of the infected and recovered individuals, and the total infectivity and susceptibility processes by establishing the scaling limits (functional law of large numbers and central limit theorems) in large populations. The limits are deterministic and stochastic Volterra integral equations, respectively. We also discuss some new PDEs models arising from the scaling limits.

MS 14–Talk 2: **On the endemic behavior of a competitive tri-virus SIS networked model**

Authors: Sebin Gracy, Mengbin Ye, Brian D.O. Anderson, and Cesar A. Uribe (Rice University)

Abstract: We study the endemic behavior of a multi-competitive networked susceptible-infected-susceptible (SIS) model. In particular, we focus on the case where there are three competing viruses (i.e., tri-virus system). First, we show that the tri-virus system is not monotone. Thereafter, we provide a necessary and sufficient condition for local exponential convergence to a boundary equilibrium (exactly one virus is alive, the other two are dead) and identify a special case that admits the existence and local exponential attractivity of a line of coexisting equilibria (at least two viruses are active). Finally, we identify a particular case (subsumed by the aforementioned special case) such that for all nonzero initial infection levels, the dynamics of the tri-virus system converge to a plane of coexisting equilibria.

MS 14–Talk 3: **Mechanistic models of Alzheimer's disease**

Authors: Travis B. Thompson (Texas Tech University)

Abstract: Can mathematics understand Alzheimer's disease (AD)? The discovery of AD, in 1906, marks a watershed at the intersection of neurology, biochemistry and neuroscience. The first AD patient exhibited a progressive loss of memory, language and behavioral control; upon death, distinctive plaques and neurofibrillary tangles were reported in the brain histology. These observations prompted questions: How, and why, do plaques form; are they the cause or consequence of cognitive aberrations; are there viable treatments for the disease? Nearly a century passed before any significant progress was made in AD research but, over the last 25 years, breakthrough discoveries have provided significant advancements. The systematic, in vivo study of human AD is ethically constrained but insights from animal models, contemporary improvements in medical imaging and novel methods from mathematics and computing are circumventing the barriers for AD research in Man. In this talk, several in vitro and histopathological observations regarding the progression of protein pathology in AD will be briefly presented. Following this, the recent *network dynamical systems* (NDS) framework for modeling neurodegenerative dynamics will be introduced; several models within the NDS framework will be surveyed and their coupling to human neuroimaging data will be discussed. Overall, we will see that mechanistic network mathematical models and scientific computing are emerging as a valuable tool for understanding AD in vivo and, with further research, are likely to provide a novel path forward for the design and testing of treatment and intervention.

MS 14–Talk 4: **Image-calibrated dynamic system for tau propagation in Alzheimer's disease**

Authors: Zheyu Wen, Ali Ghafouri, George Biros (The University of Texas at Austin)

Abstract: Alzheimer's disease (AD) is a long term scale terminal disease. PET and MRI characterize loss of gray matter and misfolded protein concentrations. Quantitatively describing how tau protein spreads in human brains can help with AD diagnosis and prognosis. Our goal is to use tau-PET images along with traditional magnetic resonance imaging to learn a dynamic model of tau propagation. In this talk we will discuss the mathematical and computational challenges of the underlying methodology as well as a set of new algorithms that enable quantification of tau spreading. We test our method on a cohort of subjects selected from publically available datasets.

MS 14–Talk 5: **Optimal experimental design for quantitative MRI with MR fingerprinting**

Authors: Bo Zhao, Evan Scope Crafts, and Hengfa Lu (University of Texas at Austin)

Abstract: Magnetic Resonance (MR) Fingerprinting is a recent breakthrough in quantitative magnetic resonance imaging, which enables the rapid quantification of multiple MR tissue parameter maps in a single imaging experiment. The original MR Fingerprinting experiments feature a randomized encoding strategy, which applies a sequence of random acquisition parameters to probe the spin system. Despite its empirical success, the optimality of this encoding scheme has not been thoroughly examined since the invention of the technique. In this talk, I will present an optimal experimental design framework to characterize and optimize the encoding process of MR Fingerprinting. Specifically, we will present a discrete-time dynamic system to model magnetization evolutions and further utilize a principled estimation-theoretic metric to optimize the acquisition parameters of MR Fingerprinting. The proposed optimal design method enables a substantial improvement of signal-to-noise efficiency of the acquisition process. In addition, our recent computational algorithm utilizing a B-spline based low-dimensional representation significantly improves the computational efficiency of the optimal design technique.

MS 14–Talk 6: **Registering MRA images to 4D flow MRI images**

Authors: Dan Lior (Baylor College of Medicine)

Abstract: A velocity field and intensity field, respectively representing blood flow and vessel tissue of a given patient, are often acquired in the same MRI series. Each of these fields contains valuable information for vessel modeling and analysis that the other lacks. There is an obvious need to combine the fields. An obstacle to this end is the misalignment of the fields. There are several factors contributing to the misalignment, one of which is a shift that can occur in the position and orientation of the patient between scans in the series. A robust method to rigidly register the two fields is based on centerline extraction. This method will be presented.

MS 14–Talk 7: **Early detection of cardiac arrest in infant with congenital heart defects using convolutional denoising autoencoders**

Authors: Arko Barman, Kunal Rai, Chiraag Kaushik, Frank Yang, Tucker Reinhardt, Andrew Pham, Aneel Damaraju, Mubbasheer Ahmed, Sebastian Acosta, Parag Jain (Rice University and Baylor College of Medicine)

Abstract: Early detection of cardiac arrest can pave the way to better outcomes for patients suffering from diseases such as hypoplastic left heart syndrome (HLHS), a severe congenital heart defect that, if left untreated, leads to death in 95% of cases within a few weeks of birth. Even after surgical treatment, these patients continue to be at high risk of sudden cardiac arrests (SCA). The difficulty in early detection of these SCAs is due to subtle irregularities of electrocardiogram (ECG) morphology in such patients, which are often missed by physicians monitoring these ECG signals. To address this problem, we propose the use of a convolutional denoising autoencoder (CDAE) architecture in conjunction with change-point detection, using a novel metric that we denote as Cumulative Reconstruction Error (CuRE). Our proposed pipeline uses 4-lead ECG data to perform early detection of patient-specific cardiac instability. The method is robust to noise due to the use of CDAE architecture and to inter-patient variability since the proposed analysis is patient-specific in nature. Our method achieves a sensitivity of 71% with an average early detection time of 1.132 +/- 0.286 (95% confidence interval) hours before cardiac arrest, with instability detection as early as 2.927 hours before cardiac arrest.

MS 14–Talk 8: **Generalized broken ray transforms in tomography**

Authors: Gaik Ambartsoumian[1] and Mohammad J. Latifi[2] (1: University of Texas at Arlington, 2: Dartmouth College)

Abstract: Mathematical models of various imaging modalities are based on integral transforms mapping a function (representing the image) to its integrals along specific families of curves or surfaces. Those integrals are generated by external measurements of physical signals, which are sent into the imaging object, get modified as they pass through its medium and are captured by sensors after exiting the object. The mathematical task of image reconstruction is then equivalent to recovering the image function from the appropriate family of its integrals, i.e. inverting the corresponding integral transform (often called a generalized Radon transform). A classic example is computerized tomography (CT), where the measurements of reduced intensity of X-rays that have passed though the body correspond to the X-ray transform of the attenuation coefficient of the medium. Image reconstruction in CT is achieved through inversion of the X-ray transform. In this talk, we will discuss several novel imaging techniques using scattered particles, which lead to the study of generalized Radon transforms integrating along trajectories and surfaces containing a "vertex". The relevant applications include single-scattering X-ray tomography, single-scattering optical tomography, and Compton camera imaging. We will present recent results about injectivity, inversion, stability and other properties of the broken ray transform, conical Radon transform and the star transform.

MS 14–Talk 9: **Estimation of aortic valve interstitial contractile behaviors using an inverse finite element approach**

Authors: Alex Khang and Michael S. Sacks (University of Texas at Austin)

Abstract: Aortic valve interstitial cells (AVICs) reside within the leaflet tissues of the aortic valve and function to replenish, restore, and remodel extracellular matrix components. AVIC contractility is brought about through the contractile properties of the underlying stress fibers and plays a crucial role in processes such as wound healing and mechanotransduction. Currently, it is technically challenging to directly investigate AVIC contractile behaviors within the dense leaflet tissues. As a result, optically clear poly (ethylene glycol) (PEG) hydrogel matrices have been used to study AVIC contractility through means of 3D traction force microscopy (3DTFM). However, the stiffness of the hydrogel material within the vicinity of the AVIC is difficult to measure directly and is further confounded by the remodeling activity of the AVIC. Ambiguity in the local hydrogel mechanical properties can lead to large errors in computed cellular tractions. Herein, we developed an inverse computational approach to estimate AVIC induced remodeling of the hydrogel material. The capabilities of the model were validated with a ground truth data set generated via a test problem comprised of an experimentally measured AVIC geometry and a prescribed modulus field containing unmodified, stiffened, and degraded regions. The inverse model was able to estimate the ground truth data set with high accuracy. When applied to AVICs assessed via 3DTFM, the model estimated regions of significant stiffening and degradation local to the AVIC. We observed that stiffening was largely localized at AVIC protrusions and was likely a result of collagen deposition as confirmed by immunostaining for collagen type 1. Degradation was more spatially uniform and present in regions further away from the AVIC surface and likely a result of enzymatic activity. Our results indicate that AVICs substantially modify the local hydrogel mechanics, which were successfully quantified by our computational model. Looking forward, the established approach will allow for more accurate computation of AVIC contractile force levels and lead to elucidation of stress fiber properties.

MS 14–Talk 10: **Control of stochastic signaling pathways in esophageal cancer**

Authors: Souvik Roy, Zui Pan and Zain Khan (University of Texas at Arlington)

Abstract: In this talk, we present a new framework for controlling aberrant signaling pathways in esophageal cancer. The dynamics of signaling pathways is given by a stochastic process that models the randomness present in the system. The stochastic dynamics is then represented by the Fokker-Planck (FP) partial differential equation that governs the evolution of the associated probability density function. We solve a FP feedback

control problem to determine the optimal combination therapies for controlling the signaling pathway states. Finally, we demonstrate the efficiency of the proposed framework through numerical results with combination drugs. This work was funded by the National Science Foundation (Award number: DMS 2212938) and the Interdisciplinary Research Program (Award number: 2021-772)

MS 14–Talk 11: **Modeling supraventricular tachycardia using dynamic computer-generated left atrium**

Authors: Bryant Wyatt, Avery Campbell, Gavin McIntosh, and Melanie Little (Tarleton State University)

Abstract: Supraventricular Tachycardia (SVT) is when the heart's upper chambers beat either too quickly or out of rhythm with the heart's lower chambers. This out-of-step heart beating is a leading cause of strokes, heart attacks, and heart failure. The most successful treatment for SVT is catheter ablation, a process where an electrophysiologist (EP) maps the heart to find areas with abnormal electrical activity. The EP then runs a catheter into the heart to burn the abnormal area, blocking the electrical signals. Much is not known about what triggers SVT and where to place scar tissue for optimal patient outcomes. We have produced a dynamic model of the left atrium accelerated on NVIDIA GPUs. An interface will allow researchers to insert ectopic signals into the simulated atria and ablate sections of the atria allowing them to rapidly gain insight into what causes SVTs and how to terminate them.

MS 14–Talk 12: **A hemodynamic comparison of single ventricle patients**

Authors: Alyssa M. Taylor-LaPole[1], Mitchel J. Colebank[2], Justin D. Weigand[3,4], Mette S. Olufsen[1], Charles Puelz[3,4] (1: NC State University, 2: University of California, Irvine, 3: Baylor College of Medicine, 4: Texas Children's Hospital)

Abstract: Hypoplastic left heart syndrome (HLHS) is a congenital heart disease that affects about 1,025 infants in the US each year. HLHS patients are born with an underdeveloped aorta and left heart, receiving a series of three surgeries to create a univentricular circulatory system called the Fontan circuit. Patients typically survive into early adulthood but suffer from reduced cardiac output leading to insufficient cerebral and gut perfusion. Currently, clinical imaging data of the neck and chest vasculature is used to assess patients, but it is difficult to use imaging data to assess deficiencies outside of the imaged region. Data from patients used in this paper include three-dimensional, magnetic resonance angiograms (MRA), time-resolved phase-contrast cardiac magnetic resonance images (4D-MRI), and sphygmomanometer blood pressure measurements. The 4D-MRI images provide detailed insight into velocity and flow in vessels within the imaged region, but they cannot predict flow in the rest of the body, nor do they provide values of blood pressure. This study combines MRA, 4D-MRI, and pressure data with a 1D fluid dynamics model to predict hemodynamics in the aorta and the peripheral vessels, including the cerebral and gut vasculature. To study the effects of surgical reconstruction of an HLHS aorta, simulations for both HLHS and matched control patients with a native aorta and double outlet right ventricle (DORV) physiology are compared. We also use perfusion plots of the liver and cerebral tissues to investigate differences in flow to these organs. Our results demonstrate the HLHS patient has hypertensive pressures in the brain as well as reduced flow to the gut. Wave-intensity analysis suggests the HLHS patient has an irregular circulatory function during light upright exercise conditions and that predicted wall-shear stresses are lower than normal.

MS 14–Talk 13: **Fast algorithms for diffeomorphic image registration**

Authors: Andreas Mang (Department of Mathematics, University of Houston)

Abstract: We will discuss the implementation and analysis of efficient numerical methods for diffeomorphic image registration. Image registration is a nonlinear, ill-posed inverse problem that poses significant mathematical and computational challenges. We seek to identify a spatial transformation that establishes point-wise correspondences between two images of the same scene. In our formulation, the spatial transformation is parametrized by a smooth, time-dependent velocity field. This velocity field is found by minimizing a variational

optimization problem governed by hyperbolic transport equations. Our contributions are the implementation of efficient numerical algorithms for evaluating forward and adjoint operators, fast second-order algorithms for numerical optimization, efficient approaches for preconditioning, and the deployment of our methodology on dedicated high-performance computing architectures. This is joint work with George Biros, Malte Brunn, Naveen Himthani, Jae-Youn Kim, and Miriam Schulte.

MS 14–Talk 14: **PocketNet: A smaller neural network for medical image analysis**

Authors: Adrian Celaya, Jonas A. Actor, Rajarajeswari Muthusivarajan, Evan Gates, Caroline Chung, Dawid Schellingerhout, Beatrice Riviere, and David Fuentes (Rice University and MD Anderson Cancer Center)

Abstract: Medical imaging deep learning models are often large and complex, requiring specialized hardware to train and evaluate these models. To address such issues, we propose the PocketNet paradigm to reduce the size of deep learning models by throttling the growth of the number of channels in convolutional neural networks. We demonstrate that, for a range of segmentation and classification tasks, PocketNet architectures produce results comparable to that of conventional neural networks while reducing the number of parameters by multiple orders of magnitude, using up to 90% less GPU memory, and speeding up training times by up to 40%, thereby allowing such models to be trained and deployed in resource-constrained settings.

MS 14–Talk 15: **Optimal transport-based segmentation and classification of ECG signals: Preliminary results and challenges**

Authors: Cesar A Uribe[1], Edward Nguyen[1], Sebastian Acosta[2], Emily Zhang[3], Jelena Lazic[1] (1: Rice University, 2: Baylor College of Medicine, 3: Wellesley College)

Abstract: In this talk, we present preliminary results on the pre-processing and classification of ECG signals based on geometric methods. Specifically, we show the advantages of using optimal transport-based metrics for reducing segmentation errors of ECG signals. Moreover, we provide evidence that indicates that optimal transport-based clustering methods improve the classification performance over Euclidean-based approaches for the task detection of Junctional Ectopic Tachycardia in postoperative children.

MS 14–Talk 16: **Using deep learning and macroscopic imaging of porcine heart valve leaflets to predict uniaxial stress-strain responses**

Authors: Luis Hector Victor, CJ Barberan, Richard G. Baranuik, and Jane Grande-Allen (Rice University)

Abstract: Heart valves consist of leaflets that normally open and shut, guaranteeing unidirectional flow; however, their proper function is limited by their degradation due to a range of disease processes. For this reason, the study of leaflet mechanics is important for understanding the effect of cardiovascular diseases,and designing prosthetics and treatments for heart valve disease. Although traditional mechanical testing of heart valve leaflets (HVLs) is the standard for evaluating mechanical behavior, it is time-intensive, tedious, technical, and requires specialized and expensive equipment. On the other hand, imaging and deep learning (DL) networks, such as convolutional neural networks (CNNs), are readily available and cost-effective, yet investigators have not leveraged these tools to study the mechanics of HVLs. In this work, we determined the influence of a curated dataset, consisting of uniaxially tensile tested porcine aortic valve (PAV) leaflets, and imaging of their aortic surface, on the ability of a CNN to predict the stress-strain response of the leaflets. We used a third-degree polynomial to fit an individual sample's stress-strain curve, which was used as the ground truth for training. Our findings indicate that our framework is robust against using relatively few samples, excellent at predicting the polynomial coefficients needed for reconstructing the toe and linear regions, and independent of the CNN used for making predictions.

MS 15: Recent advances of scientific computing and applications

Organizers: Ying Wang

There has been tremendous growth in various areas of scientific computing in the recent years. This mini-symposium intends to introduce the recent advances of scientific computing and the related interesting applications. The goal is to attract attention to scientific computing and build potential future collaborations.

MS 15–Talk 1: **Efficient numerical solutions of Laplace equations with mixed boundary conditions using Steklov eigenfunctions**

Authors: Manki Cho (University of Houston at Clear Lake)

Abstract: This talk will introduce Steklov eigenproblems on elliptic PDEs. Various ways of finding Steklov eigenpairs have been studied either analytically or numerically. This work will feature some studies of explicit Steklov eigenpairs on polygonal domains. Main results are based on the fact that Steklov eigenfunctions may construct bases of spaces of harmonic functions using only boundary conditions. Solutions of mixed boundary value problems are represented by the series of Steklov eigenfunctions where its coefficients are determined by boundary data of the problems. This idea provides pointwise error estimates in the interior of the region. Moreover, specific quantities of functions such as the central value of the solution or the magnitude of its gradient are accurately estimated by the Steklov expansion method. From the heat conduction problmes to the Dirichlet-to-Neumann operator in electrostatics, its applications will be introduced with numerical results in this talk

MS 15–Talk 2: **Exterior Finite Energy Harmonic Functions**

Authors: Giles Auchmuty[1] and Qi Han[2] (1: University of Houston, 2: Texas A&M University-San Antonio)

Abstract: A space of functions of finite-energy on an exterior domain with a compact, Lipschitz boundary is introduced. The exterior Poisson's kernel and a reproducing kernel for the harmonic function subspace are described explicitly through solutions to the exterior harmonic Steklov eigen-problems. As an application, an explicit formula for Newtonian capacity is given.

MS 15–Talk 3: **Numerical studies to the Chaplygin gas equation**

Authors: Ling Jin[1] and Ying Wang[2] (1: University of Oklahoma, 2: University of Oklahoma)

Abstract: In this talk, we will discuss the numerical solutions to the Riemann problem for Chaplygin gas equation, which is the Euler equations equipped with the state equation $p = -1/\rho$. The spatial discretization is performed using WENO reconstruction and time integration is achieved using TVD RK4. The numerical results confirm high order of accuracy.

MS 15–Talk 4: **Optimal control of Pentadesma fruit harvesting under habitat reduction**

Authors: Benito Chen-Charpentier (University of Texas at Arlington)

Abstract: The study of the synergetic effects of multiple interacting disturbances on the dynamical behavior of a biological system has received extensive attention. However, the interactions among disturbances are highly complex and the impacts are still not well understood. In this talk, we present a mathematical model based on ordinary differential equations to study the effects of exogenous pressures on the dynamics of tree ecosystems. Specifically, it incorporates the effects of non-lethal harvesting and habitat reduction. The resulting model allows the derivation of a general formula to determine the rational non-lethal harvesting level and habitat size to ensure the sustainability of the plant ecosystem. The model will be applied to fruit harvesting of pentadesma trees under different habitat sizes.

MS 16: Recent Advances in Reduced Order Models

Organizers: Matthias Heinkenschloss

The speakers in this minisymposium present recent advances in the construction, analysis, and application of projection-based reduced order models. Projection-based reduced order models (PROMs) are small-dimensional, computational efficient, accurate models obtained by systematically extracting the relevant dynamics of large-scale systems. PROMs are crucial in many query applications, such as uncertainty quantification, optimal control or parameter identification, where they replace the prohibitively expensive large-scale models. The talks in the minisymposium present recent advances the construction of data-driven, non-intrusive PROMs, modifications of PROMs that preserve structure of the underlying large-scale full order models, and applications of PROMs in large-scale optimization and parameter identification.

MS 16–Talk 1: **Operator inference for non-intrusive model reduction with quadratic manifolds**

Authors: Rudy Geelen[1] and Stephen Wright[2] and Karen Willcox[1] (1: University of Texas at Austin, 2: University of Wisconsin-Madison)

Abstract: Linear dimensionality reduction underlies a large class of model reduction techniques, including principal component analysis ? or as it known in the model reduction literature ? Proper Orthogonal Decomposition (POD). However, for many physics-based systems linear dimension reduction imposes a fundamental limitation to the accuracy that can be achieved using reduced-order models. In this talk we propose a novel approach for learning a data-driven quadratic manifold from high-dimensional data, then employing this quadratic manifold to derive efficient physics-based reduced-order models. The key ingredient of the approach is a polynomial mapping between high-dimensional states and a low-dimensional embedding. This mapping consists of two parts: a representation in a linear subspace (computed in this work using POD) and a quadratic component. The approach can be viewed as a form of data-driven closure modeling, since the quadratic component introduces directions into the approximation that lie in the orthogonal complement of the linear subspace, but without introducing any additional degrees of freedom to the low-dimensional representation. Combining the quadratic manifold approximation with the operator inference method for projection-based model reduction leads to a scalable non-intrusive approach for learning reduced-order models of dynamical systems. Applying the new approach to transport-dominated systems of partial differential equations illustrates the gains in efficiency that can be achieved over approximation in a linear subspace.

