NAHOMCon'24 and NENAD '24 Program[1]

Note: i) All invited talks are at Kemeny 008,   ii) Click the title of invited talks/sessions for details

Monday, June 17

8:40 am - 9:40 am	Invited talk: Element-based Galerkin Methods in Geophysical Fluid Dynamics Modeling by Francis X. Giraldo (Naval Postgraduate School)

Location	Kemeny 006	Kemeny 007	Kemeny 008
9:40 am - 11:10 am	MS01: Summation-by-parts: building stable discretizations since 1974 Part I • M Sayyari and Nail Yamaleev (Old Dominion University): Implicit dual time-stepping positivity-preserving entropy stable schemes for the compressible Navier-Stokes equations • Jan Glaubitz (MIT): Beyond polynomials: SBP operators for general approximation spaces • Anita Gjesteland (University of Waterloo): Injected boundary conditions for the compressible Navier-Stokes equations • Eric Ching (US Naval Research Laboratory): Positivity-preserving and entropy-bounded discontinuous Galerkin method for the multicomponent, chemically reacting Navier-Stokes equations	MS02: Scientific Machine Learning for Partial Differential Equations Part I • Yanlai Chen (UMass Dartmouth): GPT-PINN and TGPT-PINN: Linear and nonlinear model order reduction toward non-intrusive Meta-learning of parametric PDEs via Physics-Informed Neural Networks • Zhongqiang Zhang (WPI): Tensor neural networks for high-dimensional Fokker-Planck equations • Khemraj Shukla (Brown): Randomized forward mode of automatic differentiation for optimization algorithms • Qiao Zhuang (WPI): Two-scale neural networks for partial differential equations with small parameters	No Event

[1]Last update: June 17, 2024. For changes/details, contact Yoonsang Lee (yoonsang.lee@dartmouth.edu)

11:10 am - 11:25 am	Break		

Location	Kemeny 006	Kemeny 007	Kemeny 008
11:25 am - 11:55 pm	MS03: Summation-by-parts: building stable discretizations since 1974 Part II • Yulia Peet (ASU): Shock Capturing Schemes in Discontinuous Galerkin Spectral Element Formulation for Euler and Navier-Stokes Equations • Yimin Lin (Rice): High order entropy stable discontinuous Galerkin spectral element methods through subcell limiting • Carolyn Pethrik (McGill): An Assessment of Fully-Discrete Entropy Stable Flux Reconstruction for Turbulent Flows • Akil Narayan (University of Utah): Energy-stable and structure-preserving schemes for the stochastic shallow water equations	MS04: Scientific Machine Learning for Partial Differential Equations Part II • Zhicheng Wang (Dalian Univ Tech): An artificial viscosity method augmented physics informed neural networks for incompressible flow at high Reynolds number • Yeonjong Shin (NCSU): tLaSDI: Thermodynamics-informed latent space dynamics identification • Victor Churchill (Trinity): Efficient Data-Driven Modeling of PDEs • Anran Jiao (Yale): One-shot learning for solution operators of partial differential equations	Contributed Talks Session 1 • Tom Hagstrom (SMU): Spectrally convergent local algorithms for non-local problems • Yann-Meing Law (Cal State Long Beach): A Hermite Method for Nonlinear Dispersive Maxwell's Equations • Andreas Buttenschoen (Univ Mass Amherst): Graph-theoretic preconditioners for centre-based tissue models • Bowei Wu (Univ Mass Lowell): Simple quadrature for near-singular integral operators

12:55 pm - 2:10 pm	Lunch (on your own)

2:10 pm - 3:10 pm	Invited talk: Trefftz and quasi-Trefftz methods for time-harmonic wave propagation and beyond by Lise-Marie Imbert-Gérard (ASU)

Location	Kemeny 006	Kemeny 007	Kemeny 008
3:10 pm - 4:40 pm	MS05: Advances in the Construction and Use of Summation-by-Parts Operators for Time-Dependent PDEs • David Kopriva (FSU): On the Stability of Discontinuous Galerkin Spectral Element Approximations for Overset Grid Problems for Hyperbolic Systems • Jason E. Hicken (RPI): Constructing diagonal-norm summation-by-parts operators on points clouds • Jesse Chan (Rice): Sparse subcell limiting for multi-dimensional SBP operators on general elements • Ngoc Cuong Nguyen (MIT): Generative Reduced Order Modeling for Parametrized Partial Differential Equations	MS06: Design and analysis of machine learning algorithms inspired by traditional numerical methods Part I • Robert Loek Van Heyningen (MIT): Adaptive reduced-order models for high-speed flow via optimal transport • Shuhao Cao (Univ Missouri-Kansas City): Efficient Hybrid Spatio-Temporal Operator Learning • Felix Ye (Univ Albany): Robust and fast differentiation for Sinkhorn optimal transport • Wenrui Hao (PSU): Nonlinear scientific computing in machine learning	Contributed Talks Session 2 • Rick Archibald (ORNL): Federated Machine Learning for Experimental Facilities • Svetlana Tokareva (LANL): Structure-preserving matrix-free finite element method • Brian Helenbrook (Clarkson Univ): Can High-Order Convergence Be Obtained for Practical Problems in Engineering? • Catherine Mavriplis (Univ Ottawa): Implementing Immersed Boundaries in Continuous and Discontinuous Spectral Element Methods with hp-Adaptivity

