Midwest Numerical Analysis Day 2024

Department of Mathematics
University of Iowa

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https://homepage.divms.uiowa.edu/~whan/mwnaday2024.html

Abstracts (as of March 27, 2024)

1. DD-LOD

Susanne C. Brenner

Louisiana State University

DD-LOD is a multiscale finite element method for problems with rough coefficients that is based on a domain decomposition approach to the localized orthogonal decomposition methodology. I will present the construction and analysis of DD-LOD for elliptic boundary value problems with rough coefficients that only require basic knowledge of finite element methods, domain decomposition methods and numerical linear algebra. An application to elliptic optimal control problems will also be discussed.

2. Asymptotically compatible discretization of parameterized nonlocal models

Qiang Du

Columbia University

There has been much interest in nonlocal models associated with a horizon parameter δ, which characterizes the effective range of nonlocal interactions. Asymptotically compatible (AC) discretization offers robust numerical approximations for such nonlocal problems by demonstrating insensitivity to variations in the parameter δ. This presentation introduces an abstract framework for the design and mathematical analysis of AC schemes within the context of discretizing a broader class of parameterized problems. Furthermore, we explore their application to specific instances of nonlocal variational problems and nonlocal conservation laws.

3. Stability of time discretizations for semi-discrete high order schemes for time-dependent PDEs

Chi-Wang Shu

Brown University

In scientific and engineering computing, we encounter time-dependent partial differential equations (PDEs) frequently. When designing high order schemes for solving these time-dependent PDEs, we often first develop semi-discrete schemes paying attention only to spatial discretizations and leaving time t continuous. It is then important to have a high order time discretization to main the stability properties of the semi-discrete schemes. In this talk we discuss several classes of high order time discretization, including the strong stability preserving (SSP) time discretization, which preserves strong stability from a stable spatial discretization with Euler forward, the implicit-explicit (IMEX) Runge-Kutta or multi-step time marching, which treats the more stiff term (e.g. diffusion term in a convection-diffusion equation) implicitly and the less stiff term (e.g. the convection term in such an equation) explicitly, for which strong stability can be proved under the condition that the time step is upper-bounded by a constant under suitable conditions, the explicit-implicit-null (EIN) time marching, which adds a linear highest derivative term to both sides of the PDE and then uses IMEX time marching, and is particularly suitable for high order PDEs with leading nonlinear terms, and the explicit Runge-Kutta methods, for which strong stability can be proved in many cases for semi-negative linear semi-discrete schemes. Numerical examples will be given to demonstrate the performance of these schemes.

4. Quantum Joule Experiment with Neutral Atom Quantum Computer

Muhammad Asaduzzaman

University of Iowa

We investigate Quantum Joule expansion in Rydberg atom systems. The experiment is interesting in understanding eigenstate thermalization hypothesis which states that at long time the system thermalizes. Classical description of the free expansion of the ideal quantum gas states that the temperature remains unchanged following a sudden change in the volume of the gas. However, for the isolated quantum gas there is periodic revival of number density with recurrence period $T \propto L^2$, L is the system size. It is interesting to note that classical recurrence time is exponential in system size. We designed an experiment with a lattice chain of Rydberg atoms to demonstrate these features by choosing appropriate coordinates for the atom positions, Rabi frequency, and global and local detuning of the carefully. We set the parameters so that the system is initially at the disordered phase. Next, we evolve the initial vacuum state adiabatically to drive the left of the chain to Z_2 phase. Thus, we prepare an initial state $|\text{Neel}>_{\text{left}-\text{half}} \otimes |0>_{\text{right}-\text{half}}$ for our experiment. Next, the net-detuning (global+local detuning) is suddenly dropped for the left half of the atoms and the net-detuning is suddenly increased to the same value of the right half of the chain at the same time. This enables an expansion of the particles which were initially confined on the left half of the chain. Real-time density measurements after the sudden expansion facilitate the computation of recurrence times, contributing insights into quantum dynamics.

5. Modeling elements of the gut microbiota as a chemostat

Bruce P. Ayati

University of Iowa

We will discuss a recent model of three microbial species and their chemical intakes and products. These three species are representative of the major phyla prevalent in the human gut. In addition to the modeling approach, we discuss the general sensitivity analysis and its implications.

6. Risk-Averse Contextual Generation Maintenance and Operations Scheduling under Wind Energy Uncertainty

Beste Basciftci

University of Iowa

This study focuses on a risk-averse contextual predictive maintenance and operations scheduling problem with flexible generation under wind energy uncertainty. We formulate this problem as a two-stage risk-averse stochastic mixed-integer program, where

the first-stage determines the maintenance and unit commitment related decisions of the traditional generation units, whereas the second-stage determines the corresponding decisions for flexible generators along with the production related plans of all generators. To integrate contextual information in predicting wind energy, we propose a Gaussian Process Regression approach, which is leveraged into this stochastic program through a conditional expectation. Since this problem is computationally challenging to solve with a mixed-integer recourse, we utilize a progressive hedging algorithm by further extending it to the risk-averse setting. Our results on the IEEE 118-bus instance demonstrate the impact of adopting a risk-averse approach compared to risk-neutral and deterministic alternatives with a better worst-case performance, and highlight the value of integrating flexible generation and contextual information with resilient maintenance and operations schedules leading to cost-effective plans with less component failures. Furthermore, the solution algorithm provides significant speed-ups compared to the off-the-shelf solver while finding optimal solutions in the majority of the instances.