MS 16–Talk 2: **A fast and accurate domain-decomposition nonlinear reduced order model using shallow masked autoencoders**

Authors: Alejandro N. Diaz (Rice University)

Abstract: Training reduced order models (ROMs) from data typically requires access to high-dimensional full order model (FOM) simulation data. However, for so-called "extreme-scale" problems, the storage of such high-dimensional FOM simulation data renders ROM training infeasible. Domain-decomposition (DD) alleviates this issue by solving the FOM on smaller subdomains, thereby generating training data of more manageable sizes. Model reduction can then be applied to each subdomain, and the separate ROMs can be reassembled to compute a global ROM for the DD FOM. A promising model reduction approach for the DD problem is the so-called nonlinear-manifold ROM (NM-ROM). NM-ROM has provided improved accuracy over linear-subspace ROMs (LS-ROMs), particularly for advection-dominated problems. NM-ROM approximates the FOM state in a nonlinear-manifold, which is learned from training a shallow, sparse-masked autoencoder using the FOM simulation data. The shallow, sparse architecture of the autoencoder allows for hyper-reduction to be applied, yielding computational speedup. In this talk, the DD formulation of the FOM and the application of NM-ROM to each subdomain are discussed. The results of the DD NM-ROM approach with hyper-reduction are numerically compared to DD LS-ROM with hyper-reduction for the 2D steady-state Burgers' Equation.

MS 16–Talk 3: **Stabilization of linear time-varying reduced order models, a feedback controller approach**

Authors: Rambod Mojgani and Maciej Balajewicz (Rice University)

Abstract: Time-varying reduced-order models (ROMs) are results of the reduction of time-varying systems or time-invariant systems on time-varying manifolds. The latter problem is especially of our interest as we have shown the possibility of learning an optimal rank-reduction by projecting partial differential equations of travelling waves and features, (e.g., wave equations) on low-rank time-varying grids. The stability of such ROMs is not a priori guaranteed. However, a posteriori stabilization schemes can be used for accurate predictive ROMs. In this talk, we present the stabilization of linear time-varying ROMs by controlling the largest singular values of the state matrices, i.e., an extension of the eigenvalue reassignment method developed to stabilize linear time-invariant ROMs. In a post-processing step, trajectories of ROMa are controlled to enforce stability while maintaining their accuracy using a constrained nonlinear least-square minimization problem. The controller and the input signals are defined at the algebraic level, using left and right singular vectors of the reduced system matrices, to restrict the upper bound of the growth of the energy of the reduced system. The optimization problem is applied to several time-invariant, time-periodic, and time-varying problems. The method is evaluated in both reproductive and predictive (i.e., unseen inputs and the system parameters) test cases.

MS 16–Talk 4: **The Loewner framework in the time-domain**

Authors: A. C. Antoulas (Rice University Houston and Max-Planck Institute Magdeburg)

Abstract: The Loewner framework is used for building models (linear and nonlinear) from given data. The data can be frequency responses or time series. In this talk we will concentrate on the latter case and will show how time-domain responses of systems described by PDEs can be used for constructing low order models. The results will be illustrated by means of several numerical examples.

MS 16–Talk 5: **Waveform inversion via reduced order modeling**

Authors: Alexander V. Mamonov[1] and Liliana Borcea[2] and Josselin Garnier[3] and Jörn Zimmerling[4] (1: University of Houston, 2: University of Michigan, 3: Ecole Polytechnique, 4: Uppsala University)

Abstract: A novel approach to full waveform inversion (FWI), based on a data driven reduced order model (ROM) of the wave equation operator is introduced. The unknown medium is probed with pulses and the time domain pressure waveform data is recorded on an active array of sensors. The ROM, a projection of the wave equation operator is constructed from the data via a nonlinear process and is used for efficient velocity estimation. While the conventional FWI via nonlinear least-squares data fitting is challenging without low frequency information, and prone to getting stuck in local minima (cycle skipping), minimization of ROM misfit is behaved much better, even for a poor initial guess. For low-dimensional parametrizations of the unknown velocity the ROM misfit function is close to convex. The proposed approach consistently outperforms conventional FWI in standard synthetic tests.

MS 16–Talk 6: **Line-search methods for unconstrained optimization with inexactness arising from reduced order models**

Authors: Dane Grundvig and Matthias Heinkenschloss (Rice University)

Abstract: This talk discusses line-search algorithms for the solution of smooth unconstrained optimization problems that allow the use of approximate objective function and gradient information. These algorithms are motivated by the need to rigorously incorporate reduced order models (ROMs) into the solution of large-scale optimization problems governed by partial differential equations. Problems of this nature are common in many science and engineering applications. The developed algorithms are error aware and use on the fly updates to error tolerances in order to reduce the accuracy requirements on the ROM approximations. The considered algorithms require no explicit information about the underlying true model and operate entirely using error bounds on the objective and its gradient. These algorithms are implementable and provide convergence guarantees subject to some reasonable assumptions on the underlying optimization problem. Numerical results show that the proposed line-search methods, combined with ROMs, converge to local minima of the original optimization problem at a fraction of the computational cost required by traditional Newton CG algorithms.

MS 16–Talk 7: **Filtering in non-intrusive data-driven reduced-order modeling of large-scale systems**

Authors: Ionut-Gabriel Farcas[1], Rayomand P. Gundevia[2], Ramakanth Munipalli[3], and Karen E. Willcox[1] (1: The University of Texas at Austin 2: Jacobs Engineering Group, Inc., 3: Air Force Research Laboratory)

Abstract: We present a method for enhancing data-driven reduced-order modeling with a preprocessing step in which the training data are filtered prior to training the reduced model. Filtering the data prior to training has a number of benefits for data-driven modeling: it attenuates (or even eliminates) wavenumber or frequency content that would otherwise be difficult or impossible to capture with the reduced model, it smoothens discontinuities in the data that would be difficult to capture in a low-dimensional representation, and it reduces noise in the data. This makes the reduced modeling learning task numerically better conditioned, less sensitive to numerical errors in the training data, and less prone to overfitting when the amount of training data is limited. We first illustrate the effects of filtering in one-dimensional advection and inviscid Burgers' equations. We then consider large-scale rotating detonation rocket engine simulations with millions of spatial degrees of freedom for which only a few hundred down-sampled training snapshots are available. A reduced-order model is derived from these snapshots using operator inference. Our results indicate the potential benefits of filtering to reduce overfitting, which is particularly important for complex physical systems where the amount of training data is limited.

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MS 16–Talk 8: **Gaussian process subspace prediction for model reduction**

Authors: Ruda Zhang[1], Simon Mak[2], and David Dunson[2] (1: University of Houston, 2: Duke University)

Abstract: Subspace-valued functions arise in a wide range of problems, including parametric reduced order modeling (PROM), parameter reduction, and subspace tracking. In PROM, each parameter point can be associated with a subspace, which is used for Petrov–Galerkin projections of large system matrices. Previous efforts to approximate such functions use interpolations on manifolds, which can be inaccurate and slow. To tackle this, we propose a novel Bayesian nonparametric model for subspace prediction: the Gaussian process subspace (GPS) model. This method is extrinsic and intrinsic at the same time: with multivariate Gaussian distributions on the Euclidean space, it induces a joint probability model on the Grassmann manifold, the set of fixed-dimensional subspaces. The GPS adopts a simple yet general correlation structure, and a principled approach for model selection. Its predictive distribution admits an analytical form, which allows for efficient subspace prediction over the parameter space. For PROM, the GPS provides a probabilistic prediction at a new parameter point that retains the accuracy of local reduced models, at a computational complexity that does not depend on system dimension, and thus is suitable for online computation. We give four numerical examples to compare our method to subspace interpolation, as well as two methods that interpolate local reduced models. Overall, GPS is the most data efficient, more computationally efficient than subspace interpolation, and gives smooth predictions with uncertainty quantification.

MS 17: Recent Advances in Learning

Organizers: Andrea Bonito & Ming Zhong

We gather a group of speakers to present recent development and challenges in learning, in terms of both mathematical and computational aspects of discovering model questions, physical quantities, parametric structures, surrogate models, etc., from observation data.

MS 17–Talk 1: **Residual-based error correction for neural operator accelerated infinite-dimensional Bayesian inverse problem**

Authors: Lianghao Cao[1], Thomas O'Leary-Roseberry[1], Prashant K. Jha[1], J. Tinsley Oden[1], Omar Ghattas[1] (1: Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin)

Abstract: We explore using neural operators to accelerate infinite-dimensional Bayesian inverse problems (BIPs) governed by nonlinear parametric partial differential equations (PDEs). Neural operators have gained attention in recent years for their ability to approximate the parameter-to-solution mappings defined by PDEs using their numerical solutions at a limited number of parameter samples. On the one hand, the computational cost of BIPs can be drastically reduced if the large number of PDE solves required in posterior characterization are replaced with evaluations of trained neural operators. On the other hand, reducing error in the resulting BIP solutions via reducing approximation error of the neural operators in training can be challenging and unreliable. We provide an a-priori error bound result that implies certain BIPs can be ill-conditioned to the approximation error of neural operators, thus leading to inaccessible accuracy requirements in training. To reliably reduce error of neural operator predictions to be used in, but not limited to, BIPs, we consider correcting predictions of a trained neural operator by solving a linear variational problem based on the PDE residual. We show that a neural operator with error correction can possibly achieve quadratic reduction of its approximation error. Finally, we provide two numerical examples of infinite-dimensional BIPs based on a nonlinear Poisson equation and deformation of hyperelastic materials. We demonstrate that posterior representations of the two BIPs produced using neural operators are greatly and consistently enhanced by the error correction, while still retaining substantial computational speed ups.

MS 17–Talk 2: **Scalable Model Selection of Interacting Particle Models with Gaussian processes**

Authors: Jinchao Feng[1], Charles Kulick[2], Sui Tang[2] (1: Deparment of Applied Mathematics and Statistics, Johns Hopkins University; 2: Department of Mathematics, University of California, Santa Barbara)

Abstract: Interacting particle or agent systems that display a rich variety of collection motions are ubiquitous in science and engineering. A fundamental and challenging goal is to understand the link between individual interaction rules and collective behaviors. We study the data-driven discovery of distance-based interaction laws in interacting particle systems, and propose a learning approach that models the latent interaction kernel functions as Gaussian processes, which can simultaneously determine the governing equations of the dynamic systems (types of interactions & orders of the systems), and provide nonparametric inferences for the interaction kernel functions and the unknown parameters in the non-collective forces of the system. By connecting with a statistical inverse problem, we also establish an operator-theoretical framework to analyze the recoverability via the coercivity of the associated operator and provide a finite sample analysis. The numerical results on prototype systems, including the applications to two real data sets with flocking and milling patterns, show that our approach can discover the governing equations successfully, produce faithful estimators from scarce and noisy trajectory data, and make accurate predictions of the collective behaviors.

MS 17–Talk 3: **Data-Driven Learning Based Algorithms for Multiscale Problems**

Authors: Sai Mang Pun (Deparment of Mathematics, Texas A&M University)

Abstract: In this talk, we present some recent progress on the development of data-driven, machine learning algorithms for solving a class of forward and inverse problems with multiple scale features. The algorithms make use of existing multiscale solvers to build the internal structures of the whole simulator. The first part of the talk focuses on a class of parametrized and multiscale time-dependent problems. For the forward problem, we developed a multi-stage neural network architecture, containing a front-end reduction module formed by the multiscale solvers, for approximating the solutions of the problem. The second part of this talk considers a class of multiscale inverse problems. We formulate the problem into the framework of reinforcement learning and solve it with the aid of multi-level Monte Carlo Markov Chain sampling methods. Numerical results will be presented to demonstrate the efficiency and accuracy of the proposed computational methods.

MS 17–Talk 4: **Efficient Computation of Multiscale Hamiltonian Systems Aided by Machine Learning**

Authors: Rui Fang[1], Richard Tsai[1] (1: Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin)

Abstract: We introduce a data-driven approach to learn the flow map for a fixed time interval for multiscale Hamiltonian systems. In particular, we focus on appropriate training data generation and loss function design. We propose Hamiltonian Monte Carlo (HMC) based methods to sample training data from an invariant measure of the exact dynamics. Moreover, we use a multi-step loss function to improve the stability of the learned flow map when used for long-time integration. Through several numerical examples, the proposed approach is shown to have higher computational efficiency compared to classical integrators.

MS 17–Talk 5: **TNet: A Model-Constrained Tikhonov Network Approach for Inverse Problems**

Authors: Hai Van Nguyen[1], Tan Bui Thanh[1] (1: Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin)

Abstract: Deep Learning (DL), in particular deep neural networks (DNN), by default is purely data-driven and in general does not require physics. This is the strength of DL but also one of its key limitations when applied to science and engineering problems in which underlying physical properties and desired accuracy need to be achieved. DL methods in their original forms are not capable of respecting the underlying mathematical models or achieving desired accuracy even in big-data regimes. However, many data-driven science and engineering problems, such as inverse problems, typically have limited experimental or observational data, and DL would overfit the data in this case. Leveraging information encoded in the underlying mathematical models, we argue, not only compensates missing information in low data regimes but also provides opportunities to equip DL methods with the underlying physics, hence promoting better generalization. This paper develops a model-constrained deep learning approach and its variant TNet that are capable of learning information hidden in both the training data and the underlying mathematical models to solve inverse problems governed by partial differential equations. We provide the constructions and some theoretical results for the proposed approaches. We show that data randomization can enhance the smoothness of the networks and their generalizations. Comprehensive numerical results not only confirm the theoretical findings but also show that with even as little as 20 training data samples for 1D deconvolution, 50 for inverse 2D heat conductivity problem, 100 and 50 for inverse initial conditions for time-dependent 2D Burgers' equation and 2D Navier-Stokes equations, respectively. TNet solutions can be as accurate as Tikhonov solutions while being several orders of magnitude faster. This is possible owing to the model-constrained term, replications, and randomization.

MS 17–Talk 6: **Approximation with Neural Networks: advantages and limitations**

Authors: Guergana Petrova (Deparment of Mathematics, Texas A&M University)

Abstract: We discuss the approximation properties of the outputs of Neural Networks and mention some classes of functions that can be approximated with sometimes surprising accuracy by these outputs. We compare the Neural Network approximation with traditional approximation methods from the viewpoint of rate distortion and touch upon the stability of this approximation and its limitations.

MS 17–Talk 7: **Optimal Recovery from Inaccurate Data in Hilbert Spaces: Regularize, but what of the parameter?**

Authors: Simon Foucart[1], Chunyang Liao[1] (1: Deparment of Mathematics, Texas A&M University)

Abstract: In Optimal Recovery, the task of learning a function from observational data is tackled deterministically by adopting a worst-case perspective tied to an explicit model assumption made on the functions to be learned. Working in the framework of Hilbert spaces, this article considers a model assumption based on approximability. It also incorporates observational inaccuracies modeled via additive errors bounded in ℓ_2. Earlier works have demonstrated that regularization provides algorithms that are optimal in this situation, but did not fully identify

the desired hyperparameter. This article fills the gap in both a local scenario and a global scenario. In the local scenario, which amounts to the determination of Chebyshev centers, the semidefinite recipe of Beck and Eldar (legitimately valid in the complex setting only) is complemented by a more direct approach, with the proviso that the observational functionals have orthonormal representers. In the said approach, the desired parameter is the solution to an equation that can be resolved via standard methods. In the global scenario, where linear algorithms rule, the parameter elusive in the works of Micchelli et al. is found as the byproduct of a semidefinite program. Additionally and quite surprisingly, in the case of observational functionals with orthonormal representers, it is established that any regularization parameter is optimal.

MS 17–Talk 8: **Learning of Transition Operators From Sparse Space-Time Samples**

Authors: Christian Kuemmerle[1], Mauro Maggioni[2], Sui Tang[3] (1: Department of Computer Science, University of North Carolina, Charlotte; 2: Department of Mathematics and Department of Applied Mathematics and Statistics, Johns Hopkins University; Department of Mathematics, University of California Santa Barbara)

Abstract: We present a framework for the learning of a transition operator A from partial observations across different time scales. For two observation models consisting of uniformly and adaptively selected random space-time sampling locations, we show that the non-linearity of the resulting inverse problem can be addressed computationally by reformulating it as a matrix completion problem utilizing a low-rank property of a suitable block Hankel embedding matrix, which is low-rank even if the graph operator is of full rank. In particular, we show local quadratic convergence of a suitable Iteratively Reweighted Least Squares algorithm under the two observation models from $\Theta(rnlog(rn))$ space-time samples if the (n x n) transition operator is of rank r and incoherent. Furthermore, we show how our analysis informs a suitable adaptive sampling strategy to distribute a budget of spatio-temporal samples across multiple trajectories to recover a linear dynamical system based on the topology of a graph from partial information.

MS 18: Advances in theory and computation of functional optical materials

Organizers: Matthias Maier & Daniel Massatt

This mini-symposium seeks to bring together experts on theoretical modeling, phenomenological analysis, and computational simulation of novel optical materials and their applications, including 2d materials such as graphene, meta-materials, topological photonics, liquid crystals, nano optics, etc.

MS 18–Talk 1: **Dirac points for the honeycomb lattice with impenetrable obstacles**

Authors: Junshan Lin[1], Wei Li[2], Hai Zhang[3] (1: Auburn University, 2: DePaul University, 3: Hong Kong University of Science and Technology)

Abstract: Dirac points are special vertices in the band structure when two bands of the spectrum for the operator touch in a linear conical fashion, and their investigations play an important role in the design of novel topological materials. In this talk, I will discuss Dirac points for the honeycomb lattice with impenetrable obstacles arranged periodically in a homogeneous medium. I will discuss both the Dirichlet and Neumann eigenvalue problems and prove the existence of Dirac points for both eigenvalue problems at crossing of the lower band surfaces as well as higher band surfaces. In addition, quantitative analysis for the eigenvalues and the slopes of two conical dispersion surfaces near each Dirac point will be presented by a combination of the layer potential technique and asymptotic analysis.

MS 18–Talk 2: **Optimal control of the Landau–de Gennes model of nematic liquid crystals**

Authors: Shawn Walker[1] and Thomas Surowiec[2] (1: LSU, 2: Philipps University of Marburg)

Abstract: This talk presents an optimal control framework for the time-dependent, Landau–de Gennes (LdG) model of nematic liquid crystals. Since the LdG energy is non-convex, we develop parabolic, optimal control

techniques for controlling the L^2 gradient flow of the LdG energy, which is uniquely solvable. The controls are through the boundary conditions (by weak anchoring) and a body force term. We seek to find optimal controls that drive the LdG Q-tensor variable toward a desired "texture" state. The objective functional we minimize is of tracking type with additional regularization terms for the controls. To the best of our knowledge, this is the first time PDE-based optimal control has been developed for the LdG model. Existence of a minimizer for the control problem is established. Moreover, with various regularity estimates, we prove first order Frechét differentiability results for the control objective, by introducing an adjoint PDE, thus allowing gradient based optimization methods. In the talk, we highlight the analytical issues that arise, especially those due to the gradient flow being a parabolic system. We then describe a finite element discretization of the full control problem and present numerical simulations in two and three dimensions that exhibit point and line defects.

MS 18–Talk 3: **Embedded eigenvalues for discrete magnetic Schrödinger operators**

Authors: Jorge Villalobos[1] and Stephen Shipman[1] (1: LSU)

Abstract: Reducibility of the Fermi surface for a periodic operator is a key for the existence of embedded eigenvalues caused by a local defect. We consider a discrete model for a multilayer quantum system, such as stacked graphene, subject to a perpendicular magnetic field. Some techniques for constructing embedded eigenvalues extend from non-magnetic operators to magnetic ones, but the magnetic case is more complex because a typical magnetic operator on a periodic graph is merely quasi-periodic.

MS 18–Talk 4: **Effective Impedance Condition for Thin Metasurfaces**

Authors: Zachary Jermain[1], Robert Lipton[1] (1: LSU)

Abstract: Here we examine the optical response of thin metasurfaces consisting of arrangements of periodic metallic nanoparticles placed on a dielectric film layer. The dielectric film layer is composed of a Liquid Crystal Elastomer (LCE) layer which can isomerize and change its configuration for specific frequencies of incident light called the "pump frequency". With this unique property one can design a dynamic metasurface which actuates to change thickness by interaction with light alone. Ultimately one can control the optical response of an incident electromagnetic wave by controlling the thickness of the LCE layer, i.e. control light with light. We aim to help inform the design of these metasurfaces by deriving effective properties which control the optical response. Specifically, we use asymptotic methods to reduce the metasurface to an effective surface impedance condition. The impedance condition will depend on the geometry of the metallic nanoparticles, the material properties of the metal and film, the periodicity of the nanoparticles, and the thickness of the LCE layer. Finally, we look to find the relationship between the impedance condition and plasmon resonances which occur at specific frequencies of incident light.