6:00 pm -	Pizza dinner (please confirm your attendance at registration table)

Tuesday, June 18

8:40 am - 9:40 am	Invited talk: Accelerated architectures, exascale computing, and high-order finite element methods by Noel Chalmers (AMD research)

9:40 am - 10:30 am	NENAD Invited talk: Stability with Maximal Accuracy for a Hyperbolic Equation by Gilbert Strang (MIT)

Location	Kemeny 006	Kemeny 007	Kemeny 008
10:30 am - 12:00 pm	MS07: Advances in Bayesian scientific computing and its applications • Mirjeta Pasha (Tufts): Bayesian and Deterministic Methods with Edge-Preserving Priors for Spatio-Temporal Large-Scale Inverse Problems • Mathieu Le Provost (MIT): Preserving linear invariants in ensemble filtering methods • Abhishek Balakrishna (Univ South Calif): A regularity criterion for the 3D Navier-Stokes equations based on finitely many observations • Chenyi Fei (MIT): Bayesian inference of biological dynamics	MS08: Next-generation solvers using fast and high-order accurate integral equation methods • David Krantz (KTH): Accurate approximation of layer potentials evaluated near axisymmetric surfaces • Oscar Bruno (Caltech): Frequency- and Time-domain Green function methods for electromagnetic simulation, optimization, and design • Eduardo Corona (Univ Colorado Boulder): Fast algorithms for Stokesian rigid body suspensions • Thomas G. Anderson (Rice): Fast, provably high-order accurate methods for volume integral operators	Contributed Talks Session 3 • Shanyin Tong (Columbia): Policy iteration method for inverse mean field games • Ben Southworth (LANL): High-order time integration for nonlinearly partitioned multiphysics • Tongtong Li (Dartmouth): A structurally informed data assimilation approach for discontinuous state variables • Duk-Soon Oh (Chungnam Nat Univ): New Analysis of Overlapping Schwarz Methods for Vector Field Problems in Three Dimensions with Generally Shaped Domains

12:00 pm - 1:20 pm	Lunch (Dartmouth Dining Hall)

1:20 pm - 2:20 pm	Invited talk: Exponentially-convergent simulations of extreme-mass-ratio binary black hole systems: A discontinuous Galerkin method for the Teukolsky equation with singular source terms by Scott Field (University of Massachusetts Dartmouth)

Location	Kemeny 006	Kemeny 007	Kemeny 008
2:20 pm - 3:50 pm	MS09: Matrix-free Methods for Advanced High-Fidelity Simulations • Yohann Dudouit (LLNL): Overcoming the Curse of Dimensionality: Matrix-Free, High-Order Discontinuous Galerkin Methods for Advection-Diffusion in Phase Space • Tim Warburton (Virginia Tech): GPU optimization of an implicitly time-stepped high-order finite element wave solver • Yu-Hsiang Lan (UIUC): Low-Order Preconditioning for SEM-Based Advection-Diffusion Problems • Jihun Han (Dartmouth College): A stochastic approach for solving PDEs: multiscale problems and perforated domain problems	MS10: Design and analysis of machine learning algorithms inspired by traditional numerical methods Part II • Donsub Rim (Washington Univ St Louis): Low Rank Neural Representation (LRNR) for model reduction of nonlinear conservation laws • Yue Yu (Lehigh University): Projection method for causal discovery • Jonathan Siegel (TAMU): Approximation Rates for Shallow ReLU^k Neural Networks on Sobolev and Besov Spaces • Panos Stinis (PNNL): Multifidelity Scientific Machine Learning	Career Panel: Professionals working in academia, national labs, and industry will discuss various aspects of their work environment and answer questions about what steps are needed to pursue careers in these different areas Panels: Sigal Gottlieb, Andrew Christlieb, Catherine Macriplis, Svetlana Tokareva, Carol Woodward, Noel Chalmers

3:50 pm - 6:00 pm	Poster Session with Snacks (First Floor, Kemeny)

6:00 pm -	Banquet (Patio outside of Kemeny)

Wednesday, June 19

8:40 am - 9:40 am	Invited talk: High Order Adaptive Time Integration Methods and Application Through the SUNDIALS Library by Carol Woodward (LLNL)