7. An improved stable algorithm for some kernel matrix-vector multiplications

Chenyang Cao

Purdue University

Approximating kernel functions using sum-of-exponential (SoE) expansions have been studied years ago and a series of fast algorithms were proposed in 1D or 2D. In this talk, we summarize these algorithms and show a structured matrix version (sequentially semiseparable) of them in 1D. Also, we discuss the backward stability issue due to linear error propagation in matrix-vector multiplications of these structured matrices. An improved algorithm is provided by exploiting a new structure (hierarchical semiseparable) of matrix. Then the error propagation would be reduced to logarithm of problem size. We mainly focus on the Cauchy kernel to present the idea and it can be extended to other analytical kernels as well. Numerical results will be provided to validate the improved algorithm. This is joint work with Jianlin Xia.

8. The Runge–Kutta discontinuous Galerkin method with stage-dependent polynomial spaces for hyperbolic conservation laws

Qifan Chen

Ohio State University

We present a novel class of high-order Runge–Kutta (RK) discontinuous Galerkin (DG) schemes for hyperbolic conservation laws. The new method extends beyond the traditional method of lines framework and utilizes stage-dependent polynomial spaces

for the spatial discretization operators. To be more specific, two different DG operators, associated with $\mathcal{P}^k$ and $\mathcal{P}^{k-1}$ piecewise polynomial spaces, are used at different RK stages. The resulting method is referred to as the sdRKDG method and features fewer floating-point operations and may achieve larger time step sizes. We have also conducted von Neumann analysis for the stability and error of the sdRKDG schemes for the linear advection equation in one dimension. Numerical tests are provided to demonstrate the performance of the new method.

9. Computationally Efficient Structured Policy Representations in Partially Observable Markov Decision Processes

Kenneth Czuprynski

The Pennsylvania State University

A Partially Observable Markov Decision Process (POMDP) is a general model for single agent decision making. These represent an important class of optimal control problems in domains where the uncertainty must be incorporated into the model. The incorporation of uncertainty results in challenging optimization problems which limit the scalability of solution methodologies. In this talk, we discuss the use of structured policy representations as a means of inducing computationally efficient numerical structure into the underlying problem. This allows for efficient iterative and direct methods to be developed which result in more scalable algorithms. We introduce two different structured policy representations, investigate the computational benefits of each, and apply them to a suite of benchmark problems.

10. Nuclear many-body theories via quantum computing

Weijie Du

Iowa State University

Nuclear many-body problems are computationally hard on classical computers. The quantum computing techniques hold the promise to solve such problems with efficiency. In this talk, we review our recent efforts in developing quantum algorithms for solving nuclear many-body problems. Special focus is on our work of developing a novel Hamiltonian input scheme of general relativistic and nonrelativistic many-fermion systems, based on which we propose frameworks to solve the spectra and dynamics of nuclear many-body problems on future quantum computers. We also present thoughts for future development.

11. Generative Artificial Intelligence in Aerospace Engineering Applications

Xiaosong Du

Missouri University of Science and Technology

Aerodynamic design optimization plays a key role in engineering industry, including aircraft and automotive, to increase fuel efficiency and reduce pollutant emissions. However, conventional aerodynamic design adopts simulation models for a large number of evaluations, which is computationally expensive. Identifying these challenges, the presenter will introduce his research products on machine learning-enabled optimization architectures. This talk will mainly focus on the following three types: surrogate modeling with intelligent parameterization and automatic design space reduction using B-spline based generative adversarial networks; learning optimal aerodynamic designs through reduced-dimensional networks; and multi-fidelity surrogate modeling for aerodynamic design on the fly. This presenter will also briefly introduce the latest on-going research topics in his research lab.

12. A Parabolic System of Aggregation Formation in Bacterial Colonies

Zhaosheng Feng

University of Texas Rio Grande Valley

The goal of this talk is to study a fourth-order nonlinear parabolic system with dispersion for describing bacterial aggregation. Analytical solution of traveling wave is found by taking into account the dispersion coefficient. Numerically, we demonstrate that the initial concentration of bacteria in the form of a random distribution over time transforms into a periodic wave, followed by a transition to a stationary solitary wave without dispersion.

13. Circumferentially pressure-driven flow in a two-layer system: a Riemann-sum approximation

Dauda Gambo

Iowa State University

In this talk, we present the semi-analytical solution of transient viscous flow of a two-layered system in an annular duct. The flow is triggered by an imposed pressure gradient in the circumferential direction, with both the outer and inner cylinders held fixed. The model partial differential equations (PDEs) are first transformed and solved in the Laplace domain. Subsequently, the solution of the ordinary differential equations (ODEs) is then inverted to time domain using the Riemann-sum approximation. To ascertain the accuracy of the approximation employed, a comparison between steady-state solution and values derived from implicit finite difference in the transient state model is provided. Impact of the pertinent controlling parameters on the flow characteristics are also analyzed.

14. Median Filter Method for Wetting and Dewetting Dynamics with Anisotropic Surface Tension

Jiajia Guo

University of Michigan

We present new level set methods for multiphase, anisotropic (weighted) motion by mean curvature of networks, focusing on wetting-dewetting problems where one out of three phases is stationary. The new schemes are vectorial median filters: The level set values at the next time step are determined by a sorting procedure performed on the current level set values. The correct Herring angle condition at triple junctions (which include torque terms due to anisotropy) are indirectly and automatically enforced. Other standard benefits of level set methods, such as subgrid accuracy on uniform grids via interpolation and seam-less treatment of topological changes, remain intact. Convergence to the correct evolution is demonstrated via extensive numerical studies.

15. Learning Stochastic Dynamics from Data

Ziheng Guo

Illinois Institute of Technology

We present a noise guided trajectory based system identification method for inferring the dynamical structure from observation generated by stochastic differential equations. Our method can handle various kinds of noise, including the case when the components of the noise are correlated. Our method can also learn both the noise level and drift term together from trajectory. We present various numerical tests for showcasing the superior performance of our learning algorithm. To address high-dimensional cases, we have integrated deep learning techniques into our method. Additionally, a Python package encapsulating our approach has been developed.

