

# SCALA 2026: SCIENTIFIC COMPUTING AROUND LOUISIANA

FRIDAY, March 6 – 7, 2026  
LSU Campus, Digital Media Center Theater

Friday, March 6	
12:30	Registration
1:10	<b>Welcome</b>
1:15 – 2:00	<b>Keynote talk:</b> <i>Harbir Antil, George Mason University</i> <b>Digital Twins, Generative AI, and Beyond: A PDE-Constrained Optimization Perspective</b>
2:00 – 2:15	<i>Zequn Zheng, Louisiana State University</i> <b>Middle Rank Tensor Rank determination and Tensor approximation</b>
2:15 – 3:00	Coffee Break
3:00 – 3:15	<i>Davood Damircheli, Louisiana State University</i> <b>Extreme Particle Deformation in Three-Dimensional Granular Aggregates</b>
3:15 – 3:30	<i>Ying Bi, Tulane University</i> <b>Nonstandard Finite Difference methods and applications on ODEs and PDEs</b>
3:30 – 3:45	<i>Mayank Tyagi, Louisiana State University</i> <b>Machine Learning Applications for Safe and Sustainable Energy Transition</b>
3:45 – 4:00	<i>Jon Loftin, MathWorks</i> <b>MATLAB, Python, and GenAI: accelerating Teaching and Research</b>
4:00 – 4:30	Coffee Break
4:30 – 4:45	<i>Moslem Uddin, Tulane University</i> <b>Latent-DeepOKAN for low-dimensional representation of multiple asynchronous flexible fibers interaction in Stokes flow</b>
4:45 – 5:00	<i>Md Tanvir Emrose, Louisiana State University</i> <b>Reconfigurable structural color generation in multicolor pixels using phase-change materials</b>
5:00 – 5:15	<i>Joshua Agbomola, Tulane University</i> <b>Host-Parasite Dynamics: Bistability and Backward Bifurcation in Two Immune Response Models</b>
5:15 – 5:30	<i>Truc Dang, Tulane University</i> <b>Order of Accuracy for DIRK methods with Newton iterations</b>

**Saturday, Mar. 7**

9:00 – 9:45	<p><b>Keynote talk:</b></p> <p><i>Jesse Chan, University of Texas at Austin</i>  <b>High order entropy correction methods for nonlinear conservation laws</b></p>
9:45 – 10:00	<p><i>Adnan Morshed, Tulane University</i>  <b>Tortuous tales of tortuosity</b></p>
10:00 – 10:15	<p><i>Lan Trinh, Tulane University</i>  <b>Estimation of Dynamic rates using Snapshots of Biological cells</b></p>
10:15 – 10:45	<b>Coffee Break</b>
10:45 – 11:00	<p><i>Jai Tushar, Louisiana State University</i>  <b>A Conforming Virtual Element Method for a Quad-Curl Problem on Polygonal Meshes</b></p>
11:00 – 11:15	<p><i>Yangwen Zhang, University of Louisiana at Lafayette</i>  <b>Optimal <math>L^2</math> Error Estimates for Non-symmetric Nitsche's Methods</b></p>
11:15 – 11:30	<p><i>Rubaiyat Bin Islam, Tulane University</i>  <b>Interaction of Flexible Fibers with a Burgers-like Vortex</b></p>
11:30 – 11:45	<p><i>Anan Saha, Louisiana State University</i>  <b>Learning stochastic differential equations with integral-drift</b></p>
11:45 – 12:00	<p><i>Leonardo Matone, Tulane University</i>  <b>DeepVoting: Learning and Improving Voting Rules with Fine-Tuning</b></p>
12:00 – 1:00	<b>Lunch</b>
1:00 – 1:45	<p><b>Keynote talk:</b></p> <p><i>Malena Espanol, Arizona State University</i>  <b>Variable Projection Methods for Large-Scale Separable Nonlinear Inverse Problems</b></p>
1:45 – 2:00	<p><i>Hayden Bromley, Louisiana State University</i>  <b>A field theory for quasi-brittle fracture incorporating irreversible deformation</b></p>
2:00 – 2:30	<b>Coffee Break</b>
2:30 – 2:45	<p><i>Sang-Eun Lee, Tulane University</i>  <b>Collective Dynamics of Self-avoidant, Secreting Particles</b></p>
2:45 – 3:00	<p><i>Kiran Bist, Louisiana State University</i>  <b>Information Bottleneck Learning for Hyperspectral Ocean Color Inversion</b></p>
3:00 – 3:15	<p><i>Irene Eraso, Tulane University</i>  <b>Microscale flows around rigid particles under sparkle stress</b></p>
	<b>Concluding Remarks</b>