MS 18–Talk 5: **Domain wall junctions and networks in Dirac topological materials**

Authors: P. Cazeaux[1], D. Massatt[2], G. Bal[3], and S. Quinn[3] (1: Virginia Tech, 2: LSU, 3: University of Chicago)

Abstract: In this talk, we will discuss effective Dirac models for topological modes propagating along domain wall in the presence of large gapped domains, such as the AB/BA triangular domains in small-angle twisted bilayer graphene in the presence of a strong potential difference between layers, which has attracted interest in recent years. We will rigorously define topological edge invariants associated with massive Dirac operators and their robustness with respect to perturbations and geometries such as domain wall junctions, and introduce discretization strategies for these nonstandard effective Dirac equations, both for the computation of edge invariants as well as the simulation of time-dependent wavepacket propagation on the network formed by the domain walls. Using numerical simulations, we will illustrate the robust behavior in the presence of strong disorder, curved and/or intersecting domain walls.

MS 18–Talk 6: **Shape Optimization of Microstructures Governed by Maxwell's Equations**

Authors: Manaswinee Bezbaruah[1], Matthias Maier[1], Winnifried Wollner[2] (1: Texas A&M University, 2: Universitaet Hamburg, Germany)

Abstract: This talk is concerned with a class of shape optimization problems involving optical metamaterial comprised of periodic nanoscale inclusions. We will first summarize the underlying microscale model and a corresponding homogenization theory that will serve as a basis for the shape optimization problem. We then introduce an arbitrary Lagrangian-Eulerian (ALE) formulation of the cell problems and formulate an optimization problem.

MS 18–Talk 7: **Two new finite element schemes for a time-domain carpet cloak model with metamaterials**

Authors: Jichun Li[1], Chi-Wang Shu[2] and Wei Yang[3] (1: University of Nevada Las Vegas, 2: Brown University, 3. Xiangtan University)

Abstract: This talk is concerned about a time-domain carpet cloak model, which was originally derived in our previous work (Li et al., SIAM J. Appl. Math., 74(4), pp. 1136–1151, 2014). However, the stability of the proposed explicit finite element scheme is only proved under the time step constraint $\tau = O(h^2)$, which is too restricted. To overcome this disadvantage, in this new work we propose two new finite element schemes for solving this carpet cloak model: one is the implicit Crank-Nicolson (CN) scheme, and another one is the explicit leap-frog (LF) scheme. By using a totally new energy, we prove the unconditional stability for the CN scheme and conditional stability for the LF scheme under the practical CFL constraint $\tau = O(h)$. Optimal error estimates are also established for both schemes. Finally, numerical results are presented to support our analysis and demonstrate the cloaking phenomenon.

MS 18–Talk 8: **Bloch Waves for Maxwell's Equations in High-Contrast Electromagnetic Crystals**

Authors: Robert Viator (Swarthmore College)

Abstract: We investigate the Bloch spectrum of a 3-dimensional high-contrast photonic crystal. The Bloch eigen-values, for fixed quasi-momentum, are expanded in a power series in the material contrast parameter in the high-contrast limit. We achieve this power series, together with a radius of convergence, by decomposing an appropriate vectorial Sobolev space into three mutually orthogonal subspaces which are curl-free in certain subdomains of the period cell. We also identify the limit spectrum in the periodic (zero-quasi-momentum) case. Time permitting, we will describe a wide class of crystal geometries which permit the above described analytic structure of the Bloch eigenvalues.

MS 19: Modeling the heart-brain axis and age-related pathology

Organizers: Travis Thompson

The methodical study of human anatomy dates back to at least the 16th century when the Belgian physician Andreas Vesalius published his seminal work, "De humani corporis fabrica libri septem". We now understand a good deal about the large-scale mechanics and function of the many organs and systems within the human body and clinical progress has greatly extended our life spans. Extended life spans have led to new concerns, including the need to more fully understand age-related pathologies such as heart and brain diseases.

The heart and brain are central to the study of human physiology and pathology. Increasing evidence implicates the heart-brain axis in several age-related diseases and disorders, including heart failure, epilepsy, stroke and dementia, among others. The in-vivo study of the heart and brain is often invasive and impractical. Mathematical modeling, using numerical methods and medical imaging, provides an alternative means to noninvasively study the heart and brain in humans.

This minisymposium brings together an interdisciplinary community of mathematicians and medical researchers who are designing and using mathematical models, numerical methods, machine learning and imaging techniques to study important topics towards developing an understanding of the heart-brain axis and its relationship to age-related pathology, including: cardiomechanics; circulation; oxygen transport; neural network activity; neuroglia and neurodegenerative diseases.

MS 19–Talk 1: **Senescence, Sangre, Senility and Simulation: Mathematics at the intersection of the heart and the brain**

Authors: Travis B. Thompson[1] (1: Department of Mathematics and Statistics, Texas Tech University)

Abstract: The heart and the brain have long been recognized as the crucible of human life. The two are bonded together; one delivers vital nutriments to the body while the other provides the vivifying signaling milieu. The importance of both organs was recognized as early as the 5th century BC. Nearly a century later, the careful anatomical studies of Ibn al-Nafis, Andreas Vesalius and William Harvey laid the methodological groundwork for the modern era of quantitative medicine. Renaissance anatomists described the heart and central nervous system in terms of mechanical principles such as pumps, causeways, and electrical impulses ruled by the principles of physics and intelligible in terms of mathematics.

Understanding the functional and pathological relationships of the heart-brain axis is of contemporary clinical importance. The kinship between these sister organs leads to strongly associated risk factors, especially with age, for several of the leading causes of death worldwide. Animal models provide a mechanistic basis for understanding these risk factors while mathematical methods offer an ethical, non-invasive approach for analysis and for clinical testing in simulated human environments. In this talk, a perspective on the importance of the heart-brain axis, and aging, will be presented and connections between vascular factors, brain and especially neurodegenerative pathology will be discussed. Along the way, we will see an example of how mathematical modeling can be used, alongside patient-specific medical imaging data, to construct a mechanistic model of neurodegenerative disease progression that highlights how the heart of mankind can affect the aging mind.

MS 19–Talk 2: **Multi-scale computational models of cardiac and brain tissues**

Authors: Michael S. Sacks[1] and David S. Li[1] (1:Willerson Center for Cardiovascular Modeling and Simulation, Oden Institute and the Department of Biomedical Engineering, University of Texas at Austin)

Abstract: Complex organ systems such as the heart and brain are constructed and function on many structural scales. To gain deeper insights into their function, multi-scale models have been proposed. Recent developments in high resolution microscopic imaging and computational technology has lead to the ability to more fully simulate 3D structures at larger scales from smaller scale features. To demonstrate this approach, we developed a high-fidelity, micro-anatomically realistic 3D finite element model of right ventricle free wall (RVFW) myocardium by combining high-resolution imaging and supercomputer-based simulations. We first developed a representative tissue element (RTE) model at the sub-tissue scale by specializing the hyperelastic anisotropic structurally-based constitutive relations for myofibers and ECM collagen, and equi-biaxial and non-equibiaxial loading conditions were simulated using the open-source software FEniCS to compute the effective stress-strain response of the RTE. To estimate the model parameters of the RTE model, we first fitted a 'top-down' biaxial stress-strain behavior with our previous structurally based (tissue-scale) model, informed by the measured myofiber and collagen fiber composition and orientation distributions. Next, we employed a multi-scale approach to determine the tissue-level (5 x 5 x 0.7 mm specimen size) RVFW biaxial behavior via 'bottom-up' homogenization of the fitted RTE model, recapitulating the histologically measured myofiber and collagen orientation to the biaxial mechanical data. Our homogenization approach successfully reproduced the tissue-level mechanical behavior of our previous studies in all biaxial deformation modes, suggesting that the 3D micro-anatomical arrangement of myofibers and ECM collagen is indeed a primary mechanism driving myofiber-collagen interactions. We discuss how similar approaches can be used for brain tissue.mechanics.

MS 19–Talk 3: **Oscillopathies of Brain and Heart: Lessons From the Computational Medicine Clinic**

Authors: David Paydarfar[1,2] (1: Dell Medical School, Mulva Clinic for the Neurosciences 2: Oden

Institute for Computational Engineering and Sciences, The University of Texas at Austin)

Abstract: Abnormal oscillations are implicated in many disease states of the brain and heart. Examples are rhythmic discharges of neurons in epilepsy and reentrant excitation underlying ventricular tachycardia in heart disease. Biological oscillations can also be vital to normal physiology and disease states result from their loss of rhythmicity. For example, preterm infants commonly suffer from bouts of severe apnea and bradycardia due to immaturity of brainstem control of cardio-respiratory function. In this talk, Dr. Paydarfar will present theoretical, experimental, and clinical observations on the initiation and termination of neural and cardiac rhythms at the cellular, tissue and organism levels. Mathematical and computational methods can provide important insights into the etiology, prevention and treatment of oscillopathies.

MS 19–Talk 4: **Reduced models for solute transport and numerical convergence of solutions of PDEs with line source**

Authors: Beatrice Riviere[1] and Charles Puelz[2] (1: Dept. of Comp. and Appl. Mathematics, Rice University 2: Dept. of Pediatrics, Baylor College of Medicine)

Abstract: The modeling of solute exchanges between an organ and its vasculature is a key component in understanding treatment of diseases. In this talk, we first discuss reduced models of solute transport in blood vessels of varying cross-section and with arbitrary axial velocity profile. The numerical discretization uses a locally implicit discontinuous Galerkin method. Second, the numerical analysis of elliptic and parabolic partial differential equations with line source is shown for the finite element and discontinuous Galerkin methods. Optimal convergence of the numerical method is recovered away from the line source.

MS 19–Talk 5: **Hierarchical Modular Structure of the Drosophila Connectome**

Authors: Alexander B. Kunin[1,2], Jiahao Guo[1], Kevin E. Bassler[1], Xaq Pitkow[2,3] and Krešimir Josić[1] (1: University of Houston 2: Baylor College of Medicine 3: Rice University)

Abstract: The organization of neural circuitry in the brain plays a crucial role in brain function. Previous studies of the organization of the brain have generally had to trade off between coarse descriptions at a large scale and fine descriptions at small scales. We now have reconstructions of tens to hundreds of thousands of neurons at synaptic resolution, enabling investigations into the interplay between global, modular organization, and cell type-specific wiring. To do so we have applied novel community detection methods to analyze the Hemibrain data set, a synapse-level reconstruction of 21 thousand neurons and over 3.5 million synaptic connections in the brain of Drosophila. We develop an understanding of the complex structure composing the Drosophila brain by first finding the community structure at the largest scale. We then resolve the structure at increasingly finer scales, finding that the brain is organized hierarchically with smaller structures consisting mostly of subdivided larger-scale communities. The process continues until the communities become small enough for biological identification. Our methods identify well-known features of the fly brain's sensory pathways. For example, manual efforts have identified a layered structure in the fan-shaped body, with the ventral six layers thought to play a role in navigation, and the dorsal layers playing a role in sleep and modulating internal state. Our methods not only automatically recover this layered structure, but also find that the ventral two layers are distinguished from the remaining layers and from each other, reflecting distinct connectivity patterns to downstream and upstream areas. These methods show that the fine-scale, local network reconstruction made possible by modern experimental methods are sufficiently detailed to identify both large and small scale organizational features of the brain.

MS 19–Talk 6: **A deep learning framework for the automated detection and morphological analysis of GFAP-labeled astrocytes in micrographs**

Authors: Demetrio Labate[1], Yewen Huang[1], Anna Kruyer[2], Sarah Syed[1], Cihan Kayasandik[3], Manos Papadakis[1] (1: Department of Mathematics, University of Houston 2:Medical University of South Carolina 3:Istanbul Medipol University)

Abstract: Astrocytes, a subtype of glial cells with a complex star-shaped morphology, are active players in many aspects of the physiology of the central nervous system (CNS) where they provide structural and functional support to neurons. Astrocytes and neurons form tripartite synapses to establish bidirectional communications, with astrocytes modulating neuronal synaptic currents. However, there is still a major knowledge gap in understanding the highly complex role of astrocytes within the CNS, which is manifested by their morphological complexity, heterogeneity and unique ability to change size and shape. The current knowledge gap is due in part to the limitations of existing image analysis algorithms that are unable to detect and analyze astrocytes with sufficient accuracy and efficiency. To address this limitation, we introduce a new computational framework for the automated detection and segmentation of GFAP-immunolabeled astrocytes in brightfield or fluorescent micrographs. Our novel approach integrates a deep learning framework with ideas from multiscale representation to provide both accurate and interpretable results. Extensive numerical experiments using multiple image datasets show that our method performs very competitively against both conventional and state-of-the-art methods, including images where astrocytes are very dense. The ability to automatically detect astrocytes and extract reliable information about their morphology has important practical implications including the development of efficient algorithms for astrocyte analysis and classification that will advance the understanding of the role of astrocytes in the physiology of the CNS and its pathologies. In the spirit of reproducible research, our numerical code and annotated data are available open source and freely available to the scientific community.

MS 19–Talk 7: **Robust Incorporation of DTMRI Data in Soft Tissue Modeling**

Authors: Christian Goodbrake[1], Kenneth Meyer[1], Jack Hale[2] and Michael S. Sacks[1] (1: Oden Institute for Computational Engineering and Sciences and the Department of Biomedical Engineering, The University of Texas at Austin 2: The University of Luxembourg)

Abstract: Both cardiovascular and neurodegenerative diseases manifest as deleterious changes in organ structure at the individual level. This deterioration often differs markedly both between individuals and at different locations within an individual organ. As such, in order to accurately model and simulate the progression of these diseases, this changing organ and tissue structure must be accurately assessed and incorporated into these simulations and models. One prominent method of assessing organ structure is diffusion tensor magnetic resonance imaging (DTMRI), which non-invasively measures tissue's local diffusivity. Mechanical properties such as degree of anisotropy and principal tissue orientation are then inferred from this measurement, under the assumption that both a tissue's local diffusivity and its mechanical properties are reflective of its physical structure, and hence are correlated. This data possesses numerous intrinsic symmetries, which when treated naively can lead to models with spurious, unstable, or inconsistent predictions. We present a general framework for consistently and robustly incorporating DTMRI data into hyperelastic models such that the intrinsic symmetries of this data are fully respected by model's predictions, both in the generically orthotropic case, and the special cases where the data adopts stronger symmetry, such as transverse isotropy or isotropy. By representing the hyperelastic strain energy as a Taylor series in the Green Lagrange strain and the principal diffusivities, we establish the general form of strain energies of arbitrary and independent orders in diffusivity and strain. Further, we exploit the graded structure of polynomial rings to generate compatibility conditions that automatically ensure consistency when the principal diffusivities appear with greater multiplicity. We then provide a computational implementation of such a model, using automatic differentiation with FEniCSx both to perform the differentiable spectral decomposition of the diffusion tensor necessary for the forward solve, and to generate and solve the adjoint equations for gradient computation to fit model parameters to experimental data.

MS 19–Talk 8: **Computer modeling and simulation of blood flow and tissue deformation in congenital heart defects**

Authors: Charles Puelz[1], Dan Lior[1], Craig Rusin[1], Colin Edwards[2] and Silvana Molossi[1] (1: Department of Pediatrics, Division of Cardiology, Baylor College of Medicine and Texas Children's Hospital

2: Department of Mechanical Engineering, Rice University)

Abstract: This talk will focus on the computer modeling of blood flow in patients with abnormal coronary arteries. I will describe the pipeline we use to create these models, which begins with computed tomography images and ends with a computer simulation of blood flow in the aorta, aortic valve, and coronaries. The numerical approach used for these simulations is a version of the immersed boundary method that allows for the prediction of blood flow, blood pressure, and tissue deformations.

MS 19–Talk 9: **Mathematical models and methods in computational neurology**

Authors: Pedro D. Maia[1] (1: Department of Mathematics, The University of Texas at Arlington)

Abstract: The emerging field of computational neurology provides an important window of opportunity for modeling of complex biophysical phenomena, for scientific computing, for understanding functionality disruption in neural networks, and for applying machine-learning methods for diagnosis and personalized medicine. In this talk, I will illustrate some of our latest results across different spatial scales spanning a broad array of mathematical techniques such as: (i) numerical methods for nonlinear PDEs for solving inhomogeneous active cable equations, (ii) spike-train metrics for quantifying information loss on compromised neural signals, (iii) applied inverse-problem techniques for finding the origins of neurodegeneration, and (iv) data methods in medical imaging.

MS 19–Talk 10: **Telomerase Therapy Reverses Vascular Senescence**

Authors: Anahita Mojiri[1], Xu Qiu[1], Elisa Morales[1], Luay Boulahouache[1], Chiara Mancino[1], Rhonda Holgate[1], Chongming Jiang[1], Abbie Johnson[1], Brandon K. Walther[1], Guangyu Wang[1], John P. Cooke[1] MD PhD (1: Houston Methodist Research Institute)

Abstract: Hutchinson-Gilford Progeria Syndrome (HGPS) accelerates aging and vascular disease with mortality in the teen years due to myocardial infarction and stroke. In HGPS, a mutation in lamin A (progerin) alters nuclear morphology and gene expression. Differentiated endothelial cells (ECs) derived from HGPS-iPSCs exhibited hallmarks of senescence including replication arrest, DNA damage, and short telomeres. HGPS-ECs are dysfunctional and generate inflammatory cytokines that alter adjacent cells. Interestingly, HGPS-ECs compared to HGPS-vascular smooth muscle cells had a more severe senescent phenotype as assessed by telomere size and proliferation rate. We hypothesized that a telomere-directed therapy may restore telomere length and attenuate signs of senescence in human progeria cells and progeria mice models. Telomerase mRNA (hTERT) normalized HGPS-ECs morphology and functions; restored nitric oxide generation, acetylated-LDL uptake, and angiogenesis; and, reduced the expression of inflammatory cytokines. hTERT improved replicative capacity, reversed cellular senescence phenotypes such as nuclear morphology, normalized p16, p21, lamin B1 expression, reduced DNA damage signals, and restored histone protein expression in HGPS-EC. Intriguingly, the aberrant transcriptional profile observed in HGPS was normalized, and over 250 genes were fully restored by hTERT treatment. HGPS mice treated with mTERT lentivirus manifested similar improvements with a reduction in the vasculature of the inflammatory marker VCAM1, and the DNA damage marker γH2A.X. Lastly, mTERT therapy increased the lifespan of HGPS mice significantly without adverse cytopathological effects. In conclusion, vascular rejuvenation using telomerase mRNA is a promising approach for HGPS and perhaps other age-related vascular diseases. Currently, we are optimizing the lipid nanoparticles encasing the mTERT RNA for reliable delivery to the vasculature.

MS 20: Recent Developments in Model Reduction and Low Rank Algorithms

Organizers: Zhichao Peng & Min Wang

Numerical simulations of many real world scientific and engineering problems from chemically reacting flows to plasma physics involve a large number of degrees of freedom. This makes the outer-loop applications such as optimization, control, design, sensing and uncertainty quantification computationally expensive. Model reduction techniques and low rank algorithms, which explore and utilize the underlying low rank feature of the underlying problem, could dramatically accelerate these large-scale simulations. In this minisyposium, we would focus on the recent developments in model reduction and low rank algorithms such as machine learning based methods, structure preserving methods and least squares methods.

MS 20–Talk 1: **Achieving Stable Long-Term Predictions in Machine Learning Architectures with Parameterization**

Authors: Daniel Serino[1], Qi Tang[1], Joshua Burby[1] (1: Los Alamos National Labotary)

Abstract: In fields such as high energy physics and climate modeling, reduced order models (ROMs) provide a significant speed-up compared to direct numerical simulations. However, ROMs typically lack accuracy and stability for long-time predictions. Traditionally in data-based ML models, a regularization penalty term is introduced to control the behavior of the tunable weights and, in turn, improve stability. Implementing regularization often involves making a non-trivial choice of a suitable penalty function and its parameter constants. This can lead to training sub-optimal models. Instead, a novel approach is introduced where the weights of the network are parameterized to automatically enforce stability properties in the network without sacrificing regions in the parameter space which may contain an optimal solution. The stability of feed-forward neural networks is related to the singular values of the weight matrices in each layer while the stability of neural ODE networks is related to the eigenvalues of the network. Therefore, parameterization approaches involving the Singular Value Decomposition (SVD) and Block Schur Decomposition are utilized. Algorithms for parameterizing these decompositions and their building blocks will be presented. Additionally, theoretical benefits of employing these parameterizations in networks will be discussed. The model is trained on datasets involving problems in dynamical systems, high-energy physics, radiography, and climate modeling and is compared with other state-of-the-art approaches.

MS 20–Talk 2: **Contrast-independent partially explicit time discretizations for multiscale problems**

Authors: Wenyuan Li[1],Yalchin Efendiev[1], Wing Tat Leung[2] (1: Texas A&M University, 2: City University of Hong Kong)

Abstract: Multiscale nature arise in many applications and they are typically described by some parabolic partial differential equations. When the media properties are high, the flow and transport become fast and requires small time steps to resolve the dynamics. Implicit discretization can be used to handle fast dynamics. However, this requires solving large-scale nonlinear systems. Explicit methods are used when possible to avoid solving nonlinear systems. The main drawback of explicit methods is that they require small time steps that scale as the fine mesh and depend on physical parameters, e.g., the contrast. To alleviate this issue, we propose a novel algorithm called partially explicit splitting scheme. In this scheme, we split the solution space into two parts, coarse-grid part, and the correction part. Coarse-grid solution is computed using multiscale basis functions with CEM-GMsFEM. The correction part uses special spaces in the complement space (complement to the coarse space). We handle degrees of freedom from the first space implicitly and others explicitly. With this careful design of basis functions, our stability analysis shows that the time step scales as the coarse mesh size and is independent of the contrast, which provides computation savings. The numerical results also show that our proposed scheme obtains similar accuracy as the fully implicit scheme.