16. A Novel Energy Guided PINN Approach for Solving Reversible Gray-Scott type PDE systems

Baoli Hao

Illinois Institute of Technology

This talk explores the synergy between spectral methods and a novel Energy Guided Physics-Informed Neural Networks (PINNs) to solve the Reversible Gray-Scott equations in both one-dimensional (1D) and two-dimensional (2D) settings. The Gray-Scott equations are pivotal in elucidating pattern formation dynamics in various natural systems. Leveraging spectral methods, we achieve accurate and efficient solutions to the spatiotemporal evolution of the reversible Gray-Scott system. Subsequently, we employ PINNs to assimilate the spectral data into a neural network architecture, enabling

the extraction of intricate patterns and dynamics. Our study showcases the effectiveness of this integrated approach in capturing complex phenomena while providing a robust framework for analyzing reversible reaction-diffusion systems across different dimensions.

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

Xiaoming He

Missouri University of Science and Technology

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

18. Generalized Korn's inequalities for piecewise H^1 and H^2 vector fields

Qingguo Hong

Missouri University of Science and Technology

The purpose of this talk is to construct a new class of discrete generalized Korn's inequalities for piecewise H1 vector fields and piecewise H2 vector fields in three-dimensional space. The resulting Korn's inequalities are different from the standard Korn's inequalities, as they involve the trace-free symmetric gradient operator, in place of the usual symmetric gradient operator. It is anticipated that the new generalized Korn's inequalities will be useful for the analysis of a broad range of finite element methods, including mixed finite element methods and discontinuous Galerkin methods.

19. Bounds-preserving high order discontinuous Galerkin method for variable coefficient tracer transport

Yifan Hu

Iowa State University

We present a novel discontinuous Galerkin (DG) method for variable coefficient advection equation with a non-constant capacity function. This method consists of a bounds-preserving first order Finite Volume method and a high order spacetime DG method, where we design a multidimensional flux limiter based on locally optimal mixing weights. We apply this method to a density stratified fluid problem where a passive, non-reactive tracer travels with the wind over a "mountain" (non-reflective, zero-friction bottom geometry).

20. InfSupNet for solving high dimensional elliptic PDEs

Xiaokai Huo

Iowa State University

Solving high dimensional partial differential equations (PDEs) has historically posed a considerable challenge when utilizing conventional numerical methods, such as those involving domain meshes. Recent advancements in the field have seen the emergence of neural PDE solvers, leveraging deep networks to effectively tackle high dimensional PDE problems. I will talk about our recent work, InfSupNet, a model-based unsupervised learning approach designed to acquire solutions for a specific category of elliptic PDEs. The fundamental concept behind Inf-SupNet involves incorporating the inf-sup formulation of the underlying PDE into the loss function. The analysis reveals that the global solution error can be bounded by the sum of three distinct errors: the numerical integration error, the duality gap of the loss function (training error), and the neural network approximation error for functions within Sobolev spaces. To validate the efficacy of the proposed method, numerical experiments conducted in high dimensions demonstrate its stability and accuracy across various boundary conditions, as well as for both semi-linear and nonlinear PDEs.

21. Convergence of modified Newton iterations for implicit Runge-Kutta methods applied to stiff systems of differential equations

Laurent O. Jay

University of Iowa

We consider the application of implicit Runge-Kutta (IRK) methods to systems of implicit ordinary differential equations (ODEs). We are especially interested in the situation when stiffness arises. In this talk we will present some new results about sufficient conditions ensuring local contractivity, hence convergence, of modified Newton iterations of IRK methods for stiff ODEs with step size conditions independent of stiffness.

22. Solvation free energy calculation by a Nonuniform Size Modified Poisson-Boltzmann Ion Channel Model

Liam Jemison

University of Wisconsin Milwaukee

In this talk, I will introduce a software package for computing the solvation free energy of a voltage-dependent anion channel (VDAC) protein using the nonuniform size-modified Poisson Boltzmann ion channel (nuSMPBic) model. This package is developed by Prof. Dexuan Xie's research group at UWM. It includes a new irregular tetrahedral mesh generation package, the nuSMPBic finite element solver, and a novel numerical scheme for computing free energy components. I will report the free energy results generated by the package for six different VDAC proteins in a variety of ionic solutions and under various voltage and permittivity conditions, along with a comparison with two other Poisson Boltzmann ion channel models: one which assumes uniform ion sizes and one which does not incorporate any size effects. These test results demonstrate that the nuSMBPic model can perform better than the other two models in the prediction of solvation free energy. This work was done jointly with Mr. Matthew Stahl and Prof. Xie. It was partially supported by the National Science Foundation through the award number DMS-2153376.

23. q-deformations of the algebras of quantum observables

Palle Jorgensen

University of Iowa

The algebras of quantum observables are non-commutative but indexed by parameter q which reflects the particular quantum systems under consideration. We present this in detail, how the algebraic systems are indexed by a parameter q in the interval $(-1, 1)$, where the endpoints correspond to Fermions and Bosons, respectively. We show that there is stability for small values of q in the q-dependence of the isomorphism classes.

Joint work with Reinhard Werner.

24. Intrinsic Projection of Implicit Runge-Kutta Methods for DAEs

Nikita Kapur

University of Iowa

We present the new technique of Intrinsic Projection (IP) for Implicit Runge-Kutta (IRK) Methods applied to differential-algebraic equations (DAEs). IP does not require the accurate evaluation of any additional Jacobian like for standard Projected Implicit Runge-Kutta Methods and is therefore simpler to implement. IP for IRK methods is

analyzed for index 2 DAEs, in particular, we give results about existence and uniqueness, and some error estimates. For index 2 DAEs IP for IRK methods is shown to lead to the same order of error estimates as standard Projected Implicit Runge-Kutta Methods, but at a lower computational cost. Some preliminary results for index 3 DAEs will also be given.