## Keynote Talks (alphabetical by last name)

### Joshua Agbomola

*Title: Digital Twins, Generative AI, and Beyond: A PDE-Constrained Optimization Perspective*

#### Abstract:

Motivated by the dichotomy between acute and chronic phases of Chagas disease, we analyze two within-host immune response models. Both models couple identical parasite dynamics with distinct mechanisms for CD8<sup>+</sup> T-cell proliferation. While both exhibit bistability and hysteresis, the model incorporating homeostatic immune maintenance additionally permits backward bifurcation, enabling endemic persistence even when the basic reproduction number  $R_0 < 1$

### Harbir Antil

*Title: Digital Twins, Generative AI, and Beyond: A PDE-Constrained Optimization Perspective*

#### Abstract:

Digital Twins (DTs) are adaptive, real-time virtual replicas of physical systems that integrate physics-based models, sensor data, and intelligent decision-making. At their core, DTs can be rigorously framed within PDE-constrained optimization (PDECO). This talk develops a unified PDECO framework for state estimation and control, leveraging adjoint-based methods in both deterministic and stochastic settings.

To address the challenges of infinite-dimensional, large-scale optimization, we introduce novel function-space trust-region and augmented Lagrangian algorithms and explore the role of randomized methods in dynamic PDECO.

A central theme is a new connection between PDECO and Generative AI: score-based generative models can be interpreted as backward-in-time PDEs, linking ill-posed inverse problems, stability analysis, and modern machine learning. This perspective bridges physics-informed modeling with data-driven synthesis, opening the door to, for instance, score-based Digital Twins.

Applications span a wide range of domains, including structural and biomedical systems—from bridges and dams to aneurysm modeling, optimal insulation, electromagnetic cloaking, light bending, fusion, and neuromorphic computing. Together, these examples highlight a pathway toward predictive, adaptive, and trustworthy Digital Twins and AI technologies.

## Jesse Chan

*Title: High order entropy correction methods for nonlinear conservation laws*

### **Abstract:**

Entropy stable formulations improve the robustness of high order discontinuous Galerkin (DG) numerical simulations of nonlinear conservation laws by ensuring that the solution satisfies a semi-discrete entropy inequality. Most entropy stable discretizations rely on an algebraic flux differencing formulation which involves both summation-by-parts discretizations and entropy conservative two-point finite volume fluxes. However, explicit expressions for such two-point finite volume fluxes may not be available for all systems or may be computationally expensive to compute.

An alternative approach to constructing entropy stable DG methods uses entropy dissipative correction terms to offset local violations of a cell entropy inequality. The resulting methods can be implemented either as an artificial viscosity or as a flux-corrected transport type schemes and yield the same semi-discrete entropy inequality satisfied by entropy stable flux differencing DG formulations. The entropy correction coefficients are parameter-free, locally computable over each cell, and preserve high order accuracy. We compare entropy correction schemes to existing flux differencing formulations, and present extensions of such approaches to non-ideal equations of state and projection-based reduced order models.