MS 20–Talk 3: **A symplectic deep autoencoder for Hamiltonian systems**

Authors: Wei Guo[1], Qi Tang[2], Joshua Burby[2] (1: Texas Tech University, 2: Los Alamos National Labotary)

Abstract: In this talk, we introduce a novel symplectic deep autoencoder for model order reduction (MOR) of simulating parametric Hamiltonian systems with high dimensional state variables. The existing MOR techniques for parametric Hamiltonian systems suffer two limitations. First, the inherent symplectic structure of Hamiltonian systems is not necessarily inherited by the reduced order model. This may lead to instability

and blowup of the system energy. Second, due to non-dissipative nature of Hamiltonian systems, the popular global linear subspace solution representation becomes less effective, and it is related to the slow decay of the Kolmogorov n-width of the solution manifold. To overcome the difficulties, we propose a deep autoencoder using HenonNets that can preserve the symplectic structure. HenonNets are constructed by composing a sequence of Henon maps which are parametrized by neural networks. Since a Henon map is symplectic, a HenonNet preserves symplectic structures when used to learn a nonlinear embedding of the solution manifold. Hence, the reduced system is still Hamiltonian, and the system energy and long-term stability is preserved. A collection of numerical tests is presented to verify the effectiveness of the proposed MOR technique. This is a joint work with Qi Tang and Joshua Burby from Los Alamos National Laboratory.

MS 20–Talk 4: **Bayesian operator inference for data-driven reduced-order modeling**

Authors: Shane A. McQuarrie[1], Mengwu Guo[2], and Karen Willcox[1] (1: The University of Texas at Austin, 2: University of Twente)

Abstract: This work proposes a Bayesian inference method for the reduced-order modeling of time-dependent systems. Informed by the structure of the governing equations, the task of learning a reduced-order model from data is posed as a Bayesian inverse problem with Gaussian prior and likelihood. The resulting posterior distribution characterizes the operators defining the reduced-order model, hence the predictions subsequently issued by the reduced-order model are endowed with uncertainty. The statistical moments of these predictions are estimated via a Monte Carlo sampling of the posterior distribution. Since the reduced models are fast to solve, this sampling is computationally efficient. Furthermore, the proposed Bayesian framework provides a statistical interpretation of the regularization term that is present in the deterministic operator inference problem. The proposed method is demonstrated on a single-injector combustion process.

MS 20–Talk 5: **Least-squares Parametric Reduced-order Modeling**

Authors: Petar Mlinarić and Serkan Güğercin (Virginia Tech)

Abstract: In this talk, we consider reduced-order modeling for (parametric) linear time-invariant systems, based on nonlinear least-squares. We show how it is a special case of a more general $\mathcal{L}_2$-optimal parametric reduced-order modeling problem by the choice of a measure space. Based on this, we propose a gradient-based optimization algorithm for finding locally optimal reduced-order models. Then, we discuss its relation to the vector fitting method for least-squares reduced-order modeling of linear time-invariant systems. Furthermore, we present the necessary optimality conditions in the interpolation form, related to interpolatory $\mathcal{H}_2$-optimality conditions. Finally, we demonstrate the results on a number of numerical examples.

MS 20–Talk 6: **Structure-preserving machine learning moment closures for the radiative transfer equation**

Authors: Juntao Huang[1], Yingda Cheng[2], Andrew J. Christlieb[2], Luke F. Roberts[3] and Wen-An Yong[4] (1: Texas Tech University, 2: Michigan State University, 3: Los Alamos National Lab, 4: Tsinghua University)

Abstract: In this talk, we present our work on structure-preserving machine learning (ML) moment closure models for the radiative transfer equation. Most of the existing ML closure models are not able to guarantee the stability, which directly causes blow up in the long-time simulations. In our work, with carefully designed neural network architectures, the ML closure model can guarantee the stability (or hyperbolicity). Moreover, other mathematical properties, such as physical characteristic speeds, are also discussed. Extensive benchmark tests show the good accuracy, long-time stability, and good generalizability of our ML closure model.

MS 20–Talk 7: **Fast Online Adaptive Enrichment for Poroelasticity with High Contrast**

Authors: Xin Su[1], Sai-Mang Pun[1] (1: Texas A&M University)

Abstract: In this work, we develop an online enrichment strategy within the framework of the Constraint Energy Minimizing Generalized Multiscale Finite Element Method (CEM-GMsFEM) to solve the problem of

linear heterogeneous poroelasticity with coefficients of high contrast. The proposed method makes use of the fast online adaptive method to enrich the multiscale spaces for the displacement and the pressure. Additional online basis functions are computed in oversampled regions based on current residual information and are adaptively chosen to decrease the error the most. A complete theoretical analysis of the online enrichment algorithm is provided and justified by numerical experiments.

MS 20–Talk 8: **A new reduced order model of linear parabolic PDEs**

Authors: Yangwen Zhang[1], Noel Walkington[1], Franziska Weber[2] (1: Carnegie Mellon University, 2: University of California Berkeley)

Abstract: How to build an accurate reduced order model (ROM) for multidimensional time dependent partial differential equations (PDEs) is quite open. In this paper, we propose a new ROM for linear parabolic PDEs. We prove that our new method can be orders of magnitude faster than standard solvers, and is also much less memory intensive. Under some assumptions on the problem data, we prove that the convergence rates of the new method is the same with standard solvers. Numerical experiments are presented to confirm our theoretical result.

MS 21: Recent Advances of Numerical Simulations for Fluid Flows and Applications

Organizers: Yong Yang & Yonghua Yan

Numerical simulations have become vital research tools in fluid flows. This mini-symposium is dedicated to recent developments of numerical simulations for fluid flows and applications. All numerical methods including the finite difference method, the finite volume method, the finite element method, and the lattice Boltzmann method are welcome.

MS 21–Talk 1: **Study on the asymmetrical structure in late transitional boundary layer using DNS and Rortex**

Authors: Yong Yang[1], Yonghua Yan[2], and Caixia Chen[3] (1: West Texas A&M University, 2: Jackson State University, 3: Tougaloo College)

Abstract: The late transitional boundary layer is simulated by the Direct Numerical Simulation (DNS) on a flat plate at Mach number 0.5 and the asymmetrical structures are investigated. To study the source of the asymmetry from symmetric structures, we utilized the newly developed vortex visualization method, Rortex, which has an advantage in identifying vortex cores. The study shows that the origin of asymmetrical structures of the transitional flow matches with the local extreme zone of Rortex. The evolution of the asymmetrical flow structures developed along with large scale vortex cores that are defined by Rortex, which shows the generation of the asymmetry have strong correlations with fluid rotation. This study provides new insights for a deeper understanding of mechanism of turbulence.

MS 21–Talk 2: **Numerical study of the vortical structures in MVG controlled supersonic flow under different Mach numbers**

Authors: Yonghua Yan[1], Yong Yang[2], and Shiming Yuan[1] (1: Jackson State University, 2: West Texas A&M University)

Abstract: MVG (Micro Vortex generator) is a small passive control device used to control boundary layer flow. Previous study found that the ring-like vortex generated by MVG plays a very important role in reducing the separation zone caused by ramp shock waves. A clear understanding of the mechanism of the structure of vortices contributes to further understanding of SWBLI (Shock Wave Boundary Layer Interaction) and the control of flow separation. The purpose of this study was to investigate the effect of different incoming flow velocities on the vortex structure generated by the MVG. This study investigates MVG-controlled supersonic flow at five different Mach numbers ranging from 1.5 to 5.0. Numerical results show that the large eddy

structure generated by the MVG changes as the Mach number increases. At large Mach numbers, the structure in the lower boundary layer will seriously affect the vortex structure generated by the MVG, thereby affecting the formation of momentum deficit and ring-like vortices.

MS 21–Talk 3: **LBM simulation of swallowing process with dysphagia**

Authors: Caixia Chen[1], Yonghua Yan[2], Yong Yang[3], and Demetric L. Barnes[2] (1: Tougaloo College, 2: Jackson State University, 3: West Texas A&M University)

Abstract: Modeling and numerical simulation of the process of swallowing bolus food during the pharyngeal stage is conducted to understand the problems caused by dysphagia, which refers to difficulty eating or swallowing. Understanding normal swallowing mechanisms and how they are disrupted is an important patient safety goal in providing care. In this study, bolus flow is regarded as a free surface jet in hydrodynamics. The multiphase LBM (Lattice Boltzmann Method) algorithm is used to model the bolus flow. Two-dimensional numerical results of bolus flow with different flow parameters, such as viscosity and initial velocity of the flow, were obtained without considering the effect of respiration. In the absence of normal swallowing ability, the possibility of choking on water/food during swallowing was investigated. This study provides some guidance for understanding dysphagia and finding corresponding aids.

MS 21–Talk 4: **Power spectrum analysis of the interaction between large vortices and ramp shock waves in MVG controlled supersonic ramp flow**

Authors: Demetric l Banines[1], Yong Yang[2], Shiming Yuan[1], and Yonghua Yan[1] (1: Jackson State University, 2: West Texas A&M University)

Abstract: After decades of intensive research, the driving source of flow frequency instabilities in shock boundary layer interaction (SWBLI) remains unknown. In this study, high-resolution large eddy simulation (LES) was adopted to simulate supersonic ramp flow controlled by a micro-vortex generator (MVG). Power spectrum analysis of the interaction between the large-scale vortices and ramp shock waves were conducted at the ramp corner. The frequency distributions of large-scale vortex and shock oscillations at different Mach numbers in the MVG-controlled SWBLI region are investigated. In each case, the low frequencies of the flow instabilities are dominated by the frequencies of the large-scale eddies. A strong correlation is observed between the low-frequency distribution of large-scale vortices and shock oscillations. Although the vortex structure became more complex, the correlation did not decrease with larger Mach numbers.

MS 22: Stability of Solitary Waves with applications to Optics and Fluids

Organizers: Brian Choi & Ross Parker

This minisymposium presents recent advances in the stability of solitary waves motivated from nonlinear wave phenomena. Solitary waves are localized disturbances in a medium that propagate with a constant velocity. Nonlinear wave equations often exhibit solitary wave solutions whose stability properties are of interest for both mathematical and physical reasons. This session highlights these stability features via analytic and numerical approaches, featuring the fourth-order nonlinear Schrodinger equation, the generalized Lugiato-Lefever equation, and the complex Ginzburg-Landau equation.

MS 22–Talk 1: **Pure Quartic Solitons in Novel Laser Designs**

Authors: Sabrina Hetzel (Southern Methodist University)

Abstract: Pure quartic optical solitons are a special class of solitons that arise from the interaction of fourth order dispersion and the self-phase modulation due to the Kerr effect. We adapt the Lugiato-Lefever model to include purely fourth order dispersion instead of second order dispersion to consider this special class of solitons in laser systems. Investigation is done in the dynamics, bifurcation structure and stability of single and double pulse solutions. Numerical simulations are done to provide evidence of different kinds of pulse generation for

noisy initial conditions. Linear stability analysis is then conducted on these solutions to provide evidence of stable and unstable double pulse solutions. Pure quartic solitons have a unique characteristic compared to that of conventional solitons (second order dispersion), namely oscillatory tails. By looking at the interaction of individual solitons through the overlap of the tails, we locate the fixed distance between them that is related to the wavelength of these oscillations.

MS 22–Talk 2: **Stability of Ginzburg-Landau Solitons via Fredholm determinants of a Green's operator**

Authors: Erika Gallo[1], John Zweck[1], and Yuri Latushkin[2] (1: University of Texas at Dallas, 2: University of Missouri)

Abstract: Using the symmetric split-step method, we locate a soliton solution of the cubic-quintic Complex Ginzburg-Landau Equation. Linearizing the CGLE about such a solution, we classify the soliton's stability by computing eigenvalues of the linearized differential operator. We do this using the 2-modified Fredholm determinant of the associated Green's kernel, an approach which is complementary to Evans function methods for solitons. We adapt a method of Bornemann to numerically approximate the Fredholm determinant by a matrix determinant, and we quantify the error in this approximation.

MS 22–Talk 3: **Bright and Dark Multi-Solitons in a Fourth-Order Nonlinear Schrödinger Equation**

Authors: Ross Parker, Alejandro Aceves (Southern Methodist University)

Abstract: We consider the existence and spectral stability of multi-pulse solitary wave solutions to a nonlinear Schrödinger equation which incorporates both fourth and second-order dispersion terms. We do this for both the bright and the dark soliton regimes. We first show that a discrete family of multi-pulse solutions exists, which is characterized by the distances between consecutive copies of the the primary solitary wave. In the bright soliton regime, we then reduce the spectral stability problem to computing the determinant of a matrix which is, to leading order, block diagonal. Under additional assumptions, which can be verified numerically and are sufficient to prove orbital stability of the primary solitary wave, we show that all bright multi-solitons are spectrally unstable. By contrast, using a similar approach in the dark soliton regime, we find that dark multi-solitons can be spectrally neutrally stable. Finally, we show results of numerical spectral computations, which are in good agreement with our analytical results. This is supplemented with numerical timestepping experiments, which are interpreted using our spectral computations.

MS 22–Talk 4: **Continuum limit of 2-d Nonlinear Schr̈dinger Equation**

Authors: Brian Choi, Alejandro Aceves (Southern Methodist University)

Abstract: Recently, there has been an increased interest in non-local PDEs. While most of the research deals with continuum models, less is known about discrete systems showing global coupling with algebraic decay on the coupling strength. This work considers such a case in a two-dimensional lattice and centers on the question of the validity of a suitable continuum approximation. We prove that the solutions to the discrete Nonlinear Schrödinger Equation (DNLSE) with non-local algebraically-decaying coupling converge strongly in $L^2(\mathbb{R}^2)$ to those of the continuum fractional Nonlinear Schrödinger Equation (FNLSE), as the discretization parameter tends to zero. The proof relies on sharp dispersive estimates that yield Strichartz estimates that are uniform in the discretization parameter. An explicit computation of the leading term of the oscillatory integral asymptotics is used to show that the best constants of a family of dispersive estimates blow up as the non-locality parameter $\alpha \in (1, 2)$ approaches the boundaries.

MS 23: Special Topics in Mathematical Biology

Organizers: Summer Atkins & Hayriye Gulbudak

The aim of this session is to provide an opportunity for researchers to meet and discuss recent advances in mathematical biology. Such advances can be new biological findings obtained through the use of tools from the mathematical sciences or new mathematical ideas and methods that have direct applications to biological investigations. Topics include but are not limited to population dynamics, deterministic or stochastic modeling, optimal control theory, network modeling, and statistical analysis.

MS 23–Talk 1: **Complexities of the Cytoskeleton: Integration of Scales**

Authors: Keisha Cook (School of Mathematical and Statistical Sciences, Clemson University, Clemson, South Carolina, USA)

Abstract: Biological systems are traditionally studied as isolated processes (e.g. regulatory pathways, motor protein dynamics, transport of organelles, etc.). Although more recent approaches have been developed to study whole cell dynamics, integrating knowledge across biological levels remains largely unexplored. In experimental processes, we assume that the state of the system is unknown until we sample it. Many scales are necessary to quantify the dynamics of different processes. These may include a magnitude of measurements, multiple detection intensities, or variation in the magnitude of observations. The interconnection between scales, where events happening at one scale are directly influencing events occurring at other scales, can be accomplished using mathematical tools for integration to connect and predict complex biological outcomes. In this work we focus on building inference methods to study the complexity of the cytoskeleton from one scale to another.

MS 23–Talk 2: **Population dynamics under environmental and demographic stochasticity**

Authors: Alexandru Hening [1]*, Weiwei Qi[2], Zhongwei Shen[2] and Yingfei Yi[2] (1: Department of Mathematics, Texas A&M University, College Station, Texas, USA. 2: Department of Mathematics, University of Alberta, Edmonton, CA)

Abstract: This work looks at the long term dynamics of diffusion processes modelling a single species that experiences both demographic and environmental stochasticity. In this setting, the long term dynamics of the population in the absence of demographic stochasticity is determined by the sign of Λ_0 , the external Lyapunov exponent: $\Lambda_0 <$ implies (asymptotic) extinction and $\Lambda_0 >$ implies convergence to a unique positive stationary distribution μ_0. If the system is of size $\frac{1}{\epsilon^2}$ for small $\epsilon > 0$, the extinction time is finite almost surely. One must therefore analyze the quasi-stationary distribution (QSD) μ_ϵ of the system.

We look at what happens when the population size is sent to infinity, i.e., when $\epsilon \to 0$. In contrast to models that only take into account demographic stochasticity, our results demonstrate the significant effect of environmental stochasticity – it turns an exponentially long mean extinction time to a sub-exponential one.

MS 23–Talk 3: **Effect of cross-immunity in a multi-strain cholera model**

Authors: Leah LeJeune*, Cameron Browne (Department of Mathematics, University of Louisiana at Lafayette, Lafayette, Louisiana, USA)

Abstract: Observed in recent cholera outbreaks is the presence of two serotypes, strains of the cholera bacteria that mainly differ in their induced host immunity. Each serotype induces both self-immunity and a degree of cross-immunity to the other strain for some duration. We combine and extend previously studied SIRP and multi-strain models to consider the strain diversity of cholera. We explore various ways of incorporating host immunity into this deterministic multi-strain model, characterizing the dynamics and long-term behavior, particularly in the case of serotype coexistence.

MS 23–Talk 4: **Multistationarity and concentration robustness in biochemical reaction networks**

Authors: Badal Joshi[1], Nidhi Kaihnsa[2], Tung D. Nguyen[3]*, Anne Shiu[3] (1: California State University, San Marcos. 2: Brown University. 3: Texas A&M University)

Abstract: Reaction networks are commonly used to model a variety of physical systems ranging from the microscopic world like cell biology and chemistry, to the macroscopic world like epidemiology and evolution

biology. Reaction networks arising in applications often exhibit multistationarity-that is, the capacity for two or more steady states. This property is important as it is often associated with the capability for cellular signaling and decision-making. Another biologically relevant property that reaction networks can have is absolute concentration robustness (ACR), which refers to when a steady-state species concentration is maintained even when initial conditions are changed. In this project, our driving motivation is to explore the relationship between the two properties and investigate the prevalence of networks with either property. Our analysis focuses on two ends of the network-size spectrum: small networks with a few species and large networks with many species.

MS 23–Talk 5: **A switch point algorithm applied to a harvesting problem**

Authors: S. Atkins [1*], M. Martcheva[2], and W. Hager[2] (1: Department of Mathematics, Louisiana State University, Baton Rouge, Louisiana, USA. 2: Department of Mathematics, University of Florida, Gainesville, Florida, USA)

Abstract: In this talk we investigate an optimal control problem that seeks an optimal fishing strategy that maximizes the harvesting yield. The underlying question we are studying is whether marine reserves, regions in which fishing is prohibited, can be beneficial to the maximum harvesting yield. The harvesting problem is linear in the control, so parameters of this problem can be set to where the optimal harvesting strategy possesses a singular subarc. In such a scenario, Fuller's phenomenon or chattering occurs. This is the phenomenon in which the optimal control oscillates infinitely many times over a finite region. Since such a strategy cannot be realistically implemented, we will find suboptimal solutions to this problem by applying a switch point algorithm, a numerical method in which we solve for the optimal control problem with respect to the switches of the control rather than control itself. In using the switch point algorithm, we find some suboptimal harvesting strategies that lead to the incorporation of marine reserves.

MS 24: Nonlinear Physics Models and Mathematical Structures

Organizers: Vesselin Vatchev, Zhijun Qiao, Wilson Zuniga Galindo & Erwin Suazo

The aim of the mini symposium is participants to present talks and engage in a discussion of a variety of recent work and results in the area of Nonlinear Physics. The emphasis is on nonlinear PDE's, properties of their solutions, and theoretical or numerical methods for solving them with direct application to Physics Models. Topics of interest are developing models, numerical solutions and methods designed to better capture Physical characteristics of PDE's, and in more general terms providing mathematical structures to describe Physics phenomenon.

MS 24–Talk 1: **5th-order CH equation with pseudo-peakons**

Authors: Zhijun Qiao (UT Rio Grande Valley)

Abstract: In this talk, I will majorly focus on the scalar peakon models developed in the last 30 years. Most integrable peakon equations come from the negative order flow in the hierarchy. I will take some examples to explain higher order models with peakons or pseudo-peakons we proposed recently. Some open problems will also be addressed for discussion in the end.

MS 24–Talk 2: **Self-similar transformation and chirped nonlinear waves for the Davey-Stewartson I equation**

Authors: Jiefang Zhang (Communication University of Zhejiang,Hangzhou 310018,China)

Abstract: Self-similar phenomena in the nonlinear media are receiving intensive studies in diverse branches of physics. Self-similar pulse propagation in single-mode optical fibers is currently a subject of intensive theoretical and experimental studies. These self-similar waves are potentially useful for various applications in optical soliton telecommunications, since they can maintain their overall shapes but allow their amplitudes and widths to change with the modulation of the system parameters such as dispersion, nonlinearity, gain, inhomogeneity, and so on. We investigate the propagation characteristics of the chirped self-similar solitary waves in the

Davey-Stewartson I equation. This model contains many special types of nonlinear equations that appear in various branches of contemporary physics. We extend the self-similar analysis presented for searching chirped self-similar structures of the the nonlinaer Schrodinger equation in (1+1)-dimensions(one spatial and one temporal dimensions) to the Davey-Stewartson equation involving (2+1)-dimensions(two spatial and one temporal dimensions). A variety of exact linearly chirped localized solutions with interesting properties are derived in the presence of all physical effects. The solutions comprise bright, kink and antikink, and algebraic solitary wave solutions, illustrating the potentially rich set of self-similar pulses of the model. It is shown that these optical pulses possess a linear chirp that leads to efficient compression or amplification, and thus are particularly useful in the design of optical fiber amplifiers, optical pulse compressors, and solitary wave based communication links.