25. Training data studies for the cell-average-based neural network method for linear hyperbolic and parabolic equations

Tyler Kroells

Iowa State University

In this talk, we present the training data studies for the cell-average-based neural network (CANN) method for linear hyperbolic and parabolic equations. We enlarge the training data set to include representative solution trajectories such as Fourier basis functions and determine if or not the method will be improved. A perturbed stochastic gradient descent method is proposed and is verified to improve the method's stability after long-time simulations. Robustness of the method to contaminated training data is investigated. For the linear parabolic equation, the CANN method can be generalized to solve a large group of initial value problems, especially those involving high-frequency modes, while being an explicit method with a large time step size applied to evolve the solution forward in time.

This is a collaboration work with Ethan Schmidt, Changxin Qiu and Jue Yan.

26. Finite Difference Approximation with ADI Scheme for Two-dimensional Keller-Segel Equations

Yubin Lu

Illinois Institute of Technology

Keller-Segel systems are a set of nonlinear partial differential equations used to model chemotaxis in biology. In this paper, we propose two alternating direction implicit (ADI) schemes to solve the 2D Keller-Segel systems directly with minimal computational cost, while preserving positivity, energy dissipation law and mass conservation. One scheme unconditionally preserves positivity, while the other does so conditionally. Both schemes achieve second-order accuracy in space, with the former being first-order accuracy in time and the latter second-order accuracy in time. Besides, the former scheme preserves the energy dissipation law asymptotically. We validate these results through numerical experiments, and also compare the efficiency of our schemes with the standard five-point scheme, demonstrating that our approaches effectively reduce computational costs.

27. Camouflage Adversarial Attacks on Multiple Agent Systems

Ziqing Lu

University of Iowa

The multi-agent reinforcement learning systems (MARL) based on the Markov decision process (MDP) have emerged in many critical applications. To improve the robustness/defense of MARL systems against adversarial attacks, the study of various adversarial attacks on reinforcement learning systems is very important. Previous works on adversarial attacks considered some possible features to attack in MDP, such as the action poisoning attacks, the reward poisoning attacks, and the state perception attacks. In this paper, we propose a brand-new form of attack called the camouflage attack in the MARL systems. In the camouflage attack, the attackers change the appearances of some objects without changing the actual objects themselves; and the camouflaged appearances may look the same to all the targeted recipient (victim) agents. The camouflaged appearances can mislead the recipient agents to misguided actions. We design algorithms that give the optimal camouflage attacks minimizing the rewards of recipient agents. Our numerical and theoretical results show that camouflage attacks can rival the more conventional, but likely more difficult state perception attacks. We also investigate cost-constrained camouflage attacks and showed numerically how cost budgets affect the attack performance.

28. Efficient methods for time-harmonic wave propagation problems

Songting Luo

Iowa State University

In this talk, we will present some recently-developed methods for simulating high frequency wave propagation, aiming to resolve the difficulty related to the pollution effect. These methods combine Fourier pseudospectral approximations with functional evaluation iterations to balance efficiency and accuracy. Numerical experiments verify their effectiveness.

29. High order methods for wave propagation problems

Ian Morgan

Iowa State University

When dealing with the wave equation in high spatial frequencies, accurate solutions can be difficult to achieve. Asymptotic approximations may only offer localized solutions, while finite element or finite difference schemes can be susceptible to pollution errors. We are currently working on developing Fourier pseudospectral methods that

are efficient, high-order, and free from pollution. These methods involve time-stepping schemes that utilize a modified Helmholtz equation, which can be solved using either a rapidly converging Krylov subspace scheme or by structuring the inverse operator as a functional that can be evaluated numerically.

30. An improved training methodology to learn Green's function of variable coefficient elliptic PDEs

Pawan Singh Negi

Illinois Institute of Technology

Green's functions serve as fundamental solutions to PDEs for Dirac delta forcing functions. The solution to a boundary value or interface problem can be conveniently expressed as a boundary integral using the boundary condition and the Green's function. However, analytical evaluation of Green's function is highly challenging. In this study, we propose a boundary integral-based neural network approach. We utilize Green's third identity to represent the solution in terms of the forcing function, single-layer potential, and double-layer potential. Green's function is evaluated using a radial basis function-based neural network, while the density function in the layered potential is estimated using a multilayer perceptron network. The network is trained to satisfy Green's third identity for a given trial function generated from another radial basis function-based neural network with user controlled parameters. Furthermore, we generate samples from two distinct domains. For the first domain, we consider a small size, with samples finely placed near the boundary compared to the interior. For the second domain, samples are uniformly distributed over a much larger domain. We validate the solver by solving Laplace, Helmholtz, and variable coefficient PDEs for boundary value problems. Additionally, we showcase the efficacy of the learned Green's function by solving interface problems for variable coefficient elliptic PDEs.

31. Global and local growth behavior of GEPP and GECP

John Peca-Medlin

University of Arizona

Gaussian elimination (GE) remains one of the most used dense linear solvers. Error analysis of GE with selected pivoting strategies on well-conditioned systems can focus on studying the behavior of growth factors. Although exponential growth is possible with GE with partial pivoting (GEPP), growth tends to stay much smaller in practice. Support for this behavior was provided very recently by Huang and Tikhomirov's average-case analysis of GEPP, which showed GEPP growth stays at most polynomial with very high probability when using Gaussian matrices. Research on GE with complete pivoting (GECP) has also seen a lot of recent interest, with improvements to lower and upper bounds on worst-case GECP growth provided by Bisain, Edelman,

and Urschel in the last year. I am interested in studying how GEPP and GECP behave on the same linear systems, with a focus on large growth systems and orthogonal matrices. One direction will explore when GECP is less stable than GEPP, which will lead to new empirical lower bounds on how much worse GECP can behave compared to GEPP in terms of growth. Another direction will include an empirical study on a family of exponential GEPP growth matrices whose polynomial behavior in small neighborhoods limits to the initial GECP growth factor.