## Malena Espanol

*Title: Variable Projection Methods for Large-Scale Separable Nonlinear Inverse Problems*

### **Abstract:**

Many inverse problems in imaging and computational science lead to nonlinear least-squares formulations in which the forward model depends linearly on some parameters and nonlinearly on others. Variable projection is a powerful and efficient optimization approach that exploits this structure by eliminating the linear variables, thereby reducing dimensionality and improving the conditioning of the resulting problem. In this talk, I will provide an overview of the classical variable projection method and discuss its extension to large-scale inverse problems, with a particular focus on semi-blind deconvolution. I will present new regularization strategies and recent developments that incorporate approximate Jacobians computed using Krylov subspace techniques, enabling matrix-free implementations and improved scalability.

## All Abstracts (alphabetical by last name)

### Harbir Antil

*Title: Digital Twins, Generative AI, and Beyond: A PDE-Constrained Optimization Perspective*

#### Abstract:

Digital Twins (DTs) are adaptive, real-time virtual replicas of physical systems that integrate physics-based models, sensor data, and intelligent decision-making. At their core, DTs can be rigorously framed within PDE-constrained optimization (PDECO). This talk develops a unified PDECO framework for state estimation and control, leveraging adjoint-based methods in both deterministic and stochastic settings.

To address the challenges of infinite-dimensional, large-scale optimization, we introduce novel function-space trust-region and augmented Lagrangian algorithms and explore the role of randomized methods in dynamic PDECO.

A central theme is a new connection between PDECO and Generative AI: score-based generative models can be interpreted as backward-in-time PDEs, linking ill-posed inverse problems, stability analysis, and modern machine learning. This perspective bridges physics-informed modeling with data-driven synthesis, opening the door to, for instance, score-based Digital Twins.

Applications span a wide range of domains, including structural and biomedical systems—from bridges and dams to aneurysm modeling, optimal insulation, electromagnetic cloaking, light bending, fusion, and neuromorphic computing. Together, these examples highlight a pathway toward predictive, adaptive, and trustworthy Digital Twins and AI technologies.

### Ying Bi

*Title: Nonstandard Finite Difference methods and applications on ODEs and PDEs*

#### Abstract:

As first introduced in the 1980s, nonstandard finite difference (NSFD) methods are generalization of traditional finite differences that include additional degrees of freedom. It was expected that these choices could be utilized to improve the stability or the accuracy of the numerical methods. In some cases, the discretization of differential equations can generate the exact solution at the discrete nodes.

The literature contains examples of nsfd methods for specific equations and heuristics, but a coherent theory is not yet available. I will present nonstandard FD methods for second order differential equations (ode's and pde's) that make use of integrating factors, and nsfd methods for the steady state solution.

## Kiran Bist

### *Information Bottleneck Learning for Hyperspectral Ocean Color Inversion*

#### **Abstract:**

Retrieving phytoplankton absorption ( $a_{\text{v,phy}}$ ) and chlorophyll-a (Chl-a) from hyperspectral ocean-color reflectance is an ill-posed inverse problem, as different water compositions can produce nearly identical spectra, especially in optically complex coastal waters.

We present an information-theoretic approach based on the Variational Information Bottleneck (VIB), which learns a compressed representation of reflectance that retains only the information relevant for predicting phytoplankton optical properties, thereby regularizing the one-to-many inversion. The model jointly estimates spectral shape and amplitude, improving stability and reducing sensitivity to noise.

The method is compared with a Variational Autoencoder (VAE) baseline and evaluated on global hyperspectral data and unseen environments, including Lake Barataria and Lake Erie, and is further applied to NASA's PACE satellite observations. Results demonstrate improved robustness and physically consistent retrievals compared to conventional neural network approaches.

## Hayden Bromley

### *Title: A field theory for quasi-brittle fracture incorporating irreversible deformation*

#### **Abstract:**

A new field theory designed for predicting damage and fracture in quasi-brittle materials will be introduced. The model simultaneously captures the irreversible strain and elastic softening through a two-point, history dependent phase field. The initial boundary value problem satisfies energy balance and admits a positive energy dissipation rate consistent with the laws of thermodynamics. Discretization of this model allows for a mesh free analysis to computationally model fracture patterns. After an overview of the theory, numerical results will be presented exhibiting agreement with experiments both qualitatively and quantitatively. This is joint work with Robert Lipton.