MS 24–Talk 3: **Interactions of Traveling Waves in Low Order Approximations for the Two-Dimensional Euler Equations**

Authors: Julio Paez (UT Rio Grande Valley)

Abstract: In this talk, we discuss traveling waves with elastic and inelastic interactions in a low order of approximation. The waves are derived from the two-dimensional Euler equations in quadratic or linear order of approximation. A new type of inelastic interaction that is closely related to numerical study observations of the Euler equations is obtained in linear order.

MS 24–Talk 4: **Engineered Approximate Solutions to the Two-Dimensional Euler Equations**

Authors: Vesselin Vatchev (UT Rio Grande Valley)

Abstract: The two-dimensional Euler equations (EE) model wave propagation in a shallow thin channel. The relative simplicity of the physical setting allows for experimental observations, but the nonlinearity of the system is very challenging for general theoretical results. One of the most effective approaches to study EE is by using asymptotic expansion of the variables to derive an approximate system. The order of approximation is measured in the powers of the small wave amplitude. Boussinesq, KdV and Fifth order KdV, Camassa-Holm equations are a few examples obtained by using the technique with different order of approximation. The resulting systems have traveling wave solutions, but they are still approximation of the equation's order to the solutions of EE. Experiments indicate the practical importance of traveling wave solutions with special features which cannot be easily related to a solution of an approximate system. In the talk we discuss a modification of the asymptotic expansion method to engineer surface wave interactions (which are not solutions of approximate systems) that are practical, of quadratic order of approximation, and easy to study.

MS 24–Talk 5: **p-Adic Statistical Field Theory and Deep Belief Networks**

Authors: W. A. Zúñiga-Galindo (UT Rio Grande Valley)

Abstract: The talk aims to present the results of our preprint arXiv:2207.13877. In this work we initiate the study of the correspondence between p-adic statistical field theories (SFTs) and neural networks (NNs). In general quantum field theories over a p-adic spacetime can be formulated in a rigorous way. Nowadays these theories are considered just mathematical toy models for understanding the problems of the true theories. In this work we show these theories are deeply connected with the deep belief networks (DBNs). Hinton et al. constructed DBNs by stacking several restricted Boltzmann machines (RBMs). The purpose of this construction is to obtain a network with a hierarchical structure (a deep learning architecture). An RBM corresponds to a certain spin glass, thus a DBN should correspond to an ultrametric (hierarchical) spin glass. A model of such a system can be easily constructed by using p-adic numbers. In our approach, a p-adic SFT corresponds to a p-adic continuous DBN, and a discretization of this theory corresponds to a p-adic discrete DBN. We show that these last machines are universal approximators.

MS 24–Talk 6: **Quantum Control of Qubits and Qutrits**

Authors: Baboucarr Dibba (UT Rio Grande Valley)

Abstract: The main setup of quantum control is that the optimization of data output and noise decoherence and such optimality is to create certain the integrity, confidentiality, and credibility and additionally the non-interference of noise in any data transmission. Putting into consideration the coherent states with the bichromatic cavity modes, as we developed the Euler angle-dressed state used in calculating the amplitudes of the three-level quantized systems. The atom-field entanglement is taken under consideration for the measured three-level systems applying the Phoenix-Knight formalism and corresponding population inversion with an observation of the collapse and revival of different signal stages for the systems. A very impressive concept is taken through an experiment and in theory in superconducting quantum circuits, that provide a platform for manipulating microwave photons. As the optimum generation of entangled states is of great significance to quantum information science.

Theoretically, utilizing an approach centered on the widespread excited Raman-adiabatic passage technique and invariant-based shortcuts(STA) to adiabaticity achieves these objectives for quantum state transfers in common three-level systems whilst considering coupled photonic grid as a harmonic oscillator with frequency and time-varying mass. We show numerically that the technique in order with a wide set of control parameters, initiating the timescales nearer to the quantum speed limit, in addition, considering the presence of environmental disturbance.

MS 24–Talk 7: **p-adic Cellular Neural Networks: Applications to Image Processing**

Authors: Brian Zambrano (UT Rio Grande Valley)

Abstract: In this talk, we present two applications of some p-adic Cellular Neural Networks (CNN) modeled by PDEs. First, an edge detector based on p-adic CNN for gray images comparing the results with the Canny edge detector. Second, we also present a new p-adic CNN with a diffusion term. This network can be considered a p-adic generalization of a Stated Control- CNN. We use this new network to process some noised images and compare them with Perona-Malik's results.

MS 24–Talk 8: **Probabilistic solutions of fractional differential and partial differential equations and their Monte Carlo simulations**

Authors: Erwin Suazo (UT Rio Grande Valley)

Abstract: The work in this paper is four-fold. Firstly, we introduce an alternative approach to solve fractional ordinary differential equations as an expected value of a random time process. Using the latter, we present an interesting numerical approach based on Monte Carlo integration to simulate solutions of fractional ordinary and partial differential equations. Thirdly, we show that this approach allows us to find the fundamental solutions for fractional partial differential equations (PDEs), in which the fractional derivative in time is in the Caputo sense and the fractional in space one is in the Riesz-Feller sense. Lastly, using Riccati equation, we study families of fractional PDEs with variable coefficients which allow explicit solutions. Those solutions connect Lie symmetries to fractional PDEs. This is joint work with Dr. T. Oraby and graduate student H. Arrubla.

MS 25: High Order Methods for Computational Hydrodynamics

Organizers: Madison Sheridan & Bennett Clayton

The construction of accurate numerical methods is essential for simulating transport phenomena in the field of computational hydrodynamics. The aim of this mini-symposium is to discuss the current state of higher-order accurate methods for simulating realistic hydrodynamics. In particular, we are interested in numerical methods that are higher-order accurate in space and time while maintaining structure preserving properties. The partial differential equations we have in mind are those with dominant hyperbolic features such as: (i) the compressible Euler Equations; (ii) the Shallow Water Equations; (iii) the compressible Navier-Stokes Equations; (iv) radiation transport equations such as the Boltzmann Equation. These equations are often strongly nonlinear and pose numerous challenges when one tries to discretize and solve them numerically.

MS 25–Talk 1: **Energy stable state redistribution cut-cell discontinuous Galerkin methods for wave propagation**

Authors: Christina G. Taylor[1] and Jesse Chan[1] (1: Rice University)

Abstract: Cut cell methods provide the ability to represent complex geometries while maintaining the simplicity of a Cartesian mesh wherever possible. However, cut cell meshes can result in extremely small and/or skewed cut elements that severely restrict the maximum stable time step of a simulation. Special discretizations may also be required to ensure that a cut-cell method is energy stable. In this work we prove the L2 stability of state redistribution, a technique for relaxing the CFL condition when small elements are present, and combine it with a provably energy stable high order discontinuous Galerkin formulation for wave propagation problems.

MS 25–Talk 2: **Robust and efficient approximation of the compressible Navier-Stokes equations**

Authors: Matthias Maier (1: Department of Mathematics, Texas A&M University)

Abstract: Structure preserving numerical methods provide theoretical guarantees of reliability for situations where ad-hoc stabilization techniques can fail. In this talk we present a fully discrete approximation technique for the compressible Navier-Stokes equations that is second-order accurate in time and space and guaranteed to be invariant domain preserving. This means the method maintains important physical invariants and is guaranteed to be stable without the use of ad-hoc tuning parameters.

We discuss the underlying algebraic discretization technique based on collocation and convex limiting, and briefly comment on a high-performance implementation utilizing SIMD (single instruction multiple data) vectorization and OpenMPI parallelization.

MS 25–Talk 3: **A second order invariant domain preserving method for the compressible Euler equations with a tabulated equation of state**

Authors: Bennett Clayton[1], Jean-Luc Guermond[1], Matthias Maier[1], Bojan Popov[1], Eric Tovar[2] (1: Department of Mathematics, Texas A&M University 3368 TAMU, College Station, TX 77843, USA. 2: X Computational Physics, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM, 87545, USA)

Abstract: In this talk we present a second order method for approximating the compressible Euler equations with a complicated or tabulated equation of state. This method uses the so-called entropy viscosity which requires an analytic expression for the entropy. This becomes a problem if the equation of state is tabulated or incomplete. To resolve this issue, we propose a surrogate entropy which behaves similar to the physical entropy. Convex limiting is also performed on a surrogate entropy which guarantees an invariant domain preserving property.

We provide a variety of numerical illustrations with a variety of equations of state which demonstrate the second order convergence as well as convergence to solutions with composite wave structures.

MS 25–Talk 4: **High-order methods for nonlinear wave equations in second order form**

Authors: Thomas Hagstrom (Southern Methodist University)

Abstract: The theory of numerical methods for first-order hyperbolic systems in Friedrichs form is well-developed, and at least in one space dimension there are even effective methods to treat singular solutions. However, many physical theories are based on action principles which lead to second order systems. Although it is often possible to recast these as first order Friedrichs systems, with the complication of additional initial and boundary conditions and additional constraints, we would like to develop methods which treat the second order systems directly. We will illustrate our construction with examples from gravitional wave theory and compressible flows, and also discuss some new singularity phenomena which arise.

MS 25–Talk 5: **A high-order explicit Runge-Kutta method for approximating the Shallow Water Equations with sources**

Authors: Eric J. Tovar (Los Alamos National Laboratory)

Abstract: In this talk, we introduce a new higher-order in space and time approximation of the Shallow Water Equations (SWEs) with sources. In particular, we show how to construct explicit Runge–Kutta (ERK) time stepping techniques for the SWEs that are invariant-domain preserving and well-balanced with respect to rest states.

MS 25–Talk 6: **Modeling Shallow Water Flows through Obstacles with Windows**

Authors: Suncica Canic[1], Alina Chertock[2], Shumo Cui[3], Alexander Kurganov[3], Xin Liu[4], Abdolmajid Mohammadian[4] and Tong Wu[5] (1: University of California, Berkeley, and University of Houston, 2: North Carolina State University, 3: Southern University of Science and Technology, 4: University of Ottawa, and 5: The University of Texas at San Antonio)

Abstract: When flooding occurs in urban areas, water may flow into houses and other window structure obstacles. Those kinds of obstacles can be commonly found nearby the base of the raised houses as flood control structures. The investigation of such water flows plays a critical role in both flood mitigation and the planning of new urban areas. Water flows through this type of obstacle can be simulated using the incompressible 3-D Navier-Stokes equations. However, a 3-D model of an urban environment is not practical due to the high computational cost. The 2-D shallow water system is substantially less expensive, which leads us to the idea of using a multi-layer shallow water system to model the flow near the window. We have invented a strategy of locally switching back and forth between the single- and multi-layer shallow water systems, in which the total amount of water and the momentum is conserved. The designed schemes are well-balanced and positivity preserving, and the results from numerical simulations achieve good agreements with the experimental data.

MS 25–Talk 7: **A positivity-preserving and conservative high-order flux reconstruction method for the polyatomic Boltzmann–BGK equation**

Authors: Tarik Dzanic[1] (1: Texas A&M University)

Abstract: The governing equations for the majority of computational fluid dynamics solvers rely on the continuum assumption for the fluid. For many problems of interest, including rarefied gases and hypersonic flows, this assumption starts to break down, and it becomes necessary to revert to the governing equations of molecular gas dynamics which underpin the macroscopic behavior of the fluid. One such example, the Boltzmann equation, provides a statistical description of particle transport and collision which can recover the hydrodynamic equations in the asymptotic limit while providing a more detailed description of non-equilibrium systems and flows outside of the continuum regime. However, due to its high-dimensional nature, solving the Boltzmann equation comes at a computational cost that can be orders of magnitude higher than the associated transport equations for the macroscopic variables.

In this talk, we will present a numerical scheme for solving the polyatomic Boltzmann equation with the aim of increasing the applicability of the approach and drastically reducing the associated computational cost. The proposed scheme combines a positivity-preserving high-order flux reconstruction spatial discretization for unstructured meshes, guaranteeing the positivity of density and internal energy, with a nodal discrete velocity model, ensuring conservation regardless of the resolution. Furthermore, the computational cost of the collision operator is reduced through the Bhatnagar–Gross–Krook (BGK) operator, and internal degrees of freedom are included to extend the approach to polyatomic molecules and general constitutive laws. The applicability of the approach will be shown in a series of multi-scale numerical experiments, ranging from supersonic flows to compressible three-dimensional turbulence.

MS 25–Talk 8: **Greedy invariant-domain preserving approximation for hyperbolic system**

Authors: J.-L. Guermond[1], M. Maier[1], B. Popov[1], L. Saavedra[2], I. Tomas[3] (1: Department of Mathematics, Texas A&M University, 3368 TAMU, College Station, TX 77843, USA. 2: Departamento de Matemática Aplicada a la Ingeniería Aeroespacial, E.T.S.I. Aeronáutica y del Espacio, Universidad Politécnica de Madrid, 28040 Madrid, Spain. 3: Department of Mathematics and Statistics, Texas Tech University, 2500 Broadway Lubbock, TX 79409, USA.)

Abstract: In this work we propose a new way to estimate the artificial viscosity that has to be added to make explicit, conservative, and consistent numerical methods invariant-domain preserving and entropy inequality compliant. Instead of computing an estimate on the maximum wave speed in Riemann problems, we estimate a minimum wave speed in the said Riemann problems so that the approximation satisfies predefined bounds and predefined entropy inequalities. This technique eliminates non-essential fast waves from the construction of the artificial viscosity, while preserving pre-assigned invariant-domain properties and entropy inequalities. For instance, this technique eliminate accoustic waves in contact discontinuities. The resulting technique produces a methods that is invariant-domain preserving and satisfies the pre-assigned entropy inequalities.

MS 25–Talk 9: **The immersed interface method for simulating flows around rigid objects represented by triangular meshes**

Authors: Sheng Xu (Southern Methodist University)

Abstract: A rigid solid moving in a fluid can be modeled as a fluid in rigid motion enclosed by the fluid-solid interface. The velocity, the pressure and their spatial derivatives across the interface are non-smooth or discontinuous with jumps. The immersed interface method incorporates necessary jump conditions across the interface into numerical schemes to attain the sharp interface, desired accuracy and high efficiency in numerical simulation. In the past, global parametrization was used to represent an interface to ease the computation of jump conditions, but it is generally limited to smooth and simple interfaces. In this talk, we present how to compute jump conditions on a triangular mesh that represents an interface. The interface can be non-smooth and complex. The immersed interface method with triangular mesh representation is robust to simulate flows around multiple moving non-smooth complex rigid solids. We simulate various flows to demonstrate the accuracy, efficiency and robustness of the method.

MS 25–Talk 10: **A parallel high-order overset framework for compressible turbulent flows**

Authors: Amir Akbarzadeh[1], Lai Wang[1], Freddie Witherden[2], Antony Jameson[1,2] (1: Texas A&M University, Department of Aerospace Engineering, 1: Texas A&M University, Department of Ocean Engineering)

Abstract: A parallel high-order overset framework is developed to simulate moving object problems such as rotorcrafts and wind turbines. Here, we implement overset grid connectivity developed in TIOGA library into PyFR for simulating compressible flows. The framework is developed to be used with many GPUs on both linear and high-order curved hex grids. Moreover, using high-order interpolations, the framework is capable of visualizing flow fo all grids on the background grid, which alleviates the flow visualization in the case of presence of multiple grids. The framework is validated against benchmarks such as turbulent Taylor-Green vortex with a moving grid, and a spinning sphere.

MS 25–Talk 11: **Guaranteed upper bound for the maximum speed of propagation in the Riemann problem**

Authors: Bennet Clayton[1], Jean-Luc Guermond[1], Bojan Popov[1] (1: Department of Mathematics, Texas A&M University, 3368 TAMU, College Station, TX 77843, USA.)

Abstract: We will present a derivation of a guaranteed upper bound for the maximum speed of propagation in the Riemann solution for the Euler system of gas dynamics in Eulerian or Lagrangian frame with the Extended Noble-Abel Stiffened-Gas Equation of State. The novelty is that an accurate upper bound on the speed is given explicitly, hence no iterative solver is needed, and the algorithm can be used in both Eulerian and Lagrangian frame. Moreover, the upper bound can be used to define a first order invariant domain preserving method for the Euler system even when the equation of state is tabulated. This is a joint work with Bennet Clayton and Jean-Luc Guermond.

MS 25–Talk 12: **Higher-order methods for phase-resolving wave/structure interaction**

Authors: Chris Kees and Wen-Huai Tsao and Rebecca Schurr (Louisiana State University)

Abstract: We consider viscous, inviscid, and depth-averaged models of non-hydrostatic coastal wave propagation over submerged and emergent structures. Our aim is to model wave height attenuation and momentum dissipation through marsh vegetation and over coastal protective structures. Each model requires a significantly different set of numerical methods to achieve higher-order accuracy in a robust manner, and we will discuss several of these, including CutFEM and flux limiting. Finaly we present results on experimental data obtained from physical models of wave/structure interaction.

MS 26: Scientific Deep Learning

Organizers: Hai Nguyen, Tan Bui-Thanh & C. G. Krishnanunni

The fast growth in practical applications of deep learning in a range of contexts has fueled a renewed interest in deep learning methods over recent years. Subsequently, scientific deep learning is an emerging discipline that merges scientific computing and deep learning. Whilst scientific computing focuses on large-scale models that are derived from scientific laws describing physical phenomena, deep learning focuses on developing data-driven models which require minimal knowledge and prior assumptions. With the contrast between these two approaches follows different advantages: scientific models are effective at extrapolation and can be fitted with small data and few parameters whereas deep learning models require a significant amount of data and a large number of parameters but are not biased by the validity of prior assumptions. Scientific deep learning endeavors to combine the two disciplines in order to develop models that retain the advantages from their respective disciplines. This mini-symposium collects recent works on scientific deep learning methods covering theories, algorithms, and engineering and sciences applications.

MS 26–Talk 1: **Deep Learning of the Evolution of Unknown Systems**

Authors: Victor Churchill, Dongbin Xiu (The Ohio State University)

Abstract: Many phenomena in science and engineering are observable but not yet explainable. That is, we can observe solution data generated from many physical systems, but the actual physics, e.g. an ordinary or partial differential equation model, are unknown. In this case, developing a deep neural network based model that replicates the system's behavior is desirable. Hence in this talk, we'll explore how to learn the time evolution of unknown ODE and PDE systems from their solution data using deep neural networks. The specific neural network architectures used are grounded in numerical methods for solving ODEs and PDEs. We also consider the case of partially observing the solution vector, where a time history of the observed variables are required.

MS 26–Talk 2: **Development of a Physics-Informed Machine Learning Method for Pressure Transient Test**

Authors: Daniel Badawi, Eduardo Gildin (Petroleum Engineering Department, Texas A&M University)

Abstract: Physics-Informed Machine Learning (PIML) have recently emerged with some interesting and unique features that can be applied to reservoir engineering. In reservoir engineering, well testing is performed to determine reservoir and well properties such as reservoir average permeability, well skin factor, boundary distance, and reservoir average pressure. Well testing is an inverse problem where bottom-hole pressure or production rates are recorded and then matched with the solution of the diffusivity equation that best describes the flow regime. The diffusivity equation is a stiff partial differential equation (PDE) and often very challenging to solve or approximate using traditional numerical methods. Perhaps the most popular test in well testing is the buildup test. In short, a buildup test is the measurement and analysis of bottom-hole pressure data acquired after a producing well is shut in, then the pressure data is matched with a set of approximated solutions to the diffusivity equation which enables the estimation of reservoir and well properties mentioned above. In this talk, we will show the power physics-informed neural networks (PINNs) for determining reservoir properties without having to actually run the well test. To this end, we show how to tackle the stiffness of the PDE that governs the diffusivity equation in porous media flow. Also, we show the inverse capabilities of PINNs for accurately determining reservoir intrinsic properties.

MS 26–Talk 3: **Learning Data-driven Subgrid-Scale Models: Stability, Extrapolation, and Interpretation**

Authors: Pedram Hassanzadeh, Yifei Guan, Ashesh Chattopadhyay, Adam Subel (Rice University)

Abstract: To make simulations of these turbulent flows or other high-dimensional multi-scale systems computationally tractable, processes with scales smaller than the typical grid size of numerical solvers have to be parameterized. Recently, there has been substantial interest (and progress) in using deep learning techniques to develop data-driven subgrid-scale (SGS) parameterizations for many canonical dynamical systems and turbulent flows. However, for these data-driven SGS parameterizations to be useful and reliable in practice, a number of major challenges have to be addressed. These include: 1) instabilities arising from the coupling of data-driven SGS parameterizations to coarse-resolution solvers, 2) learning in the small-data regime, 3) interpretability, and 4) extrapolation to different parameters and forcings. Using several setups of 2D turbulence, as well as two-layer quasi-geostrophic turbulence and Rayleigh-Benard convection as test cases, we introduce methods to address (1)-(4). These methods are based on combining turbulence physics and recent advances in theory and applications of deep learning. For example, we will use backscattering analysis to shed light on the source of instabilities and incorporate physical constraints to enable learning in the small-data regime. We will further introduce a novel framework based on spectral analysis of the neural network to interpret the learned physics and will show how transfer learning enables extrapolation to flows with very different physical characteristics. In the end, we will discuss scaling up these methods to more complex systems and real-world applications, e.g., for SGS modeling of atmospheric gravity waves.