Location	Kemeny 006	Kemeny 007	Kemeny 008
9:40 am - 11:10 am	**MS11: Recent Advances in Finite Element Methods for Flow Problems** • Yang Yang (Michigan Tech Univ): A reinterpreted discrete fracture model for Darcy-Forchheimer flow in fractured porous media • • Raven Shane Johnson (Rice): High order entropy stable methods for blood flow simulations • Lu Zhang (Rice): An energy-based discontinuous Galerkin method for stochastic wave equations in second-order form	**MS12: High-order methods for computational relativity** • Geoffrey Lovelace (Calif State Univ Fullerton): Simulating binary black holes with higher order methods using SpECTRE • Keefe Mitman (Caltech): Extracting physics from black hole simulations with Cauchy-characteristic evolution • Sizheng Ma (Perimeter Institute): Higher order boundary conditions in numerical relativity through Cauchy-characteristic matching • Francois Foucart (Univ New Hampshire): Simulating binary neutron star mergers with mixed Discontinuous Galerkin - Finite Volume methods	**Contributed Talks Session 4** • Gustaaf Jacobs (SDSU): High-order Lagrangian algorithms for Liouville models • Catherine Mavriplis (Univ Ottawa): A Parallel hp-Adaptive Discontinuous Galerkin Spectral Element Method Solver for Acoustic Problems in Curvilinear Geometries with Dynamic Load Balancing • Jonah A Reeger (Air Force Insititute of Technology): Local Adaptivity in Kernel Methods • Ngoc Cuong Nguyen (MIT): Discontinuous Galerkin Methods for Hypersonic Flows

11:10 am - 11:25 am	Break

Location	Kemeny 006	Kemeny 007	Kemeny 008
11:25 am - 12:55 pm	Contributed Talks Session 5 • Zheng Sun (University of Alabama): The Runge–Kutta Discontinuous Galerkin Method with Stage-Dependent Polynomial Spaces for Hyperbolic Conservation Laws • Bosu Choi (Dartmouth College): Enhanced data assimilation based on the energy spectrum of nonlinear chaotic dynamics • Phil Roe (University of Michigan): Stencils and Representations that Promote High-Order Accuracy • Iman Samani (University of Michigan): Fifth-order Active Flux Methods for Wave Propagation	MS13: Highly Accurate Machine Learning Methods for Solving PDEs • Wei Zhu (UMass Amherst): Data-driven discovery of independent conservation laws through neural deflation • Zezheng Song (Univ Maryland): A Finite Expression Method for Solving High-Dimensional Committor Problems • Shikai Fang (Univ Utah): Solving High Frequency and Multi-Scale PDEs with Gaussian Processes • Lizuo Liu (Dartmouth): DeepProp-Net - A Recursive Deep Neural Network Propagator for Learning Evolutionary PDE Operators	No Event

12:55 pm - 2:10 pm	Lunch (Dartmouth Dining Hall)

2:10 pm - 3:10 pm	Invited talk: The need for mathematical innovation around design and optimization of non-equilibrium plasmas by Andrew Christlieb (MSU)

Invited Talks

Element-based Galerkin Methods in Geophysical Fluid Dynamics Modeling

Francis X. Giraldo (Naval Postgraduate School)

In this talk, I will present the role that element-based Galerkin (EBG) methods have had in GFD but more specifically in atmospheric modeling. I will describe the experiences of my group and collaborators to remedy the identified weaknesses and emphasize the strengths. Among EBG methods, I will describe not only spectral element and discontinuous Galerkin methods, but also flux differencing which invariably must include a discussion on kinetic-energy-preserving and entropy-stable methods. I will also touch on the time-integration strategies required for constructing efficient solutions for global, regional, and Large-Eddy-Simulation (LES) modeling and will show results for these regimes. I will briefly discuss the future of these methods in regards to the changing landscape in high-performance computing and discuss our experience with using neural networks to represent LES processes in GFD models.. This talk is motivated by my group and collaborators' research in building operational weather prediction models as well as advancing the field for application in climate, space weather, and ocean dynamics. A list of publications on these topics can be found at: `https://frankgiraldo.wixsite.com/mysite/` publications.

Trefftz and quasi-Trefftz methods for time-harmonic wave propagation and beyond

Lise-Marie Imbert-Gérard (Arizona State University)

In the field of numerical partial differential equations (PDEs), many methods rely on standard bases, like polynomial bases, but other methods rely on problem-dependent bases. Trefftz methods rely, in broad terms, on the idea of approximating solutions to PDEs via Galerkin-type formulations discretized with basis functions solving exactly the governing PDE locally, making explicit use of information about the ambient medium. They are of particular interest for wave propagation problems, for example with plane wave bases with the wave number depending on the propagation medium. The presentation will start with an introduction to Trefftz methods. However, in general, for problems modeled by PDEs with variable coefficients, no exact solutions are available. Hence quasi-Trefftz methods have been introduced to address this problem: they rely not on exact solutions to the PDE but instead on high order approximate solutions constructed locally. We will discuss some of the fundamental properties of these numerical methods for problems governed by the Helmholtz equation. Finally we highlight the main difficulty in developing quasi-Trefftz methods for time-harmonic electromagnetic wave propagation, and present recent developments to problems governed by a class of elliptic equations.