## Jesse Chan

*Title: High order entropy correction methods for nonlinear conservation laws*

### **Abstract:**

Entropy stable formulations improve the robustness of high order discontinuous Galerkin (DG) numerical simulations of nonlinear conservation laws by ensuring that the solution satisfies a semi-discrete entropy inequality. Most entropy stable discretizations rely on an algebraic flux differencing formulation which involves both summation-by-parts discretizations and entropy conservative two-point finite volume fluxes. However, explicit expressions for such two-point finite volume fluxes may not be available for all systems or may be computationally expensive to compute.

An alternative approach to constructing entropy stable DG methods uses entropy dissipative correction terms to offset local violations of a cell entropy inequality. The resulting methods can be implemented either as an artificial viscosity or as a flux-corrected transport type schemes and yield the same semi-discrete entropy inequality satisfied by entropy stable flux differencing DG formulations. The entropy correction coefficients are parameter-free, locally computable over each cell, and preserve high order accuracy. We compare entropy correction schemes to existing flux differencing formulations, and present extensions of such approaches to non-ideal equations of state and projection-based reduced order models.

## Davood Damircheli

*Title: Extreme Particle Deformation in Three-Dimensional Granular Aggregates*

### **Abstract:**

We introduce a high-fidelity three-dimensional computational framework for modeling the bulk mechanical response of granular assemblies composed of deformable, brittle grains. Unlike classical discrete element methods (DEM), the proposed approach resolves both inter-particle interactions and intra-particle deformation through a nonlocal continuum formulation based on peridynamics. Individual grains are meshed directly from level-set descriptions, allowing accurate elastic behavior and fully autonomous fracture evolution without the need for explicit crack tracking or fragment reconstruction.

The framework is validated against a series of benchmark problems, including the Kalthoff-Winkler fracture test, crushing of hollow spheres, and combined impact-crushing scenarios. It is further applied to large granular assemblies containing up to 1000 irregular sand grains reconstructed from three-dimensional X-ray computed tomography. The simulations demonstrate convergence of the bulk stress response under compression, indicating the viability of defining representative volume elements (RVEs) for multiscale analysis. Finally, the method exhibits excellent strong and weak scaling performance, with simulations executed on up to 1600 cores, highlighting its suitability for large-scale, high-performance computing applications.

## Truc Dang

*Title: Order of Accuracy for DIRK methods with Newton iterations*

### **Abstract:**

Diagonally implicit Runge-Kutta (DIRK) methods are efficient time integrators for solving stiff differential equations and offer improved stability compared to explicit methods. At each timestep, DIRK methods require nonlinear solves, which are typically handled by an inexact Newton method. We study how the choice of Newton iteration affects the formal order-of-accuracy of a DIRK method. Based on this analysis, we demonstrate the challenges that arise when naively applying a Newton solver, and construct several new DIRK methods that preserve their order-of-accuracy while requiring only a single Newton iteration per stage.

## Md Tanvir Emrose

*Title: Reconfigurable structural color generation in multicolor pixels using phase-change materials*

### **Abstract:**

We introduce multilayer structures based on phase-change materials for reconfigurable structural color generation. These structures can produce multiple distinct colors within a single pixel. Specifically, we design structures that generate either two or four maximally distinct structural colors. We employ a memetic optimization algorithm coupled with the impedance method to identify the optimal combination of materials and layer thicknesses that maximizes the distinctiveness of the generated colors. We demonstrate that our design approach achieves strong color contrast between the generated colors. The proposed multilayer design eliminates the need for subwavelength lithography, making it highly suitable for large-scale applications. Our results could lead to a new class of single-cell multicolor pixels which retain each color without power consumption, making them particularly appealing for low refresh rate displays.