MS 26–Talk 4: **Deep Learning Enhanced Geophysical Inversion Schemes**

Authors: Jiefu Chen, Yanyan Hu, Xuqing Wu, Yueqin Huang (University of Houston)

Abstract: Using joint inversion to reveal underlying geology has drawn considerable research attention due to the availability of multiple geophysical datasets, ever-increasing computational resources, advanced inversion methodologies, and reduced uncertainties. We propose a deep learning enhanced joint inversion framework to simultaneously reconstruct different models by fusing different types of geophysical data. A key issue of joint inversion is to develop effective strategies to fuse different geophysical data in a unified mathematical framework. In our work, we enforce the constraint of structural similarity by a deep neural network (DNN) during the learning process. The framework is designed to combine the DNN and the traditional separate inversion workflow together and improve the joint inversion results iteratively. In each iteration, the separately inverted models will be input into the well-trained network, get improved by the network, and then perform as the initials of the separate inversions in the next iteration. A weighting and cooling strategy is adopted during this process to obtain reasonable and guaranteed inversion results (where the coefficients α_{EM} and α_S are involved). The network can be easily extended to incorporate multi-physics without structural changes. In addition, this learning-based framework demonstrates excellent flexibility when the sensing configuration changes or different discretization is used for different models. We will show several numerical experiments to demonstrate that our deep learning enhanced joint inversion framework can reconstruct more accurate both physical property values and structural features of the anomalous bodies than separate inversions and traditional cross-gradient based joint inversion.

MS 26–Talk 5: **A Model-Constrained Tangent Manifold Learning Approach for Dynamical Systems**

Authors: Hai Nguyen and Tan Bui-Thanh (University of Texas at Austin)

Abstract: Real-time accurate solutions of large-scale complex dynamical systems are in critical need for control, optimization, uncertainty quantification, and decision-making in practical engineering and science applications. This paper contributes in this direction a model-constrained tangent manifold learning (mcTangent) approach. At the heart of mcTangent is the synergy of several desirable strategies: i) a tangent manifold learning to take advantage of the neural network speed and the time-accurate nature of the method of lines; ii) a model-constrained approach to encode the neural network tangent with the underlying governing equations; iii) sequential learning strategies to promote long-time stability and accuracy; and iv) data randomization approach to implicitly enforce the smoothness of the neural network tangent and its likeliness to the truth tangent up second order derivatives in order to further

enhance the stability and accuracy of mcTangent solutions. Both semi-heuristic and rigorous arguments are provided to analyze and justify the proposed approach. Several numerical results for transport equation, viscous Burger's equation, and Navier-Stokes equation are presented to study and demonstrate the capability of the proposed mcTangent learning approach.

MS 26–Talk 6: **Exploiting the local parabolic landscapes of adversarial losses to accelerate black-box adversarial attack**

Authors: Hoang Tran, Dan Lu and Guannan Zhang (Oak Ridge National Laboratory)

Abstract: Machine learning models, and convolutional neural networks (CNNs) in particular, have demonstrated remarkable performance in many classification tasks. However, deep learning technology also exposed certain security risks, as they are susceptible to malicious inputs, which are small, human-imperceptible perturbations to the inputs designed to fool the model prediction. In this talk, we present an investigation into the vulnerability of CNN classifiers from the shape of the loss's landscape perspective. We theoretically and experimentally justify that the adversarial losses of many standard and robust image classifiers behave like parabolas with respect to perturbations in the Fourier domain, but not in the pixel domain. Then, we exploit the parabolic landscape to design a new black-box adversarial attack methods with improved query efficiency, compared to the other state-of-the-art baselines. To mitigate the security risk of the neural networks and avoid overconfident predictions on noisy or malicious inputs, we integrate a recent UQ method, called PI3NN, into CNN to quantify prediction uncertainty and identify out-of-distribution inputs of classification models. The performance of this approach will be demonstrated on the problem of identification of transient location in power systems.

MS 26–Talk 7: **The approximation of the wave equation operator using deep learning**

Authors: Ziad Aldirany[1], Marc Laforest[1], Régis Cottereau[2] and Serge Prudhomme[1] (1: Polytechnique Montréal, 2: Centrale Marseille)

Abstract: The solution of the wave equation is required in a wide variety of fields, such as seismology, electromagnetism, and acoustics. In the last few years, a number of deep learning methods have been developed for the solution of PDE-based problems, with the objective of producing techniques that are more flexible and faster than the traditional FEM, FD, FV approaches. Deep operator networks (DeepONet) attempt to solve PDEs by learning the inverse of the differential operator for a wide class of initial data, rather than learn a single solution. However, this approach is especially expensive for problems containing high frequencies, such as those with the linear wave equation. For the approximation of the homogeneous wave equation, we present a neural network architecture that is based on the integral representation formula of the wave equation. This architecture yields a faster learning and a better generalization error when compared to the classical DeepONet architecture. Moreover, with the proposed architecture, a trained network can be retrained for solutions with higher frequencies which results in an efficient learning strategy for high frequency functions. Numerical results in 1D and 2D will be presented to analyze frequency dependent convergence of the proposed approach.

MS 26–Talk 8: **Strengthening Gradient Descent by Sequential Motion Optimization for Deep Neural Networks**

Authors: Thang Duc-Le[1], Quoc-Hung Nguyen[2], Jaehong Lee[1] and H. Nguyen-Xuan[3] (1: Deep Learning Architecture Research Center, Sejong University, Seoul 05006, Republic of Korea, 2: Department of Computational Engineering, Vietnamese-German University (VGU), Binh Duong City, Viet Nam, 3: CIRTech Institute, HUTECH University, Ho Chi Minh City, Viet Nam)

Abstract: In this report, we introduce a new optimization framework named Sequential Motion Optimization (SMO) to strengthen gradient-based methods. The key idea of SMO comes from a movement mechanism in a recent metaheuristic method called Balancing Composite Motion Optimization (BCMO). Specifically, SMO establishes a sequential motion chain of two gradient-guided individuals including a leader and a follower to enhance the effectiveness of parameter updates in each iteration. A surrogate gradient model is theoretically presented to estimate the gradient of the follower by that of the leader through chain rule during the training process. Experimental results in terms of training quality on both fully-connected multilayer perceptrons (MLPs) and convolutional neural networks (CNNs) with respect to three popular benchmark datasets including MNIST, Fashion-MNIST and CIFAR-10 show the superior performance of the proposed framework in comparison with the vanilla stochastic gradient descent (SGD) implemented via back-propagation (BP) algorithm. Although this study only introduces the vanilla gradient descent (GD) as a main gradient-guided factor in SMO for deep neural networks (DNNs) training application, it has great potential to combine with other gradient-based variants to improve its effectiveness and solve other large-scale optimization problems in practice.

MS 26–Talk 9: **Leveraging Data-driven Surrogates to Enable Efficient Density Estimation of Sparse Observable Data on Low-dimensional Manifolds**

Authors: Tian Yu Yen and Tim Wildey (Sandia National Laboratories)

Abstract: Non-parametric density estimation is well-known to suffer from the curse of dimensionality. When the dimension of observable data is large, the number of samples required for reliable density estimates becomes prohibitively expensive, especially in physical applications where limited data is available. However, in realistic scenarios, the manifold hypothesis suggests that observable data lies on a low-dimensional manifold embedded in this high-dimensional space. In this talk, we propose utilizing physics-based surrogate models to learn an approximate low-dimensional manifold for the data. By restricting the density estimation problem to this lower-dimensional manifold, we are able to perform efficient density estimation in contexts where observational data is sparse. We demonstrate the proposed approach on both idealized scenarios and realistic physical applications, e.g., fluid flow in porous media.

MS 26–Talk 10: **Layerwise Sparsifying Training and Sequential Learning Strategy for Neural Architecture Adaptation**

Authors: C. G. Krishnanunni and Tan Bui-Thanh (University of Texas at Austin)

Abstract: This work presents a two-stage framework for progressively developing neural architectures to adapt/generalize well on a given training data set. In the first stage, a manifold-regularized layerwise sparsifying training approach is adopted where a new layer is added each time and trained independently by freezing parameters in the previous layers. In order to constrain the functions that should be learned by each layer, we employ a sparsity regularization term, manifold regularization term and a physics-informed term. We derive the necessary conditions for the trainability of a newly added layer and analyze the role of manifold regularization. In the second stage of the Algorithm, a sequential learning process is adopted where a sequence of small networks is employed to extract useful information from the residual produced in stage I and thereby making robust and more accurate predictions. Numerical investigations with fully connected network on prototype regression problem, physics-informed neural network (PINNs) problems, and classification problem demonstrate that the proposed approach can outperform adhoc baseline networks.

MS 26–Talk 11: **Scalable neural network approximation for high-dimensional inverse problems**

Authors: Jinwoo Go, Peng Chen (Georgia Institute of Technology)

Abstract: High-dimensional inverse problems governed by large-scale models, e.g., partial differential equations, are challenging to solve. In this talk, we present a scalable method using invertible neural networks to solve model-constrained high-dimensional inverse problems. In particular, we investigate the impact of different loss functions for the training of forward neural networks as approximation of the parameter-to-observable map and inverse neural networks as approximation of the observable-to-parameter map, both in latent spaces.

MS 26–Talk 12: **Finite Expression Method for Solving High-Dimensional PDEs**

Authors: Haizhao Yang (University of Maryland, College Park)

Abstract: Designing efficient and accurate numerical solvers for high-dimensional partial differential equations (PDE) remains a challenging and essential topic in computational science and engineering, mainly due to the "curse of dimensionality" in designing numerical schemes that scale in dimension. This talk introduces a new methodology that seeks an approximate PDE solution in the space of functions with finitely many analytic expressions and, hence, this methodology is named the finite expression method (FEX). It is proved in approximation theory that FEX can avoid the curse of dimensionality. As a proof of concept, a deep reinforcement learning method is proposed to implement FEX for various high-dimensional PDEs in different dimensions, achieving high and even machine accuracy with a memory complexity polynomial in dimension and an amenable time complexity. An approximate solution with finite analytic expressions also provides interpretable insights into the ground truth PDE solution, which can further help to advance the understanding of physical systems and design postprocessing techniques for a refined solution.

MS 27: Challenges and opportunities in computational science and engineering: Perspectives from data-driven learning and model reduction

Organizers: Ionut Farcas, Marco Tezzele & Aniketh Kalur

The high computational cost of realistic simulations of real-world phenomena - even on parallel supercomputers - renders tasks that require ensembles of such simulations, i.e., outer-loop applications, such as uncertainty quantification, control, parameter inference or design optimization, computationally infeasible. To this end, model-order reduction can be used to construct fast and accurate reduced models of complex simulations and therefore speed up outer-loop applications. In addition, primarily due to the tremendous recent advances in computing, data-driven learning and modeling emerged as a viable and practically feasible way of addressing the computational challenges in the aforementioned complex tasks as well. The aim of the mini-symposium is to foster discussion on data-driven methods, system identification, model order reduction, and uncertainty quantification for complex applications in computational science and engineering. The talks will present methodological developments as well as applications from different engineering fields.

MS 27–Talk 1: **Reduced Order Modeling for a LES filtering approach**

Authors: M. Girfoglio[1] and A. Quaini[2] and G. Rozza[1] (1: International School for Advanced Studies, 2: University of Houston)

Abstract: It is well known that the extension of reduced order models (ROMs) to turbulent flows presents several challenges. We choose to work with a large eddy simulation (LES) approach that describes the small-scale effects by a set of equations to be added to the discrete Navier-Stokes equations. This extra problem acts as a low-pass differential filter. We propose a Proper Orthogonal Decomposition (POD)-Galerkin based ROM when a linear filter is used and a hybrid projection/data-driven strategy in the case of a nonlinear filter. The novelties of our ROMs include: 1) the use of a ROM differential filter, i.e. a ROM spatial filter that uses an explicit lengthscale, 2) the computation of the pressure field at the ROM level, 3) the use of a finite volume method for the space discretization, which is common in many commercial codes, and 4) the use of different POD coefficients and bases to approximate the intermediate and end-of-step velocities. The performance of the proposed methods is assessed through 2D and 3D test cases.

MS 27–Talk 2: **Adaptive Model Order Reduction for Turbulent Reacting Flows**

Authors: Cheng Huang[1] (1: University of Kansas)

Abstract: Even with exascale computing capabilities, high-fidelity simulations of turbulent combustion in realistic applications such as rocket combustion remain computationally expensive and inaccessible for many-query applications. Projection-based model order reduction (PMOR) has shown promise in greatly improving computational efficiency. However, classical MOR methods that seek reduced solutions in static low-dimensional subspaces fail for realistic turbulent combustion problems because reacting flows feature extreme stiffness, sharp gradients, and multi scale transport, which pose great challenges in deriving effective low order representations and developing predictive reduced-order models (ROMs). In this talk, an adaptive reduced-order modeling method is introduced which updates the low-dimensional space on the fly, thus circumventing representation

barriers faced by static reduced dimensional spaces. The method leverages model-form preserving least-squares projections with variable transformation (MP-LSVT) for improved robustness of ROM and adapt the low-dimensional subspaces based on the evaluated dynamics during online calculations to enable predictive ROMs for turbulent reacting flows.

MS 27–Talk 3: **A low-order nonlinear model of a stalled airfoil from data: Exploiting sparse regression with physical constraints**

Authors: A. Leonid Heide[1],Katherine J. Asztalos[2],Scott T. M. Dawson[2], and Maziar S. Hemati[1] (1: University of Minnesota, 2: Illinois Institute of Technology)

Abstract: This work uses data-driven sparsity-promoting methods to obtain low-order governing equations for the wake of a stalled airfoil. Direct numerical simulation data of a NACA-0009 airfoil at an angle of attack of $\alpha = 15°$ is utilized in this study, with actuation being performed by injecting momentum into the flow near the airfoil's leading edge. Proper Orthogonal Decomposition (POD) is used to obtain a reduced order representation of the flow field. The Sparse Identification of Nonlinear Dynamics (SINDy) framework is then implemented to obtain low-order quadratic governing equations for the flow over the stalled airfoil. The SINDy model is constrained to preserve the energy-conserving property of the quadratic nonlinearity and associated triadic energy-transfer mechanisms. Low-order nonlinear models of the unsteady flow field associated with the stalled airfoil are obtained and cross-validated using off-design data. Furthermore, an output equation that predicts the lift coefficient is also identified and cross-validated. These low-order nonlinear models are expected to facilitate future developments in model-based analysis and control of separated flows.

MS 27–Talk 4: **Dimensionality reduction for spatial-temporal fields beyond POD and CNN**

Authors: Shaowu Pan[1,2], Steve Brunton[2], Nathan Kutz[2] (1: Rensselaer Polytechnic Institute, 2: University of Washington, Seattle)

Abstract: Fluid dynamics exhibits complex, multi-scale spatial structure, chaotic dynamics in time, and bifurcation in the relevant parameters. Among these challenges, spatial complexity is the major barrier for modeling and control of fluid dynamics, which motivates the need of dimensionality reduction. Existing paradigms, such as proper orthogonal decomposition or convolutional autoencoders, both struggle to accurately and efficiently represent flow structures for problems requiring variable geometry, non-uniform grid resolution (e.g., wall-bounded flows, flow phenomenon induced by small geometry features), adaptive mesh refinement, or parameter-dependent meshes. To resolve these difficulties, we propose a general framework called *Neural Implicit Flow* (NIF) that enables a compact and flexible dimension reduction of large-scale, parametric, spatial-temporal data into mesh-agnostic fixed-length representations. This work complements existing meshless methods, e.g., physics-informed neural networks, and we focus specifically on obtaining effective reduced coordinates where modeling and control tasks may be performed more efficiently. We apply our mesh-agnostic approach to several fluid flows, including flow past a cylinder, sea surface temperature data, 3D homogeneous isotropic turbulence, and a transonic 3D flow over ONERA M6 wing. In these examples, we demonstrate the utility of NIF for parametric surrogate modeling, efficient differentiable query in space, learning non-linear manifolds, and the interpretable low-rank decomposition of fluid flow data.

MS 27–Talk 5: **Discovering Model Error with interpretability and Data-Assimilation: Sparse observations of multi-scale flows**

Authors: Rambod Mojgani[1], Ashesh Chattopadhyay[1], Pedram Hassanzadeh[1] (1: Rice University)

Abstract: We are developing a framework for discovering structural model errors from temporally and spatially sparse data to improve accuracy of climate models. Inaccuracies in the models of the Earth system, i.e., structural and parametric model errors, lead to inaccurate predictions. Such errors may have originated from unresolved phenomena due to a low numerical resolution, as well as misrepresentations of physical phenomena or boundaries (e.g., orography). While calibration methods have been introduced to address parametric uncertainties, representing structural uncertainties in models of the Earth system remains a major challenge.

Therefore, along with the increases in both the amount and frequency of observations, algorithmic innovations are required to identify interpretable representations of the model errors. We have introduced Model Error Discovery with Interpretability and Data-Assimilation (MEDIDA), a flexible, general–purpose framework to discover interpretable model errors. Here, we show its performance on a canonical prototype of geophysical turbulence, the two–level quasi–geostrophic system. Accordingly, a Bayesian sparsity–promoting regression framework is used to select the relevant terms from a library of interpretable kernels. As calculating the library from noisy and sparse data (e.g., from observations) using conventional techniques leads to interpolation and numerical errors, here we propose using a coordinate-based multi–layer embedding to impute the sparse observations. We demonstrate the importance of alleviating spectral bias, especially with the multi–scale nature of turbulent flows, and show a random Fourier feature layer can sufficiently increase accuracy of the kernel terms to enable an accurate discovery. Our framework successfully identifies structural model errors due to linear and nonlinear processes (e.g., radiation, surface friction, advection), as well as misrepresented orography.

MS 27–Talk 6: **Compiler-based Differentiable Programming for Accelerated Simulations**

Authors: Ludger Paehler[1,2] and Jan Hueckelheim[2] and Johannes Doerfert[3] (1: Technical University of Munich, 2: Argonne National Laboratory, 3: Lawrence Livermore National Laboratory)

Abstract: With the ever accelerating advances of modern machine learning techniques such as implicit differentiable layers, and deep equilibrium models the desire to extend these techniques to traditional simulations for the purpose of acceleration or the improvement of outer-loop applications becomes ever stronger. While in some areas it may be feasible to rewrite simulations in differentiable domain specific languages such as Jax, PyTorch or DiffTaichi, this is entirely infeasible for traditional simulations which have been built up, and validated over the past decades. In this talk we build on our recent work on compiler-based automatic differentiation enabling the synthesization of gradients, and vectorization of computation for simulations written in C/C++, Fortran, Julia, Rust, etc. to extend these modern techniques to traditional simulations, and enable the acceleration thereof.

MS 27–Talk 7: **Advances in parameter space reduction with applications in naval engineering**

Authors: M. Tezzele[1] and G. Rozza[2] (1: University of Texas at Austin, 2: International School for Advanced Studies)

Abstract: Active subspaces (AS) method is one of the most widespread linear methods to reduce the dimensionality of the input design space. In this talk we introduce a new localization version of AS exploiting a supervised distance metric for regression and classification tasks. With this technique we are able to find local rotations of the parameter space so to unveil low-dimensional structures of the function. We also present a multi-fidelity extension to increase the accuracy of Gaussian process response surfaces by incorporating a low-dimensionality bias without the need of running low-fidelity simulations. This allows us to extract more information from the same set of initial high-fidelity data. Finally, we show how to incorporate parameter space reduction into a non-intrusive reduced order modelling framework for the structural optimization of passenger ship hulls.

MS 28: Modeling of air flow and droplet transport for biomedical applications

Organizers: Vladimir Ajaev & Andrea Barreiro

Mathematical and computational modeling of air flow in the respiratory system is important for a range of applications including prevention of infectious diseases such as tuberculosis and COVID-19, understanding the functioning of the olfactory system, and improving therapeutic efficiency of drugs delivered by aerosol inhalation. The mini-symposium will focus on recent progress in the computational modeling of air flow in nasal cavity and respiratory airways, as well as the transport of microscale droplets which can carry infections or inhaled medication. The physics of evaporation and condensation of such droplets will be discussed with implications to their trajectories and ultimate locations of their deposition. After deposition, the transport of components of droplet through mucus layer is of interest and can be studied using the methods of computational fluid mechanics. Potential applications of machine learning in combination with the standard numerical solutions of the Navier-Stokes equations, as well as other future research directions in the field will among the topics for the mini-symposium.

MS 28–Talk 1: **Building the Next-Generation Physiologically Realistic Human Respiratory Digital Twin System for Pulmonary Healthcare**

Authors: Yu Feng (Oklahoma State University)

Abstract: Nowadays, "personalized medicine" is starting to replace the current "one size fits all" approach. The goal is to have the right drug with the right dose for the right patient at the right time and location. An example of personalized pulmonary healthcare planning is the targeted pulmonary drug delivery methodology. However, traditional in vitro and in vivo studies are limited and not sufficient for the precision medicine plan development. Specifically, due to the invasive nature and imaging limitations, most animal studies and clinical tests lack operational flexibility and cannot provide high-resolution patient-specific data. Therefore, alternative methods should be developed to conquer these bottlenecks. Models based on the computational fluid-particle dynamics (CFPD) method play a critical role in exploring alternate study designs and provide high-resolution data in a noninvasive, cost-effective, and time-saving manner. The in silico methodologies can fill the knowledge gap due to the deficiency of the traditional in vitro and in vivo methods, as well as make breakthroughs to pave the way to establish a reliable and efficient numerical investigation framework for pulmonary healthcare on a patient-specific level. A physiologically realistic CFPD-based human respiratory system modeling framework has been developed. This clinically validated elastic whole-lung model has been successfully applied to (1) Provide in silico evidence to regulatory authorities by evaluating the comparability between two dry powder inhalers to accelerate the approval process, (2) Optimize mitigation plans to reduce the airborne transmission of SARS-CoV-2 laden droplets in various indoor spaces, (3) Quantify the influence of lung disease progression on inhaled medication transport and delivery, (4) Predict the pharmacokinetics (PK) and human immune system responses after the inhaled medications or infectious virus deposited in the human respiratory system, (5) Assist the development of a new diagnostic method to detect airway obstruction location effectively, and (6) Assist on the development of personalized targeted pulmonary drug delivery to designated lung sites. It can make breakthroughs to establish a reliable and efficient computational modeling framework to drastically reduce the time to boost medical innovation in pulmonary healthcare and risk assessment on a subject-specific level, without compromising human subject safety.