32. Discrete real time path integrals

Wayne Polyzou

University of Iowa

Quantum computers are finite quantum systems with a finite number of qbits. Computations involve real time evolution of these finite quantum systems. In this talk I discuss a path integral representation of unitary time evolution for finite quantum systems. Operators are represented using an irreducible pair of unitary operators. When the number of quantum states is 2^N the irreducible pairs can be decomposed into tensor products of local irreducible pairs that act on each qbit. Time evolution is represented by the expectation value of a complex probability [1] on a set of cylinder sets. For a finite number (M) of time steps the number of cylinder sets is finite and the complex probability for each cylinder set exactly factors into a product of (M) one time step complex probabilities, which reduces the compution to the M^{th} power of a finite matrix. I illustrate the method with applications to potential scattering and local quantum field theory [2].

[1] Ekaterina S. Nathanson and E.T. Jørgensen, Palle. A global solution to the Schrödinger equation: From Henstock to Feynman. J. Math. Phys., 56:092102, 2015.

[2] W. N. Polyzou, Path integrals and the discrete Weyl representation, arxiv:2108.12494

33. Locally-implicit discontinuous Galerkin schemes for kinetic Boltzmann-BGK

James Rossmanith

Iowa State University

The kinetic Boltzmann equation with the Bhatnagar-Gross-Krook (BGK) collision operator allows for the simulation of gas dynamics over a wide range of Knudsen numbers with a simplified collision operator. Efficient numerical methods for Boltzmann-BGK should be asymptotic-preserving, which allows the numerical method to be stable at fixed mesh parameters for any value of the Knudsen number, including in the fluid (very small Knudsen numbers), slip flow (small Knudsen numbers), transition (moderate Knudsen numbers), and free molecular flow (large Knudsen numbers) regimes. In

this work, we develop a novel approach for solving the Boltzmann-BGK equation for achieving both arbitrary high-order and the asymptotic-preserving property. The proposed method is a locally-implicit discontinuous Galerkin (LIDG) scheme with careful modification in both the prediction and correction steps to achieve the asymptotic-preserving property. Some key advantages of the proposed schemes are: (1) no splitting between macroscale and microscale components of the distribution function is required; (2) only a single unified time-discretization is required; and (3) arbitrary high-order in both space and time can be achieved simply by increasing the spatial polynomial order in each element. Several numerical examples are shown to demonstrate the effectiveness of the proposed numerical scheme.

34. Asymptotic-Preserving Scheme for the Kinetic Boltzmann-BGK Equation

Preeti Sar

Iowa State University

The kinetic Boltzmann equation with the Bhatnagar-Gross-Krook (BGK) collision operator describes the motion of a fluid for the simulation of gas dynamics over a wide range of Knudsen numbers with a simplified collision operator. The small scales in kinetic and hyperbolic equations lead to different asymptotic regimes which are expensive to solve numerically. Asymptotic preserving schemes are efficient in these regimes, which preserve at the discrete level, the asymptotic limit which drives the microscopic equation to its macroscopic equation. Such schemes allow the numerical method to be stable at fixed mesh parameters for any value of the Knudsen number, including in the fluid (very small Knudsen numbers), slip flow (small Knudsen numbers), transition (moderate Knudsen numbers), and free molecular flow (large Knudsen numbers) regimes. In this work, we develop an approach for solving the Boltzmann-BGK equation for achieving both arbitrary high-order and asymptotic preservation. This numerical scheme is applied to multidimensional flows and hence is an extension to previous work done in one dimension.

35. Starting Approximations for SIRK Methods Applied to Index 2 DAEs

Joseph R. Small

University of Iowa

In this presentation, we look at applications of IRK methods to index 2 DAEs, henceforth referred to as specialized implicit Runge-Kutta (SIRK) methods. We are particularly interested in developing high order starting approximations for the internal stages to minimize the number of fixed-point/Newton type iterations needed at each step to solve the nonlinear system within the desired error bounds. We use reverse

SIRK methods to simplify the analysis and fix some errors that have appeared in previous papers on the topic. Our analysis also leads us to new convergence results for these reverse methods.

36. Fast Gaussian Process Regression with Derivative Information

Aleksei Sorokin

Illinois Institute of Technology

Gaussian process regression, or kriging, is a method for high dimensional interpolation which has gained popularity thanks to the ability to encode assumptions about the underlying simulation into the covariance kernel and the ability to quantify prediction uncertainty. A significant drawback is that fitting a kriging model to n data points typically costs $O(n^3)$ as it is required to solve a system involving the $n \times n$ Gram matrix of pairwise covariance kernel evaluations. Hickernell and Jagadeeswaran show in their 2019 and 2022 papers on fast automatic Bayesian cubature that when one has control over the design of numerical experiments then specially chosen sampling locations and matching covariance kernels yield structured Gram matrices for which we can complete all necessary computations in $O(n \log n)$. Specifically, lattice and digital sequences from Quasi-Monte Carlo paired with matching kernels yield circulant and block-Toeplitz Gram matrices respectively.

We have extended the cubature rules implemented in QMCPy to surrogate modeling with support for noisy observations and derivative information. We present methods and Julia software for fitting these fast kriging models in $O(n \log n)$, including software to generate Quasi-Monte Carlo point sets. The software is demonstrated by modeling the solution process of a PDE with random coefficients.