## Irene Erazo

*Title: Microscale flows around rigid particles under sparkle stress*

### **Abstract:**

This study models the dynamic behavior of small spherical particles immersed in a viscous fluid under the influence of thermal fluctuations. Using the Regularized Stokes Images outside a sphere, we perform theoretical and numerical analyses of particle diffusion to characterize their motion across varying particle sizes. The objective is to determine whether the fluid-particle coupling for rigid spheres adheres to the Stokes-Einstein scaling relation.

## Malena Espanol

*Title: Variable Projection Methods for Large-Scale Separable Nonlinear Inverse Problems*

### **Abstract:**

Many inverse problems in imaging and computational science lead to nonlinear least-squares formulations in which the forward model depends linearly on some parameters and nonlinearly on others. Variable projection is a powerful and efficient optimization approach that exploits this structure by eliminating the linear variables, thereby reducing dimensionality and improving the conditioning of the resulting problem. In this talk, I will provide an overview of the classical variable projection method and discuss its extension to large-scale inverse problems, with a particular focus on semi-blind deconvolution. I will present new regularization strategies and recent developments that incorporate approximate Jacobians computed using Krylov subspace techniques, enabling matrix-free implementations and improved scalability.

## Rubaiyat Bin Islam

*Title: Interaction of Flexible Fibers with a Burgers-like Vortex*

### **Abstract:**

An important category of microscale fluid-structure interactions concerns how flexible fibers deform and interact with fluid flows. Specifically, the dynamics of passive fibers such as passive planktons, and the navigation of motile microorganisms in external flows, a phenomenon known as rheotaxis, are often modeled under the simplifying assumption that local background flows exhibit constant vorticity. Many experimental and numerical studies have therefore focused on these interactions in simple external flows such as shear flows. Here we move away from this assumption and study the morphological evolution of slender fibers in a zero Reynolds number analog of a Burgers vortex. We reveal novel shapes exhibiting three-dimensional symmetric deformations, which are absent in typical shear flow experiments. We also investigate the rheotaxis of swimming microorganisms, modeled as flexible actuated fibers, in these complex flows to better understand how they navigate through hydrodynamic environments.

## Jenita Jahangir

*Title: A backward bifurcation in discrete-time epidemic models*

### **Abstract:**

We develop a discrete-time SIS model with vaccination, in which vaccination reduces but does not eliminate the risk of infection. We establish the stability of the disease-free equilibrium and determine the conditions under which a branch of backward bifurcating branch of endemic equilibria exists via an extension of the Fundamental Bifurcation Theorem. When vaccination is partially effective, backward bifurcation has been observed in the SIS model with vaccination at  $R_0 = 1$ , where a stable endemic equilibrium coexists with a stable disease-free equilibrium when the vaccine reproduction number ( $R_0$ ) is less than one. When vaccination is completely effective, the disease dies out when  $R_0 < 1$ , and it may persist when  $R_0 > 1$ . We observe that imperfect vaccination and recovery of infected individuals are necessary for the existence of backward bifurcation. We compare our findings to those of a continuous-time counterpart and examine how specific modeling assumptions influence endemic dynamics.

## Sang-Eun Lee

*Title: Collective Dynamics of Self-avoidant, Secreting Particles*

### **Abstract:**

Motivated by autophoretic droplet swimmers that move in response to a self-produced chemical gradient, here we examine the collective dynamics of individual motile agents using a reaction-diffusion system. The agents have an unlimited supply of a chemical, secrete it at a given rate, but are anti-chemotactic so move at a given speed in the direction of maximal decrease of this chemical. In both one- and two-dimensional periodic domains, we find intriguing long-time behavior of the system. Depending upon a non-dimensional parameter that involves secretion rate, agent velocity, domain size and diffusion, we find that the position of the agents either relax to regularly spaced arrays, approach these regular arrays with damped oscillation, or exhibit undamped, periodic trajectories. We examine the progression of particles that are initially seeded randomly, and we also examine the stability of the steady and periodic states. In addition, we will present results when these agents are embedded in an incompressible fluid, thus adding advection of the chemical field to the dynamics of this complex system.