MS 28–Talk 2: **Computational Prediction of Transport, Deposition, and Resultant Immune Response of Nasal Spray Vaccine Droplets to Potentially Prevent COVID-19**

Authors: Hamideh Hayati[1], Yu Feng[1], Xiaole Chen[2], Emily Kolewe[3], Catherine Fromen[3] (1:Oklahoma State University2:Nanjing Normal University, China, 3:University of Delaware)

Abstract: Intranasal vaccination against COVID-19 caused by SARS-CoV-2 could be highly advantageous over conventional intramuscular vaccination, which can benefit children who are afraid of needles. However, the effectiveness of the intranasal vaccine is highly dependent on the delivery dose to the designated site, i.e., the olfactory region (OR), which is the Angiotensin-converting enzyme 2-rich region. Many factors can influence the aerosolized vaccine transport in the nasal passage and the delivery dose, such as nasal spray cone angle, droplet initial velocity, and composition. Unfortunately, no computational effort has been made to investigate how administration strategies can influence the deposition of vaccine droplets in the nasal cavity, especially for children. This study focuses on the transport, deposition, and triggered immune response of intranasal vaccine droplets to the OR in the nasal cavity of a 6-year-old female to possibly prevent COVID-19. To investigate how administration strategy can influence the nasal vaccine delivery efficiency to OR, a validated multiscale model (i.e., computational fluid-particle dynamics (CFPD) and host-cell dynamics (HCD) model) was employed. Droplet deposition fraction, size change, residence time, and the area percentage of OR covered by the vaccine droplets and triggered immune system response were predicted with different spray cone angles, initial droplet velocities, and compositions. Numerical results indicate that droplet initial velocity and composition have negligible influences on the vaccine delivery efficiency to OR. In contrast, the spray cone angle can significantly impact vaccine delivery efficiency. The triggered immunity is not significantly influenced by the administration investigated due to the low percentage of OR area covered by the droplets. To enhance the effectiveness of the intranasal vaccine to prevent COVID-19 infection, it is necessary to optimize the vaccine formulation and administration strategy so that the vaccine droplets can cover more epithelial cells in OR to minimize the available receptors for SARS-CoV-2.

MS 28–Talk 3: **Analytical Solutions for Fluid Flow and Diffusion around a Slowly Condensing Levitating Liquid Droplet**

Authors: Jacob E. Davis, Vladimir S. Ajaev (Southern Methodist University)

Abstract: Studies of interaction of microscale droplets with moist air flow are important for applications such as tranmission of infectious diseases and drug delivery by aerosol inhalation. We consider a slowly condensing droplet levitating near a surface of evaporating liquid and develop a mathematical model to describe diffusion, heat transfer, and fluid flow in the system. The method of separation of variables in bipolar coordinates is used to obtain series expansions for all physical quantities. This framework allows us to determine temperature profiles and condensation rates at the surface of the droplet. We find that the dependence of the equilibrium concentration on temperature is necessary to accurately model the phase change at the surface of the liquid. The condensation of vapor leads to the temperature in the droplet being, on average, higher than the surrounding air.Temperature and concentration gradients lead to significant differences between phase change rates at the top and bottom of the droplet. Fluid flow is described in terms of the Stokes stream function expressed in bipolar coordinates. Force acting on the droplet from the moist air flow is calculated as a function of distance between the droplet and the surface of evaporating liquid. Supported by NSF grant DMS-2009741.

MS 28–Talk 4: **Predicting Transport and Deposition of Multicomponent E-cigarette Aerosols in a Subject-specific Airway Model with Different Nicotine Forms: An in silico Study**

Authors: Ted Sperry, Yu Feng (Oklahoma State University)

Abstract: Predicting the transport and deposition of e-cigarette aerosols in the human respiratory system is essential to understanding how initial e-liquid compositions, especially different nicotine forms in new generations of e-cigarette products, can influence the absorption of nicotine in the human lung. Using a newly developed computational fluid dynamics (CFD) based numerical method which integrated the species transport and discrete phase (DPM) models, this study simulated and compared the transport dynamics of multicomponent e-cigarette aerosols in a subject-specific human respiratory system, and investigated how nicotine forms, nicotine mass fraction, PG/VG ratio, and acid/nicotine ratio in the e-liquids can influence the transport, evaporation/condensation dynamics, and deposition/absorption patterns in the human airway from mouth to generation 6 (G6). Specifically, the experimentally calibrated and validated CFPD model is able to predict the gas-liquid phase change dynamics of water, PG, VG, and nicotine in the aerosols during their transport through the pulmonary route. Freebase nicotine and nicotine salt were both investigated, with different PG/VG ratios and benzoic or lactic acids. Simulation results indicate that compared with free-based nicotine e-liquid, using nicotine salt with Benzoic and Lactate Acids will reduce the headspace nicotine saturation pressure, thereby reducing the evaporation rate of nicotine, which leads to lower nicotine absorption in the human upper airway and higher nicotine absorption in small airways. In addition, increasing PG/VG ratio will also reduce the headspace nicotine saturation pressure, further reducing the evaporation rate of nicotine. In summary, a CFD-based species transport-DPM model has been developed and validated to quantify how e-liquid composition can influence the transport, evaporation/condensation, and deposition/absorption of inhaled multicomponent e-cigarette aerosol in human respiratory systems. Future work will include (1) investigating

how disease-specific lung airway deformation kinematics can influence the inhaled nicotine distributions, and (2) quantifying the pharmacokinetics of nicotine after deposition/absorption in the human body.

MS 28–Talk 5: **Mathematical Modeling of Phase Change in Respiratory Droplets**

Authors: Vladimir S. Ajaev, Art Taychameekiatchai, James Barrett (Southern Methodist University)

Abstract: Infectious diseases transmitted by tiny droplets of respiratory fluids affect tens of millions of people worldwide. Better understanding of the mechanism of transmission of infections can lead to improvements in both treatment and protection strategies. The focus of our work is on understanding how phase change processes such as evaporation and condensation affect the overall dynamics of respiratory droplets and the deposition of these droplets in the airways. We start by considering phase change in a spherical droplet surrounded by moist air. We find droplet radius over time in the framework of a model that accounts for the diffusion process, Stefan flow, presence of solutes, and changes in ambient humidity/temperature. Conditions are defined when droplets remain large enough to carry viable pathogens, but small enough to be rapidly carried by air. We then develop a lubrication-type model of sessile droplets containing solutes such as salt. The model incorporates nonequilibirum effects during evaporation from the liquid surface and an increase of solute concentration as a result of solvent evaporation. The presence of solute leads to reduction of the evaporation rates at initial stages of evolution but the trend is reversed at the later stages, resulting in lower lifetimes of evaporating droplets. Evaporative cooling is also considered in the framework that accounts for heat conduction in the substrate and shown to increase the droplet lifetime. Extensions of the model to the more realistic descriptions of respiratory droplets are discussed. Supported by NSF grant DMS-2009741.

MS 28–Talk 6: **Investigating the Impact of Mechanosensation on Retronasal Olfaction**

Authors: Abdullah Saifee[1], Andrea Barreiro[1],Cheng Ly[2],Woodrow Shew[3] (1:Southern Methodist University, 2:Virginia Commonwealth University, 3:University of Arkansas)

Abstract: Retronasal olfaction, which refers to the perception of odors that occurs during exhalation, accounts for partial flavor perception. But unlike orthonasal olfaction (smells during inhalation), retronasal olfaction is still rather poorly understood. There have been studies which indicate that even for identical odors, the brain activations that occur are different between the two types of olfaction. Prior experiments showed that synaptic inputs to the olfactory bulb from the nose are different for ortho- and retronasal olfaction in rats. How the nasal epithelium is stimulated for the two types of olfaction is still to be identified. Our hypothesis is that at the sensory periphery, the retro and ortho nasal stimuli produce distinct spatiotemporal patterns of mechanosensory excitation of olfactory receptor neurons. Experiments show that mechanical forces by air flow can lead to robust neural responses in the olfactory bulb. So it is likely that the airflow patterns will be quite different for retronasal flow compared to orthonasal flow, leading to different mechanical forces on olfactory receptor neurons (ORNs) and different input to olfactory bulb (OB). Ultimately, we will test this hypothesis with fluid dynamics simulations in experimentally obtained, animal-specific nasal cavity models. Today we will show preliminary results demonstrating that shear stress forces differ for orthonasal vs. retronasal air flow; i.e., inspiration vs. exhalation, in an idealized model of a nasal cavity.

MS 29: Applications and Computation in Algebraic Geometry

Organizers: Jordy Lopez Garcia, Josué Tonelli-Cueto & Thomas Yahl

Many applied problems, such as the description of the position of a robotic arm or the equilibria points of a biochemical reaction network, can be formulated in terms of polynomials. Therefore, to deepen our understanding of these problems, we need to develop computational methods that exploit the appearing algebraic and geometric structures. In this mini-symposium, we gather researchers working at the intersection of algebraic geometry, computation, and applications.

MS 29–Talk 1: **On the geometry of geometric rank**

Authors: Runshi Geng[1] (1: Texas A&M University)

Abstract: Geometric Rank of tensors was introduced by Kopparty et al. as a useful tool to study algebraic complexity theory, extremal combinatorics and quantum information theory. In this talk I will introduce Geometric Rank and results from their paper, in particular showing the relation between geometric rank and other ranks of tensors. Then I will present recent results of our study on geometric rank, including the connections between geometric rank and spaces of matrices of bounded rank, and classifications of tensors with geometric rank one, two and three.

MS 29–Talk 2: **Approximate Rank for Real Symmetric Tensors**

Authors: Alperen Ergur[1] (1: University of Texas at San Antonio)

Abstract: We investigate the effect of an epsilon–room of error tolerance to real symmetric tensor rank. We provide two main results and three algorithms for approximate rank estimation. Our aim is to exploit the specific nature of real geometry, rather than using complex algebraic tools, so we rely on ideas from convexity, additive combinatorics, and probability. This is joint work with Petros Valettas and Jesus Rebollo Bueno. https://arxiv.org/pdf/2207.12529.pdf

MS 29–Talk 3: **Computing Galois groups of Fano problems**

Authors: Thomas Yahl[1] (1: Texas A&M University)

Abstract: A Fano problem consists of enumerating linear spaces of a fixed dimension on a variety, generalizing the classical problem of 27 lines on a cubic surface. Those Fano problems with finitely many linear spaces have an associated Galois group that acts on these linear spaces and controls the complexity of computing them in coordinates via radicals. Galois groups of Fano problems were first studied by Jordan, who considered the Galois group of the problem of 27 lines on a cubic surface. Recently, Hashimoto and Kadets nearly classified all Galois groups of Fano problems by determining them in a special case and by showing that all other Fano problems have Galois group containing the alternating group. We use computational tools to prove that several Fano problems of moderate size have Galois group equal to the symmetric group, each of which were previously unknown.

MS 29–Talk 4: **The Point Scheme and Line Scheme of a Certain Quadratic Quantum $\mathbb{P}^3$**

Authors: José Lozano[1] (1: University of Texas at Arlington)

Abstract: In the past 35 years, some research in noncommutative algebra has been driven by attempts to classify regular algebras of global dimension four, also known as quantum $\mathbb{P}^3$s. In this presentation, we consider a certain quadratic quantum $\mathbb{P}^3$ having a finite point scheme and a line scheme that is a union of three distinct lines, with multiplicities 8, 6, and 6, respectively.

MS 29–Talk 5: **The dimension of the semirings of polynomials and convergent power series.**

Authors: Kalina Mincheva[1], Netanel Friedenberg[2] (1: Tulane University, 2: Tulane University)

Abstract: In this talk I will define the Krull dimension of a (topological) semiring as the number of strict inclusions in a chain of prime congruences. I will compute the dimensions of the polynomial semirings with coefficients in the tropical numbers or in any of its sub-semifields. I will also give bounds for the dimension of the semiring of convergent power series with coefficients in the tropical numbers or any of its sub-semifields. I will explain how these computations align with our geometric intuition (from tropical geometry).

MS 29–Talk 6: **Generating random points uniformly distributed on a parametric curve**

Authors: Josué Tonelli-Cueto[1], Apostolos Chalkis[2], and Christina Katsamaki[3] (1: The University of Texas at San Antonio 2: Quantagonia, 3: Inria Paris & IMJ-PRG)

Abstract: Given a polynomial parametric curve $\gamma : [-1, 1] \to \mathbb{R}^n$, we want to sample random points $\mathfrak{x} \in \gamma([-1, 1])$ uniformly distributed with respect the arc-length. However, even assuming that we can sample random points uniformly in $[-1, 1]$ and perform exact arithmetic operations, sampling such points is not an easy task. In this talk, we discuss an algorithm for sampling points approximately uniformly by paying special attention to controlling the error (with respect to the total variation distance).

MS 29–Talk 7: **Algebraic, Geometric, and Combinatorial Aspects of Unique Model Identification**

Authors: Brandilyn Stigler[1] (1: Southern Methodist University)

Abstract: Biological data science is a field replete with many substantial data sets from laboratory experiments and myriad diverse methods for analysis and modeling. Given the abundance of both data and models, there is a growing need to group data sets to reveal salient features of the data and ultimately of the underlying network. For discrete data, a special class of discrete models called *polynomial dynamical systems* (PDSs) can be used to capture all models which fit the given data from a network with n nodes. Typically a data set can have a large number of associated models, requiring model selection as a post-processing step. In parallel experimental design can be utilized as a preprocessing step to minimize the number of resulting models

In this talk we consider two problems related to inferring PDSs from an experimental design point of view. First, we aim to characterize data sets that uniquely determine a PDS. More specifically, we study input sets viewed as affine varieties V over a finite field F as well as the corresponding ideal of points $\mathbb{I}(V)$ so that the associated quotient ring $F[x_1, \dots, x_n]/\mathbb{I}(V)$ has a unique basis (up to scalar multiple) as a vector space over F. Here we connect geometric properties of V with algebraic aspects of Gröbner bases for $\mathbb{I}(V)$.

Next we relax the condition of requiring a unique PDS and focus on identifying data sets with a unique *wiring diagram*, that is a directed graph representing the connections in the network. In fact we show how to select minimal sets of edges using only the input data, extending previous results. We present algebraic conditions on $\mathbb{I}(V)$ that guarantee that there is a *unique* minimal set. We also provide a geometric condition on the data that guarantees the existence of *multiple* minimal sets.

An outcome of this joint work with E. Dimitrova, C. Fredrickson, N. Rondoni, and A. Veliz-Cuba is a much-reduced number of models

to validate experimentally since we connect sparsest model selection with optimal data selection.

MS 29–Talk 8: **Identifiability of Cycle Compartmental Models With Two Leaks and Identifiability of Submodels**

Authors: Dessauer, Paul R[1], Tanisha Grimsley[2], Jose Lopez[3] (1. Department of Mathematics, University of Texas El Paso, El Paso, Texas 2. Department of Mathematics, Juniata College, Huntingdon, Pennsylvania 3. Department of Mathematics, California State University - Fresno, Fresno, California)

Abstract: Directed cycle models are comprised of compartments, inputs, outputs, leaks, and edges to model how a substance flows within a network. These models are said to be identifiable if and only if the rank of the Jacobian matrix for the coefficient map of the edges and leaks is equal to the number of compartments plus the number of leaks. We proved that a submodels coefficient map is obtainable through transformations done on the coefficient map of its parent model. Furthermore, for models comprised of two leaks, the identifiability of a parent model does not always imply the identifiability of the submodel; and we conjecture which cases do preserve identifiability. Additionally, we wrote a program that determines identifiability for any model with one output; using this program, a database was constructed with the identifiability status of all two leak models with three, four, five, and six compartments. With this database, we conjecture that all cycle compartmental models with two leaks and one output are identifiable if and only if the output location is between the leak locations.

MS 30: Data-driven and Nonlinear Model Reduction Methods for Physical Sciences and Engineering

Organizers: Rudy Geelen & Shane McQuarrie

The rapidly increasing demand for computer simulations of complex physical, chemical, and other processes poses significant challenges and opportunities for computational scientists and engineers. Despite the remarkable rise of available computer resources and computing technology, the need for model order reduction to cope with highly complex problems is an ever-present reality. While the field of model reduction is relatively mature for linear systems, reducing nonlinear and parametric systems remains an active area of research, especially for large-scale problems. This mini-symposium highlights recent theoretical and algorithmic advancements in data-driven methods and related machine learning techniques for nonlinear model reduction in scientific applications. Such advancements include nonlinear dimensionality reduction, operator learning and inference, scientific machine learning, and physics-informed learning of dynamical systems.

MS 30–Talk 1: **A mixture of experts approach for efficient representation of combustion manifolds**

Authors: Ope Owoyele[1,2] Pinaki Pal[2] (1: Argonne National Laboratory, 2: Louisiana State University)

Abstract: Direct numerical modeling of turbulent combustion with detailed chemical kinetics is challenging, due to the vast number of chemical scalars involved, the existence of a wide range of spatio-temporal scales, and the complex interactions between chemical kinetics and turbulent flow. To mitigate these challenges, physically-derived reduced-order models that rely on *a priori* tabulation of chemistry (such as the tabulated flamelet model) have been developed. These models, however, suffer from the curse of dimensionality, where the size of the table and the interpolation complexity increases exponentially as more independent variables are added. In response to these issues, an approach for learning turbulent combustion tables in the context of the flamelet model has been the developed. In this approach, multiple neural networks (called experts) are trained concurrently, each neural network attempting to adversely alter the training of the other competing experts. In this way, the thermochemical space of interest is divided amongst the neural networks, with each one being an expert in specific regions of the thermochemical domain. The proposed approach is applied to the combustion of *n*-dodecane in air, showing improved speed and accuracy compared to the conventional use of single neural networks.

MS 30–Talk 2: **Neural Ordinary Differential Equations with Physics-Informed Architectures and Constraints for Dynamical Systems Modeling**

Authors: Cyrus Neary[1], Franck Djeumou[1], Eric Goubault[2], Sylvie Putot[2] and Ufuk Topcu[1] (1: University of Texas at Austin, 2: LIX, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, France)

Abstract: Effective inclusion of physics-based knowledge into deep neural network models of dynamical systems can greatly improve data efficiency and model robustness. Such a priori knowledge might arise from physical principles (e.g., conservation laws) or from the system's design (e.g., the Jacobian matrix of a robot), even if large portions of the system dynamics remain unknown. We develop a framework to learn dynamics models from trajectory data while incorporating a priori system knowledge as inductive bias. More specifically, the proposed framework uses physics-based side information to inform the structure of the neural network itself and to place constraints on the values of the outputs and the internal states of the model. It represents the system's vector field as a composition of known and unknown functions, the latter of which are parametrized by neural networks. The physics-informed constraints are enforced via the augmented Lagrangian method during the model's training. We experimentally demonstrate the benefits of the proposed approach on a variety of dynamical systems – including a suite of robotics environments featuring large state spaces, nonlinear dynamics, external forces, contact forces, and control inputs. By exploiting a priori system knowledge, the proposed approach learns to predict the system dynamics two orders of magnitude more accurately than a baseline approach that does not include prior knowledge, while also enforcing physics-based constraints.

MS 30–Talk 3: **Derivative informed neural operators for PDE-constrained optimization under uncertainty**

Authors: Dingcheng Luo[1], Thomas O'Leary-Roseberry[1], Peng Chen[2] and Omar Ghattas[1] (1: University of Texas at Austin, 2: Georgia Institute of Technology)

Abstract: When optimizing the performance of systems governed by PDEs, the presence of uncertainty in the model parameters lead to optimization under uncertainty (OUU) problems, where the optimization cost is defined in terms of risk measures of a quantity of interest. OUU problems are often orders of magnitude more expensive to solve compared to their deterministic counterparts due to the need to evaluate the risk measure by stochastic integration. This can require many evaluations of the governing PDE at every optimization iteration, rendering its solution computationally prohibitive for complex PDEs. In this talk, we present a novel framework for constructing derivative informed neural operator surrogates for the purpose of OUU. In particular, the PDE solution mapping from the uncertain parameters and optimization variables to the state is approximated by a neural operator. Sensitivity information from the PDE is used to determine reduced bases for input and output dimension reduction. Furthermore, we also incorporate the derivatives in a Sobolev-type training loss to ensure that the neural operator has accurate derivatives with respect to the optimization variable, such that they are amenable to derivative based optimization algorithms when solving the OUU problem. Here, we will discuss the construction of such neural operators and its use as surrogates for OUU, demonstrating its capabilities over a suite of numerical examples.