37. Finite Element Exterior Calculus for Hamiltonian PDEs

Ari Stern

Washington University in St. Louis

We consider the application of finite element exterior calculus (FEEC) methods to a class of canonical Hamiltonian PDE systems involving differential forms. Solutions to these systems satisfy a local multisymplectic conservation law, which generalizes the more familiar symplectic conservation law for Hamiltonian systems of ODEs, and which is connected with physically-important reciprocity phenomena, such as Lorentz reciprocity in electromagnetics. We characterize hybrid FEEC methods whose numerical traces satisfy a version of the multisymplectic conservation law, and we apply this characterization to several specific classes of FEEC methods, including conforming Arnold–Falk–Winther-type methods and various hybridizable discontinuous Galerkin (HDG) methods. Interestingly, the HDG-type and other nonconforming methods are

shown, in general, to be multisymplectic in a stronger sense than the conforming FEEC methods. This substantially generalizes previous work of McLachlan and Stern [Found. Comput. Math., 20 (2020), pp. 35–69] on the more restricted class of canonical Hamiltonian PDEs in the de Donder–Weyl grad-div form.

38. **Ridge function machines**

David Stewart

University of Iowa

Ridge functions have the form $\mathbf{x} \mapsto \varphi(\mathbf{w}^T\mathbf{x})$ for a weight vector $\mathbf{w} \in \mathbb{R}^n$ and a function $\varphi\colon \mathbb{R} \to \mathbb{R}$. While these form an infinite dimensional space of functions, we propose a finite dimensional class of functions that approximates this space, and can be used in machine learning systems instead of fixed-activation function neural networks. Approximation of data with these functions can be performed efficiently, and can be adapted to give greater or lesser refinement according to the data available.

39. **Functional Equivariance and Modified Vector Fields**

Sanah Suri

Washington Univeristy in St. Louis

Certain numerical integrators preserve geometric properties of the flow of differential equations. In particular, the preservation of linear and quadratic first integrals has been studied extensively. McLachlan and Stern introduced the idea of F-functional equivariance providing a new framework to talk about the preservation of first integrals as well as other notable observables of a dynamical system. This talk will extend the idea of F-functional equivariance to backward error analysis and modified vector fields. We generalize results on invariant preservation and describe the numerical evolution of non-invariant observables.

40. **Dynamic behavior for the AGEM algorithm**

Xuping Tian

Iowa State University

In this talk we investigate a novel gradient algorithm, AGEM, using both energy and momentum, for addressing general non-convex optimization problems. The solution properties of the AGEM algorithm, including aspects such as uniformly boundedness and convergence to critical points, are examined. The dynamic behavior is studied through a comprehensive analysis of a high-resolution ODE system. This ODE system, being nonlinear, is derived by taking the limit of the discrete scheme while preserving the momentum effect through a rescaling of the momentum parameter. The paper

emphasizes the global well-posedness of the ODE system and time-asymptotic convergence of solution trajectories. Furthermore, we establish a linear convergence rate for objective functions that adhere to the Polyak-Łojasiewicz condition. This is a joint work with Hailiang Liu (ISU).

41. Data-driven multi-scale models for materials-by-design of energetic materials

H. S. Udaykumar

University of Iowa

Multi-scale modeling of energetic material sensitivity requires telescoping physics from the nano- and micro- and meso-scales to make predictions of their macro-scale response. While atomistic simulations must inform meso-scale models, meso-scale models must provide closure to macro-scale simulations. Scale bridging in multi-scale simulations can be achieved through a variety of machine learning algorithms, providing data-driven closures which upscale key (localization) physics from subgrid (unresolved) scales. This talk will indicate work done thus far to develop a route to materials-by-design of energetic materials, where structure-property-performance (S-P-P) relationships are established through different approaches: 1) a technique based on surrogate modeling while relies on an ensemble of meso-scale calculations; 2) a deep learning approach. We also show how modern deep learning approaches can be employed in a design loop where in silico S-P-P frameworks can be constructed to optimize microstructures. In addition, ongoing work on transfer learning and multi-fidelity modeling strategies will also be highlighted, as these are useful for crossing species, i.e., employing knowledge about one material in a family of energetic materials to speed up learning the behavior of another material.

42. Numerical experiments using the barycentric Lagrange treecode

Lei Wang

University of Wisconsin, Milwaukee

To account for hydrodynamic interactions among solvated molecules, Brownian dynamics simulations require correlated random displacements $\mathbf{g} = D^{1/2}\mathbf{z}$, where D is the $3N \times 3N$ Rotne-Prager-Yamakawa diffusion tensor for a system of N particles and $\mathbf{z}$ is a standard normal random vector. The Spectral Lanczos Decomposition Method (SLDM) computes a sequence of Krylov subspace approximations $\mathbf{g}_k \to \mathbf{g}$, but each step requires a dense matrix-vector product $D\mathbf{q}$ with a Lanczos vector $\mathbf{q}$, and the $O(N^2)$ cost of computing the product by direct summation (DS) is an obstacle for large-scale simulations. This work employs the barycentric Lagrange treecode (BLTC) to reduce the cost of the matrix-vector product to $O(N \log N)$ while introducing a controllable

approximation error. Numerical experiments compare the performance of SLDM-DS and SLDM-BLTC with particular attention on the effect of the BLTC approximation error.

43. An Extreme Learning Machine-Based Method for Computational PDEs in Higher Dimensions

Yiran Wang

Purdue University

We present two effective methods for solving high-dimensional partial differential equations (PDE) based on randomized neural networks. Motivated by the universal approximation property of this type of networks, both methods extend the extreme learning machine (ELM) approach from low to high dimensions. With the first method the unknown solution field in d dimensions is represented by a randomized feed-forward neural network, in which the hidden-layer parameters are randomly assigned and fixed while the output-layer parameters are trained. With the second method the high-dimensional PDE problem is reformulated through a constrained expression based on an Approximate variant of the Theory of Functional Connections (A-TFC), which avoids the exponential growth in the number of terms of TFC as the dimension increases. The free field function in the A-TFC constrained expression is represented by a randomized neural network and is trained by a procedure analogous to the first method.