## Jonathon Loftin

*Title: MATLAB, Python, and GenAI: Accelerating Teaching and Research*

### **Abstract:**

As computational workflows grow more interdisciplinary, educators and researchers increasingly rely on tools that enable flexibility, performance, and accessible innovation. This talk highlights how MATLAB and Python can be used together to create seamless, productive research and teaching environments. We will explore practical interoperability workflows that allow researchers to combine MATLAB's high-level analytics, visualization, and engineering toolboxes with Python's extensive open source ecosystem. The session also examines the latest deep learning capabilities in MATLAB, including model training, visualization, and integration with popular Python frameworks, enabling engineers and scientists to build, evaluate, and deploy AI models efficiently. Finally, we will discuss strategies for teaching with MATLAB in an era shaped by generative AI—illustrating how instructors can design meaningful learning experiences, integrate AI-assisted tools such as MATLAB Copilot responsibly, and help students build computational intuition while maintaining academic integrity. Together, these themes demonstrate how MATLAB, Python, and generative AI can support modern research, accelerate classroom innovation, and prepare students for an increasingly AI-driven future.

## Lovelyn Madu

*A Novel Double-Inertia Adaptive Step-Size Method for the Split Variational Inequality Problem.*

### **Abstract:**

This work presents a CQ-type projection and contraction method that integrates a double inertial extrapolation step together with self-adaptive step sizes for solving split variational inequality problems with quasi-monotone operators in real Hilbert spaces. We establish strong convergence of the proposed algorithm under mild and standard assumptions. Furthermore, numerical experiments confirm that our method achieves superior performance compared to several related algorithms in the literature. Additional comparisons in image processing and image restoration tasks further demonstrate the efficiency and practical advantages of the proposed approach.

## Leonardo Matone

*Title: DeepVoting: Learning and Improving Voting Rules with Fine-Tuning*

### **Abstract:**

Preference aggregation problems frequently center around identifying functions which provide desirable axiomatic properties. However, for many sets of axioms, functions which never violate the axioms are known to not exist; these are classically called impossibility results. Recent work on learning novel rules to minimize axiom violations shows the effectiveness of machine learning but explores a limited class of axioms. In this work we quantify the effectiveness of using standard social choice data structures as features for learning existing voting rules, resulting in networks that have better accuracy than past approaches while using an order of magnitude fewer parameters. Subsequently, we demonstrate a novel approach for measuring axiom satisfaction as a machine learning loss function. We employ transfer learning to fine-tune learned rules with new axiomatic properties and significantly reduce the number of axiom violations while maintaining highly accurate learned approximations of standard voting rules.

## Adnan Morshed

*Title: Tortuous tales of tortuosity*

### **Abstract:**

The geometric concept of tortuosity of a curved path has enjoyed a lot of room in the literature for being imprecisely defined. Due to the abundance of problems in biofluids - from porous media, retinal, and aortic flows, to microswimmer navigation in confined geometries - that make use of the concept of tortuosity, it becomes necessary to precisely pin down the application-dependent subjectivities to gain any objective benefit out of the data analysis. This talk will focus on some traditional as well as exotic definitions of tortuosity and will attempt to navigate some dangerous bends en route to arrive at an appropriate definition for microswimmer elastohydrodynamics.

## Anan Saha

*Title: Learning stochastic differential equations with integral-drift*

### Abstract:

Stochastic differential equations (SDEs) with integral drift arise naturally in multiscale systems and in applications where the effective dynamics emerges from averaging over latent or unobserved variables. In such models, the drift admits the representation

$$\bar{b}(x) = \int b(x, y) \pi(dy),$$

where  $\pi$  is an unknown probability measure on the latent space. A key challenge is that  $\pi$  is typically non-identifiable from observations of the marginal process  $X_t$ . Rather than attempting to recover  $\pi$ , our objective is to perform nonparametric estimation of the averaged drift  $\bar{b}$  directly from discrete observations of  $X$ . To this end, we develop a Bayesian methodology based on normalizing flows, which provides a flexible prior over the latent measure and enables scalable inference for  $\bar{b}$  in complex settings. Finally, we demonstrate the effectiveness of the proposed framework through numerical experiments on representative integral-drift SDE models.