MS 30–Talk 4: **Prediction of numerical homogenization using deep learning for the Richards equation**

Authors: Sergei Stepanov[1], Denis Spiridonov[1] and Tina Mai[2] (1: North-Eastern Federal University, 2: Duy Tan University and Texas A&M University)

Abstract: We investigate a coarse-scale approximation based on numerical homogenization for the nonlinear Richards equation as an unsaturated flow over heterogeneous media. Using deep neural networks (DNNs), this approach provides frequent and rapid calculations of macroscopic parameters. To be more precise, during training a neural network, we utilize a training set of stochastic permeability realizations and accordingly computed macroscopic targets (effective permeability tensor, homogenized stiffness matrix, and right-hand side vector). The treatment for the nonlinearity of Richards equation is incorporated in the (predicted) coarse-scale homogenized stiffness matrix, as a novelty in our proposed deep learning method, which creates nonlinear maps between such permeability fields and macroscopic features. Numerous numerical experiments in two-dimensional model problems show how well this technique performs, in terms of predictions of the macroscopic properties and consequently solutions

MS 30–Talk 5: **Why are deep learning-based models of geophysical turbulence long-term unstable?**

Authors: Ashesh Chattopadhyay[1] and Pedram Hassanzadeh[1] (1: Rice University)

Abstract: Deep learning-based data-driven models of geophysical turbulence, e.g., data-driven weather forecasting models, have received substantial attention recently. These models, trained on observational data, are competitive with numerical weather prediction (NWP) models in terms of short-term performance. Such data-driven weather predictions models, trained on observational data are devoid of numerical biases and can be used for probabilistic forecasts with a large number of ensemble members, as well as efficient data assimilation at a computational cost which is several orders of magnitude smaller than that of NWP models. However, these data-driven models do not remain stable when integrated for a long time period (decadal time scales). This hinders their usefulness to simulate long-term climate statistics with synthetically generated data that could be used for studying the physical mechanisms of extreme events. A physical cause of this instability in data-driven models of weather, and generally turbulence, is yet-so-far unknown and several ad-hoc strategies are often adopted for improving their stability. In this work, we propose a causal mechanism for this instability through the lenses of physical and deep learning theory and propose a mitigation strategy to obtain long-term stable models of weather, climate, and generally geophysical turbulence.

MS 30–Talk 6: **Smoothness and Sensitivity of Principal Subspace-valued Map**

Authors: Ruda Zhang[1] (1: University of Houston)

Abstract: Proper orthogonal decomposition (POD) is a popular method to construct bases for reduced order modeling (ROM) of nonlinear systems. It confines the high-dimensional dynamics to a subspace spanned by the principal components of some state snapshots. When POD is used for the local bases of a parametric ROM, the mapping from model parameters to POD subspaces needs to be approximated. The sample complexity of function approximation, however, depends on the smoothness of such principal subspace-valued maps. In this talk, I give some smoothness results on principal subspace-valued maps: (1) sufficient conditions for the map to be analytic (C^ω)and continuous (C^0), respectively; (2) sensitivity of the map in terms of the Frechet derivative; (3) in case the map is discontinuous, the continuity gap and its improvement when we use a probabilistic version of the principal subspaces. Remarkably, the full probabilistic version of the map is always continuous. Numerical examples illustrate how these results affect approximation accuracy. Our results apply to any type of principal subspace-valued maps, including POD and parametric principal component analysis (PCA).

MS 30–Talk 7: **Adaptive planning for digital twins**

Authors: Marco Tezzele[1] and Karen Willcox[1] (1: University of Texas at Austin)

Abstract: Digital twins are rapidly spreading and are used in many engineering applications. With digital twin we intend a dynamically updating virtual representation of a physical asset of interest throughout its operational lifespan. Possible applications are predictive maintenance, optimization, and planning. In this talk we present a digital representation of an unmanned aerial vehicle, focusing on its structural health, in the framework of autonomous aerial cargo missions. We focus on how to incorporate adaptive planning, assimilating information during the operational regime. The idea is to exploit a Beta-Bernoulli process to easily update the posterior distribution of the state transition probability of the underlying Markov decision process. This is accomplished without the need of numerical integration. A new policy is selected dynamically using the most recent transition probability estimation. The resulting digital twin is thus adapting the planning strategy online during the mission.

MS 31: Mathematical modeling and robust numerical algorithmsin various biological processes

Organizers: Shuang Liu

Computational and mathematical biology are important new areas in the biological sciences. Recognizing this, I propose a mini–symposium on the topic of computational and mathematical biology entitled mathematical modeling and robust numerical algorithms in various biological processes,which aims to bring the attention of researchers to the broad biological research area and at the same time focuses on a few specific subjects: the growth of brain tumor, cell polarization, cell movement, cell migration, and patterning and tissue formation within the body.Various efficient computational tools and robust numerical algorithms, like powerful machine learning methodologies, phase-field method, and level-set method, have enabled the capability of capturing complicated dynamics in various biological processes.The mini-symposium session consists of 4 invited talks, which are from the perspective of developing mathematical models of complex biological processes, as well as capturing complicated mechanisms with extensive numerical and computational simulations.

MS 31–Talk 1: **Pattern formation and bistability in a synthetic intercellular genetic toggle**

Authors: Bárbara de Freitas Magalhães[1], Gaoyang Fan[2], Eduardo Sontag[3], Krešimir Josić[2], and Matthew R. Bennett[1] (1:Rice University, 2: University of Houston, 3: Northeastern University)

Abstract: Differentiation within multicellular organisms is a complex process that helps to establish spatial patterning and tissue formation within the body. Often, the differentiation of cells is governed by morphogens

and intercellular signaling molecules that guide the fate of each cell, frequently using toggle-like regulatory components. Here, we couple a synthetic co-repressive toggle switch with intercellular signaling pathways to create a "quorum-sensing toggle." We show that this circuit not only exhibits population-wide bistability in a well-mixed liquid environment, but also generates patterns of differentiation in colonies grown on agar containing an externally supplied morphogen. We develop a mechanistic mathematical model of the system, to explain how degradation, diffusion, and sequestration of the signaling molecules and inducers determine the observed patterns.

MS 31–Talk 2: **Cell Polarity and Movement with Reaction-Diffusion and Moving Boundary**

Authors: Shuang Liu[1], Li-Tien Cheng[1], and Bo Li[1] (1:University of California, San Diego)

Abstract: Cell polarity and movement are fundamental to many biological functions. Experimental and theoretical studies have indicated that interactions of certain proteins lead to the cell polarization which plays a key role in controlling the cell movement. We study the cell polarity and movement based on a class of biophysical models that consist of reaction-diffusion equations for different proteins and the dynamics of moving cell boundary. Such a moving boundary is often simulated by a phase-field model. We first apply the matched asymptotic analysis to give a rigorous derivation of the sharp- interface model of the cell boundary from a phase-field model. We then develop a robust numerical approach that combines the level-set method to track the sharp boundary of a moving cell and accurate discretization techniques for solving the reaction-diffusion equations on the moving cell region. Our extensive numerical simulations predict the cell polarization under various kinds of stimulus, and capture both the linear and circular trajectories of a moving cell for a long period of time. In particular, we have identified some key parameters controlling different cell trajectories that are less accurately predicted by reduced models. Our work has linked different models and also developed tools that can be adapted for the challenging three-dimensional simulations.

MS 31–Talk 3: **Computational Modeling of Cell Migration in Microfluidic Channel**

Authors: Zengyan Zhang[1], Yanxiang Zhao[2], and Jia Zhao[1] (1: Utah State University, 2: George Washington University)

Abstract: Cell migration plays an important role in various biological processes, such as tissue morphogenesis, wound healing and cancer metastasis, etc.. The mechanisms underlying cellular motility involve generating protrusive patches on the moving interfaces and determining moving directions under the guidance of chemotaxis. In our work, we proposed a phase-field model coupled with a reaction-diffusion system to keep track of the morphology changes of the cell membrane and steer the cell by gradients of attractive chemicals. In this talk, I will introduce our phase-field model for the migration of cell through complex channels and some numerical simulation results will be elaborated.

MS 31–Talk 4: **Parameter Inference in Diffusion-Reaction Models of Glioblastoma Using Physics-Informed Neural Networks**

Authors: Zirui Zhang[1], Andy Zhu[2], John Lowengrub[1] (1: University of California, Irvine, 2: Carnegie Mellon University)

Abstract: Glioblastoma is an aggressive brain tumor that proliferates and infiltrates into the surrounding normal brain tissue. The growth of Glioblastoma is commonly modeled mathematically by diffusion-reaction type partial differential equations (PDEs). These models can be used to predict tumor progression and guide treatment decisions for individual patients. However, this requires parameters and brain anatomies that are patient specific. Inferring patient specific biophysical parameters from medical scans is a very challenging inverse modeling problem because of the lack of temporal data, the complexity of the brain geometry and the need to perform the inference rapidly in order to limit the time between imaging and diagnosis. Physics-informed neural networks (PINNs) have emerged as a new method to solve PDE parameter inference problems efficiently. PINNs embed both the data the PDE into the loss function of the neural networks by automatic differentiation, thus seamlessly integrating the data and the PDE. In this work, we use PINNs to solve the diffusion-reaction

PDE model of glioblastoma and infer biophysical parameters from numerical data. The complex brain geometry is handled by the diffuse domain method. We demonstrate the efficiency, accuracy and robustness of our approach.

Tutorial

A hands-on tutorial for data-driven Full Waveform Inversion

Description: Understanding subsurface velocity structures is critical to a myriad of subsurface applications, such as carbon sequestration, reservoir identification, subsurface energy exploration, earthquake early warning, etc. They can be reconstructed from seismic data with full waveform inversion (FWI), which is governed by partial differential equations (PDEs).
Data-driven FWI leverages neural networks to learn the inverse mapping from seismic data to velocity maps. In this tutorial, we will walk through the anatomy of two data-driven FWI networks: InversionNet and VelocityGAN. The codes written in Pytorch are available on GitHub and examples of the Jupyter notebook will be given for attendees to get hands-on practice. The attendees would run experiments and make modifications to see how they are trained with an open-access seismic FWI dataset, OpenFWI. The broader goal of this tutorial is to provide a deeper understanding of how machine learning methods are implemented in solving scientific inverse problems.

Dr. Youzuo Lin
Team Leader and Staff Scientist, Sensors and Signatures Team
Geophysics Focus Lead, Center for Space and Earth Sciences
Earth and Environmental Sciences
Los Alamos National Laboratory

Dr. Shihang Feng
PostDoc
Los Alamos National Laboratory

Poster Presentations

Poster Session A: Saturday 12:00–01:00*
Location: Houston Room, Student Center South

** There will be an additional opportunity to informally present and discuss poster contributions F1—U14 during the Coffee Break in the afternoon (3:00–3:30). We recommend that the presenters in this session set up the posters prior the poster session (e.g., during the Coffee Break from 10:30 to 11:00).*

F1 **Probabilistic bounds on best rank-one approximation ratio**.
Presenter: Josué Tonelli-Cueto (Department of Mathematics, The University of Texas at San Antonio).

F2 **Group table and Sudoku puzzles**.
Presenter: Qingquan Wu (College of Engineering, West Texas A&M University).

F3 **Elements of disease in a changing world: modelling feedbacks between infectious disease and ecosystems**.
Presenter: Lale Asik (Department of Mathematics and Statistics, University of the Incarnate Word).

F4 **Scalability analysis of direct and iterative solvers used to model charging of non-insulated superconducting pancake solenoids**.
Presenter: Muhammad Mohebujjaman (Department of Mathematics and Physics, Texas A&M International University, and Plasma Science and Fusion Center, Massachusetts Institute of Technology).

F5 **Role of machine learning in the game of cricket: A systematic review and a meta-analysis**.
Presenter: Indika Wickramasinghe (Department of Mathematics, Prairie View A&M University).

F6 **Validity of angles in generalized circle/sphere theorems**.
Presenter: Jordan Alexander (Mathematics Department, Lone Star College-CyFair).

F7 **On the inf-sup stability of Crouzeix-Raviart Stokes Elements in 3D**.
Presenter: Celine Torres (Department of Mathematics, University of Houston).

F8 **Accounting for ethnicity improves the outcomes of vaccine prioritization strategies**.
Presenter: Md Rafiul Islam (Department of Mathematics and Statistics, University of the Incarnate Word).

F9 **Distributed generalized wirtinger flow for interferometric imaging on networks**.
Presenter: Sean Farrell (Department of Electrical and Computer Engineering, Rice University).

H1 **Comparative analysis of sustainable carbon capture technologies through their carbon footprints—Who's watching the watchmen?**.
Presenter: Anya Choudhary (East Brunswick High School).

H2 **Classifying melanoma using convolutional neural networks**.
Presenter: Tejasvi Tyagi (Baton Rouge Magnet High School).

U1 **Analyzing Dallas County eviction data**.
Presenter: Michala Gradner (Department of Mathematics, Texas State University).

U2 **Comparing Activation Functions to Corresponding B-functions**.
Presenter: John Breedis (Oden Institute, The University of Texas at Austin).

U3 **Robust principal component analysis and k-means on video footage for motion detection**.
Presenter: Saad Rafiq (Department of Mathematics, Texas State University).

U4 **Convergence of a modified Galerkin method for solutions of cantilevered structures**.
Presenter: Alyssa Blount (Department of Mathematics, Southeastern Louisiana University).

U5 **Investigating packing configurations of DNA in viral capsids**.
Presenter: Bridgett Slone (Center for Computation and Technology REU, Louisiana State University).

U6 **Hyperbolicity of surfaces of positive curvature**.
Presenter: Katherine Wong (Department of Mathematics, University of Houston).

U7 **Regulating autonomous drone fly-overs via authorization-based zoning**.
Presenter: Abdullah Kamal (Department of Computer Science, Texas State University).

U8 **On invertibility of passive 1D cloaking systems**.
Presenter: Damon Spencer (Department of Mathematics and Department of Electrical and Computer Engineering, University of Houston).

U9 **A mathematical model of onchocerciasis resistance and treatment**.
Presenter: Dashon Mitchell (Department of Mathematics, Tarleton State University).

U10 **Mathematical modeling of nematic liquid crystals**.
Presenter: Andrew Fisher (Department of Computer Science, Tufts University).

U11 **Bayesian methods to infer parameters for ODE models of disease spread**.
Presenter: Derek Hopkins (Tarleton State University).

U12 **An immunological model for COVID-19**.
Presenter: Teddie Swize (Louisiana State University).

U13 **N-soliton solutions to the KdV equation**.
Presenter: Omar Saldana (The University of Texas Rio Grande Valley).

U14 **Analyzing the effectiveness of the gang reduction youth development program using dynamic mode decomposition**.
Presenter: Axel Sanchez Moreno (Department of Mathematics, Texas State University).

U15 **Modelling supraventricular tachycardia using a dynamic computer-generated left atrium**.
Presenter: Gavin McIntosh (Department of Mathematics, Tarleton State University).

Poster Session B: Saturday 7:30–
Location: Houston Room, Student Center South

G1 **The global active subspace method**.
Presenter: Ruilong Yue (Department of Mathematics, Florida State University).

G2 **Predictive models of arsenic and phosphorus contamination in the Dickinson Bayou watershed**.
Presenter: Ida B. Nielsen (Department of Mathematics, Tarleton State University).

G3 **Active score Shapley for global sensitivity analysis**.
Presenter: Hui (Alyssa) Duan (Department of Mathematics, Florida State University).

G4 **C0 interior penalty methods for an optimal control problem with a general tracking function and pointwise state constraints**.
Presenter: SeongHee Jeong (Department of Mathematics, Louisiana State University).

G5 **Imaging of 3D objects with real data using orthogonality sampling methods**.
Presenter: Trung Truong (Department of Mathematics, Kansas State University).

G6 **Einstein's model with traveling band of biological systems and it's localization properties**.
Presenter: Rahnuma Islam (Department of Mathematics & Statistics, Texas Tech University).

G7 **Model-informed generative adversarial network (MI-GAN) for learning optimal power flow**.
Presenter: Yuxuan Li (School of Industrial Engineering and Management, Oklahoma State University).

G8 **An application of multivariate analysis tools**.
Presenter: Charu Rajapaksha (Department of Mathematics & Statistics, Texas Tech University).

G9 **Deep learning and statistical multivariate analysis for inferring breast cancer**.
Presenter: Fahad Mostafa (Department of Mathematics & Statistics, Texas Tech University).

G10 **Consensus ADMM-based distributed simultaneous imaging & communication**.
Presenter: Nishant Mehrotra (Department of Electrical & Computer Engineering, Rice University).

G11 **A conservative low-rank tensor method for the Vlasov–Maxwell system**.
Presenter: Shadi Heenatigala (Department of Mathematics & Statistics, Texas Tech University).

G12 **Accelerated distributed optimization for multi-agent synchronization**.
Presenter: Miguel F. Arevalo-Castiblanco (Electrical and Computer Engineering, Rice University).

G13 **A Local Macroscopic Conservative (LoMaC) low rank tensor method with the discontinuous Galerkin method for the Vlasov dynamics**.
Presenter: Jannatul Ferdous Ema (Department of Mathematics, Texas Tech University).

G14 **Model of Disease Spread Using Stochastic Processes on Networks**.
Presenter: David Baldwine Osei (Tarleton State University).

G15 **TNet: A model-constrained Tikhonov network approach for inverse problems**.
Presenter: Hai Nguyen (Department of Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin).

G16 **Automatic classification of deformable shapes**.
Presenter: Radmir Sultamuratov (Department of Mathematics, University of Houston).

G17 **Formative assessment of middle grades students' proportional reasoning**.
Presenter: Oghale Okuda (Department of Mathematics, Tarleton State University).

G18 **Einstein's model on the movement of small particles in a stationary liquid revisited**.
Presenter: Isanka Garli Hevage (Texas Tech University).

G19 **Simulating implicitly solvated biomolecules with atomic polarizable multipoles**.
Presenter: Xin (Sharon) Yang (Department of Mathematics, Southern Methodist University).

G20 **Structure-preserving finite element schemes for the Euler-Poisson equations**.
Presenter: Jordan Hoffart (Department of Mathematics, Texas A&M University).

G21 **Fast evaluation of PDE operators for optimization and uncertainty quantification in problems governed by transport equations**.
Presenter: Jae Youn Kim (Department of Mathematics, University of Houston).

G22 **Trajectory optimization of hypersonic vehicles via a Radau pseudospectral method**.
Presenter: Jonathan Cangelosi (Department of Computational Applied Mathematics and Operations Research, Rice University).

G23 **Rogue wave solutions to the Sasa-Satsuma equation**.
Presenter: Changyan Shi (School of Mathematical and Statistics Sciences, The University of Texas Rio Grande Valley).

G24 **Model-based group testing**.
Presenter: Ivan Lau (Department of Electrical and Computer Engineering, Rice University).

G25 **Predicting shallow water dynamics using recurrent neural network and transfer learning**.
Presenter: Mohammad Shah Alam (Department of Mathematics, University of Houston).

G26 **Critical angle for nanopattern formation in ion-irradiated thin films**.
Presenter: Tyler Evans (Department of Mathematics, Southern Methodist University).

G27 **Imbalanced machine learning technique to predict heart disease**.
Presenter: Md Saiful Islam Saif (Department of Mathematics & Statistics, Texas Tech University).

G28 **Model selection for zero inflated count data from Demographic Health Survey**.
Presenter: Naima Alam (Department of Mathematics & Statistics, Texas Tech University).

G29 **A new diagonalization based method for parallel-in-time solution of linear-quadratic optimal control problems**.
Presenter: Nathaniel Kroeger (Computational and Applied Math, Rice University).

G30 **Modeling and numerical analysis of cholesteric shells**.
Presenter: Andrew Hicks (Department of Mathematics, Louisiana State University).

G31 **Bayesian nonparametric learning of stochastic differential equations**.
Presenter: Jinpu Zhou (Department of Mathematics, Louisiana State University).

G32 **Scalable average consensus with compressed communications**.
Presenter: Mohammad Taha Toghani (Department of Electrical and Computer Engineering, Rice University).

G33 **On the performance of gradient tracking with local updates**.
Presenter: Edward Duc Hien Nguyen (Department of Electrical and Computer Engineering, Rice University).

G34 **Model of disease spread using stochastic processes on networks**.
Presenter: David Baldwine Osei (Department of Mathematics, Tarleton State University).

G35 **The area law for XXZ quantum spin systems**.
Presenter: Lee Fisher (Department of Mathematics, University of California Irvine).

G36 **Waves in black hole geometries: An energy-based discontinuous Galerkin method**.
Presenter: Jaryd Domine (Department of Mathematics, Southern Methodist University).

G37 **Interactive image segmentation for brain tumors**.
Presenter: Alex T. Balsells (Department of Computational Applied Mathematics and Operations Research, Rice University).

G38 **Predicting voting behavior of minority groups from publicly available census data**.
Presenter: Cody Drolet (Department of Mathematics, Tarleton State University).

G39 **Local stochastic factored gradient descent for distributed quantum state tomography**.
Presenter: Junhyung Lyle Kim (Computer Science Department, Rice University).

G40 **A novel way to compute the numerical flux terms in nodal Discontinuous Galerkin (DG) methods for multiscale physics**.
Presenter: Marc de Vernon (Computer Science Department, Rice University).

G41 **New numerical schemes for the Q-tensor model of nematic liquid crystals**.
Presenter: Justin Swain (Department of Mathematics, University of North Texas).

G42 **A face-oriented stabilized Nitsche-type extended variational multiscale method for incompressible two-phase flow**.
Presenter: Himali Gammanpila (Department of Mathematics and Statistics, Texas Tech University).

G43 **Parameter inference for the Fitzhugh-Nagumo model through artificial neural networks**.
Presenter: German Villalobos (Department of Mathematics, University of Houston).

G44 **Smart materials model with hysteresis and thermodynamic compatibility: Parameter identification**.
Presenter: Md Sakhawat Hossain (Department of Mathematics and Statistics, Texas Tech University).

G45 **Bayesian methods to infer parameters for ODE models of disease spread**.
Presenter: Joseph Douglas (Tarleton State University).

G46 **Classification performance of supervised machine learning methods on multivariate normal mixture models**.
Presenter: Dip Das (Department of Mathematics and Statistics, Texas Tech University).

G47 **Comparison of AI models for automatic liver segmentation**.
Presenter: Rachel Glenn (The University of Texas MD Anderson Cancer Center).

G48 **On chaotic non-stationary steady-states and biological processes**.
Presenter: Gessner Soto (Continuing Education, University of Colorado).