44. Full weak Galerkin FEMs for linear poroelasticity problems on quadrilateral meshes

Zhuoran Wang

University of Kansas

In this talk, we present full weak Galerkin solvers for linear poroelasticity problems. The Darcy pressure and the linear elasticity are approximated by scalar- or vector-valued polynomials. We establish discrete weak gradient and numerical velocity in the (vector- or matrix-version) Arbogast-Correa spaces. We formulate the fully-discrete system using implicit Euler time discretization or Crank-Nicolson method for higher order methods. Numerical experiments are presented for validating the optimal order convergence rates and the locking-free property of the new solvers. This is a joint work with Dr. James Liu, Dr. Simon Tavener, and Dr. Ruishu Wang.

45. Fast solvers for neural network least-squares approximations

Jianlin Xia

Purdue University

Neural networks provide an effective way to approximate functions, especially for some challenging situations with discontinuities, large variations, and sharp transitions. In our recent development of a novel block Gauss-Newton method for least-squares approximations via ReLU shallow neural networks, some dense linear systems arise in the iterations for finding some linear and nonlinear parameters. The coefficient matrices are shown to be symmetric and positive definite. We can further show that they are highly ill conditioned, and the condition numbers get even worse for some challenging function approximations. The ill-conditioned dense linear systems are thus difficult to solve by traditional direct and iterative solvers. On the other hand, we prove that the matrices have some interesting features that we can explore so that the systems can be solved efficiently and accurately. This is joint work with Zhiqiang Cai, Tong Ding, Min Liu, and Xinyu Liu.

46. An Efficient Finite Element Solver for a Nonuniform Size Modified Poisson-Nernst-Planck Ion Channel Model

Dexuan Xie

University of Wisconsin–Milwaukee

In this talk, I present an efficient finite element iterative method for solving a nonuniform size modified Poisson-Nernst-Planck ion channel (SMPNPIC) model and a corresponding software package that works for an ion channel protein with a three-dimensional crystallographic structure and an ionic solvent with multiple species. An efficient iterative scheme is also introduced to solve each related nonlinear algebraic system to further improve the efficiency of the method. Numerical results for a voltage-dependent anion channel (VDAC) in an ionic solvent of four species will be reported to demonstrate the method's convergence, the package's high performance, and the importance of considering nonuniform ion size effects. This work is partially supported by the National Science Foundation, USA, through award number DMS-2153376 and the Simons Foundation, USA, through research award 711776.

47. A reinterpreted discrete fracture model for Darcy-Forchheimer flow in fractured porous media

Yang Yang

Michigan Technological University

We propose a novel hybrid-dimensional model for the Darcy–Forchheimer flow in fractured rigid porous media, with a natural applicability to non-conforming meshes. Motivated by the previous work on the reinterpreted discrete fracture model (RDFM) for Darcy flows, we extend its key idea to non-Darcy flows. Coupling the Darcy's law in the matrix and the Forchheimer's law in the fractures through the introduction of

the Dirac-functions to characterize the fractures, we derive a relationship between the total flow velocity in the porous media and the fluid velocity in the fractures. With this relation, it is natural to model the Darcy–Forchheimer flow in the whole computational domain by one equation. The local discontinuous Galerkin method is applied for numerical discretization of the steady-state single-phase flow problem and a time-marching method is adopted to find the solution of the resulting nonlinear system. Besides, we construct a direct solver for the nonlinear equation of the fluid velocity in fracture to save computational cost. As an application, we discuss a simple transport model coupled with the flow equation. Several numerical experiments validate the performance of the model with its effectiveness on non-conforming meshes. We observe that the Darcy–Forchheimer model effectively reduces the flow rates and makes the predictions more realistic in case of excessive fracture velocities.

48. Nonconforming FEM for a Stokes Hemivariational Inequality

Yuan Yao

University of Iowa

In recent years, modeling, analysis, and numerical solution of hemivariational inequalities have attracted much attention in the research communities. Through the formulation of hemivariational inequalities, application problems involving nonmonotone, nonsmooth and multivalued constitutive laws, forces, and boundary conditions can be treated successfully. In this talk, we present a nonconforming finite element method for a Stokes hemivariational inequality arising in the study of a viscous incompressible fluid flow subject to a non-monotone slip boundary condition of the friction type. We consider the $CR-P_1$ element pair for the numerical approximation and use the pressure projection technique to stabilize the numerical solution. We use the Uzawa algorithm for the numerical simulation, and will present numerical results for the performance of the method.

This is a joint work with Weimin Han.

49. An Efficient and Spectrally Accurate Numerical Approach for Solving the Fractional Fokker-Planck Equation Under the Dirac-Delta Initial Condition and Its Applications

Qihao Ye

University of California, San Diego

The Fokker-Planck Equation (FPE), a cornerstone in statistical physics and various applied mathematics fields, has been extensively explored, leading to a profound understanding of its implications and solutions. In contrast, the Fractional Fokker-Planck Equation (FFPE), which generalizes the classic FPE by incorporating anomalous diffusion and nonlocal effects, remains an area of active and ongoing research. This study

presents an efficient and spectrally accurate numerical approach for solving the FFPE, focusing on scenarios with a Dirac-delta initial condition. The utility of this approach extends to the domain of reinforcement learning, where it underpins a model-based approach for continuous-time policy evaluation with unknown Lévy process dynamics. This application provides a first step to continuous-time model-based reinforcement learning, particularly in scenarios characterized by irregular, heavy-tailed dynamics.