## Lan Trinh

*Title: Estimation of Dynamic rates using Snapshots of Biological cells*

### Abstract:

In our work, we bring statisticians' perspective to what would classically be an inverse Partial Differential Equation (PDE) problem, but the data exhibits intrinsic randomness. Particularly, we have been working on static snapshot data that capture the discrete spatial positions of micro-particles whose motions are governed by a stochastic differential equation. The observed particles, confined within a single domain, ultimately follow a Poisson spatial point process whose intensity function is described by a PDE. The goal is to find the maximum likelihood estimators as well as study their asymptotic behavior, of the dynamic rates appearing in the PDE using only these snapshot observations. In implementing this framework, a major challenge stems from the fact that the associated PDE cannot be solved analytically, prompting the use of an efficient numerical method to approximate it before incorporating the result into the likelihood function. We also investigate the impact of heterogeneity and spatial information on the efficiency of the estimators and reveal that they enhance the estimation quality.

## Jai Tushar

### *A Conforming Virtual Element Method for a Quad-Curl Problem on Polygonal Meshes*

#### **Abstract:**

High-order curl operators appear in electromagnetic modeling and are closely related to Maxwell's transmission eigenvalue problem. In this talk, we present a  $C^0$ -conforming virtual element method for a two-dimensional quad-curl boundary value problem. We discuss treatment of both simply and multiply connected polygonal domains discretized using general polygonal meshes. Our approach is built on a Hodge-decomposition based reduction of the quad-curl problem to a sequence of second-order elliptic problems, that can be discretized using  $H^1$ -conforming finite element spaces.

## Mayank Tyagi

### *Title: Machine Learning Applications for Safe and Sustainable Energy Transition*

#### **Abstract:**

Increasing emissions of greenhouse gases (GHGs) have resulted in pressing concerns about climate change and increased investments in decarbonization. Therefore, it is imperative that the currently prevalent petroleum resources must make way for several alternate (and hopefully sustainable) energy solutions for society. However, the challenges for the safer and sustainable energy transition will require addressing not only the technological issues but also the socio-political concerns. Progress in artificial intelligence (AI) and machine learning (ML) has provided a strong economic motivation to many industrial sectors such as healthcare, retail etc. Applications of machine learning to petroleum engineering during the energy transition provide a unique opportunity to help train the workforce on translational skillsets and yet achieve the goal for safer and sustainable energy transition. In this talk, several examples of machine learning applications will be discussed to highlight Smart decision-making, Safety of operations, and Sustainability of subsurface energy resources that will be relevant to the energy transition. Rig state identification to reduce the invisible lost time (ILT) on offshore drilling platforms will be presented as ML example of smart decision making. Early kick detection (EKD) using ML based multi-class alarm system for an offshore drilling platform is shown as an example of operational safety. Lastly, the physics-informed neural networks (PiNNs) for the production datasets of an offshore reservoir field will be shown as an example for reduced-order models (ROMs) for waterflooding operations. Future directions of ML applications to geothermal reservoir engineering will be presented as an example of sustainable energy transition.

### *Latent-DeepOKAN for low-dimensional representation of multiple asynchronous flexible fibers interaction in Stokes flow*

#### **Abstract:**

Neural operators harness the capabilities of neural networks (NN) to learn nonlinear operators from data, enabling predictions of unseen outputs. The Deep Operator Network (DeepONet) effectively learns mappings by using a feedforward NN, making it suitable for solving partial differential equations (PDEs) resulting from complex physical systems. DeepONet utilizes two networks, namely the branch and trunk, to learn mappings. The branch takes inputs (e.g., initial conditions, boundary conditions, training parameters), while the trunk takes evaluation locations where the learned map will be evaluated (can be spatial, temporal, or both). As system complexities grow, DeepONet faces challenges in generating accurate predictions and incurs higher computational costs. To tackle these issues, Kolmogorov Arnold networks (KAN) are utilized in the recently proposed DeepOKAN instead of NN, which offers improved approximation with reduced computational expense in many cases. In this talk, we will introduce Latent-DeepOKAN, which employs data compression techniques like NN-based autoencoder-decoder and singular value decomposition (SVD) to derive effective latent representations for high-dimensional data, combined with KAN for enhanced operator learning. Using the test problem of multiple asynchronous flexible fibers locomotion in a viscous fluid modeled utilizing the Stokes' equation, we evaluate the computational performance of Latent-DeepOKAN. The ground truth data is generated utilizing the method of regularized Stokeslet segments, a strategy that is widely used to study flexible fiber locomotion in Stokes flow. We will share preliminary results that indicate that Latent-DeepOKAN enables better prediction capability with less computational cost as compared to standard DeepOKAN. Furthermore, we will discuss challenges and directions for further improvements.

## Yangwen Zhang

*Title: Optimal  $L^2$  Error Estimates for Non-symmetric Nitsche's Methods*

### **Abstract:**

Nitsche's method is widely used to weakly impose Dirichlet boundary conditions in finite element discretizations. While the symmetric formulation is well understood, the non-symmetric counterpart is often preferred because it avoids large penalty parameters and, in many settings, works naturally without additional stabilization; nevertheless, its  $L^2$ -error theory remains unsatisfactory. Existing analyses predict a suboptimal half-order loss in the  $L^2$  norm, in contrast with the optimal convergence that is consistently observed in numerical experiments.

In this work, we close this theoretical gap. We show that the suboptimal estimates arise from a lack of adjoint consistency in the standard duality argument. By constructing a new dual problem tailored to the non-symmetric formulation, together with refined regularity results for associated Robin boundary value problems, we recover full optimal  $L^2$  convergence. Our analysis covers both the stabilized and the penalty-free variants of the method, and applies on general shape-regular meshes without assuming quasi-uniformity. Three-dimensional numerical experiments validate the sharpness of the derived estimates.

## Zequn Zheng

*Title: Middle Rank Tensor Rank determination and Tensor approximation*

### **Abstract:**

Tensor rank determination and tensor approximation are fundamental problems in multilinear algebra with broad applications in signal processing, machine learning, and scientific computing.

The difficulty of those problems depends on the rank of tensors.

In this paper, we introduce a new framework for middle-rank tensor rank determination and tensor approximation.

Our method leverages generating polynomials and utilize linear algebra to detect the rank when the tensor's true rank is below certain bound.

Numerical experiments demonstrate that our algorithm can produces accurate tensor approximations without requiring prior knowledge of the rank.

*Title: A finite element framework for simulating residential burglary in realistic urban geometries*

### **Abstract:**

We consider a partial differential equation (PDE) model to predict residential burglary derived from a probabilistic agent-based model through a mean-field limit operation. The PDE model is a nonlinear, coupled system of two equations in two variables (attractiveness of residential sites and density of criminals), similar to the Keller-Segel model for aggregation based on chemotaxis. Unlike previous works, which applied periodic boundary conditions, we enforce boundary conditions that arise naturally from the variational formulation of the PDE problem, i.e., the starting point for the application of a finite element method. These conditions specify the value of the normal derivatives of the system variables at the boundary. For the numerical solution of the PDE problem discretized in time and space, we propose a scheme that decouples the computation of the attractiveness from the computation of the criminal density at each time step, resulting in the solution of two linear algebraic systems per iteration. Through numerous numerical tests, we demonstrate the robustness and computational efficiency of this approach. Leveraging the flexibility allowed by the finite element method, we show results for spatially heterogeneous model parameters and a realistic geometry (city of Chicago). The paper includes a discussion of future perspectives to build multiscale, 'multi-physics' models that can become a tool for the community. The robust and efficient code developed for this paper, which is shared open-source, is intended as the solid base for this broader research program.