50. Control of Instability in a Vlasov-Poisson System

Yukun Yue

University of Wisconsin, Madison

The Vlasov-Poisson equation serves as a fundamental model for simulating plasma dynamics. Within this framework, there exist two equilibrium states that are inherently unstable, namely the Two-Stream and Bump-on-Tail instabilities. Suppressing these instabilities is often a desirable objective in numerous practical applications. This paper aims to achieve such suppression by the implementation of an external field. When minor perturbations are introduced into these equilibrium states, they have the potential to instigate rapid growth, resulting in substantial disruptions of the equilibrium. To address this challenge, we introduce two distinct strategies for applying an external field to stabilize these inherently unstable distributions. The first strategy focuses on neutralizing the electric field generated within the plasma system. This approach effectively restricts the movement of the particles in a free-drifting state. The second strategy adopts a more comprehensive approach, leveraging linear analysis to investigate various methods for the application of the external field, inclusive of the first method. We provide numerical evidence to substantiate the efficacy of these proposed methodologies.

51. A Simple And Efficient Convex Optimization Based Bound-Preserving Limiter

Xiangxiong Zhang

Purdue University

For time-dependent PDEs, the numerical schemes can be rendered bound-preserving without losing conservation and accuracy, by a post processing procedure of solving a constrained minimization in each time step. Such a constrained optimization can be formulated as a nonsmooth convex minimization, which can be efficiently solved by first order optimization methods, if using the optimal algorithm parameters. By analyzing the asymptotic linear convergence rate of the generalized Douglas–Rachford splitting method, optimal algorithm parameters can be approximately expressed as a simple function of the number of out-of-bounds cells. We demonstrate the efficiency of

this simple choice of algorithm parameters by applying such a limiter to cell averages of a discontinuous Galerkin scheme solving phase field equations for 3D demanding problems. Numerical tests on a sophisticated 3D Cahn–Hilliard–Navier–Stokes system indicate that the limiter is high order accurate, very efficient, and well-suited for large-scale simulations. For each time step, it takes at most 20 iterations for the Douglas–Rachford splitting to enforce bounds and conservation up to the round-off error, for which the computational cost is at most 80N with N being the total number of cells. Preliminary results for compressible Navier-Stokes equations will also be reported.

52. Quantitative CT-based Cluster-informed Assessment of Airway Resistance and Particle Deposition in Asthma Patients

Xuan Zhang

University of Iowa

Joint work with Frank Li, Prathish K. Rajaraman, Alejandro P. Comellas, Eric A. Hoffman, and Ching-Long Lin.

RATIONALE: A cluster-informed computational fluid and particle dynamics (CFPD) framework is proposed to investigate airway resistance and particle deposition within clusters of pulmonary diseases, including COVID-19 survivors. Here, clusters are also known as subgroups, sub-populations, and subtypes. In this study, we apply this framework to study asthma subjects.

METHODS: The study included 42 participants with asthma who underwent CT scans, with 6 of them having Single-photon Emission Computerized Tomography (SPECT) images. Additionally, 105 participants with CT scans were recruited as healthy controls. We employed a previously established simple decision scheme based on four quantitative CT (qCT) variables to classify these subjects into four clusters. These variables are: Jacobian (deformation of an image voxel between inspiration and expiration scans), percentage of air trapped voxels (AirT%), normalized hydraulic airway diameter (D_h^*), and normalized airway wall thickness (W_T^*). The clusters were designated as follows: Cluster 1 (C1, $n = 11$), Cluster 2 (C2, $n = 14$), Cluster 3 (C3, $n = 9$), and Cluster 4 (C4, $n = 8$).

We analyzed multiscale qCT metrics, encompassing airway diameter, homothety ratio, AirT%, fSAD%, percentage of emphysema voxels (Emph%), and Jacobian within clusters. Furthermore, we assessed clinical variables such as FEV1% predicted and FEV1/FVC ratios. To predict airway resistance and particle deposition for these cluster subjects, we implemented a subject-specific whole-lung CFPD model based on CT imaging. This airway model includes about 20 generations of conducting airways and 8 generations of respiratory airways. A support vector regression model was then utilized to predict the enhancement factor, which accounts for the impact of inspiratory turbulent jet flow on particle deposition.

RESULTS: The results revealed a significant rise in AirT% solely among Asthma-C4 subjects, despite both Asthma-C4 and Asthma-C3 subjects being classified as moderate to severe asthmatics. This increase predominantly stemmed from elevated fSAD%, as indicated by the coefficients of variation (CV) derived from CFPD predictions and SPECT measurements.

CONCLUSION: The cluster-informed CFPD framework proposed here opens up new avenues for understanding the interplay between imaging, clinical, and CFPD variables in individuals with asthma. It holds promise for enhancing our understanding of the mechanisms underlying the effectiveness of inhaled medications and the impact of air pollutants on individuals, paving the way for more customized and personalized treatment approaches.

53. Learning Collective Behaviors from Observation

Ming Zhong

Illinois Institute of Technology

We present a series of learning methods used to understand collective behaviors (clustering, flocking, swarming, synchronization) from observation data. We exploit the high dimensional structure and able to achieve efficient convergence rate for our estimators. We can work on complicated geometric structure, with missing feature map and with stochastic noise. Numerical examples and theoretical insights will be given. Software demo can be also provided.

54. Efficient Uncertainty Quantification for Physics-Informed Neural Networks and Operator Learning via Ensemble Kalman Inversion

Xueyu Zhu

University of Iowa

Uncertainty quantification (UQ) for Physics Informed Neural Networks (B-PINNs) have gained significant attention for PDE-based inverse problems. Existing UQ approaches are either computationally expensive for high-dimensional posterior inference or provide unsatisfactory uncertainty estimates. In this paper, we present a new efficient inference algorithm for B-PINNs that uses Ensemble Kalman Inversion (EKI). We find that our proposed method can achieve inference results with informative uncertainty estimates comparable to Hamiltonian Monte Carlo (HMC)-based B-PINNs with a much reduced computational cost. Besides, we shall also discuss the extension of the proposed method to operator learning, such as DeepONets.