Accelerated architectures, exascale computing, and high-order finite element methods

Noel Chalmers (AMD research)

The use of accelerators has become ubiquitous in the largest supercomputers in the world, typically providing much higher main memory bandwidth and floating-point operations per second (FLOPS) than their host CPUs. In modern accelerators, specialized sections of hardware, such as matrix cores, further accelerate certain computational workloads leading to increased FLOPS throughput and power efficiency. For finite element methods, which are very often bound by main memory bandwidth, such specialized hardware does not appear to offer much potential performance benefit or is not easily leveraged. On the other hand, high-order methods have operations which naturally map to matrix cores and see significant performance gains. In this talk, I will discuss performance modelling and bottlenecks of high-order finite element operations on accelerators, the details of matrix cores and their architecture, and show how the use of matrix cores can significantly improve the performance of some of these operator kernels.

NENAD Invited talk: Stability with Maximal Accuracy for a Hyperbolic Equation

Gilbert Strang (MIT)

We describe a long-ago result for explicit difference methods of maximum accuracy for the simplest hyperbolic equation $du/dt = du/dx$. Lax and Wendroff compute each value $U(t + \Delta t, n\Delta x)$ from three previous values $U(t, (n + k)\Delta x), k = -1, 0, 1$. This has 2nd order accuracy and it is stable for $\Delta t \leq \Delta x$. The extension uses $2N + 1$ previous values $k = -N$ to N at each step. Its accuracy is of order $2N$. The key question is stability: It is stable for $\Delta t \leq \Delta x$ but not for $\Delta t \leq N\Delta x$.

Exponentially-convergent simulations of extreme-mass-ratio binary black hole systems: A discontinuous Galerkin method for the Teukolsky equation with singular source terms

Scott Field (University of Massachusetts Dartmouth)

Gravitational wave signals from extreme mass ratio binary (EMRB) systems are a crucial target for space-based gravitational wave detectors. In such systems, a smaller black hole orbits around a supermassive black hole. These systems are typically modeled as a

distributionally-forced Teukolsky equation that describes the evolution of spacetime metric perturbations and gravitational radiation emitted to the far-field. This equation poses two computational challenges: (i) the source terms feature not only a Dirac delta distribution but also its first, second, and third derivatives and (ii) we need to supply appropriate outer boundary conditions (conditions of complete transparency) and access the far-field signal on a finite computational domain. In this talk, we describe a multi-domain discontinuous Galerkin method for this problem. To handle the Dirac delta, we expand the solution in spherical harmonics and recast the sourced Teukolsky equation as a first-order system by using distributional auxiliary variables. This allows us to derive the method's numerical flux to correctly account for the distributional right-hand side and achieve spectral convergence even at the location of the distributional source terms. To connect the near-field to the distant far-field, we use the hyperboloidal layer method, allowing us to supply outer boundary conditions and provide direct access to the gravitational wave signal. We also observe superconvergence in the extracted gravitational waveform. Several benchmark numerical examples will be presented. Linear wave equations with source terms containing Dirac delta functions and their derivatives occur in other areas of engineering and physics, and generalizations of our method to other PDEs sourced by arbitrary nth-order derivatives of a Dirac delta distribution will also be discussed.

High Order Adaptive Time Integration Methods and Application Through the SUNDIALS Library

Carol S. Woodward (LLNL), Cody J. Balos (LLNL), David J. Gardner (LLNL)
Daniel R. Reynolds (SMU), and Steven B. Roberts (LLNL)

The SUNDIALS library of time integrators and nonlinear solvers has long provided adaptive step and order linear multistep time integration methods. Several years ago, the ARKODE package of additive multistage methods allowing for high order, adaptive diagonally implicit, explicit, and implicit/explicit (ImEx) methods was added to SUNDIALS. Recently, we have released new implementations of multirate methods which allow for advancing partitions of the differential equation right-hand-side function with a small time step and other partitions with a large time step, yet still retaining high order accuracy. I will overview the SUNDIALS library, including its high order, adaptive implementations of multistep, multistage, and multirate methods then show examples of their use within several scientific applications.

The need for mathematical innovation around design and optimization of non-equilibrium plasmas

Andrew Christlieb (Michigan State University)

Many of the viable fusion energy concepts involve control of non equilibrium plasmas. When seeking to optimize such systems, one needs models that go beyond the classic 5 moment model of gas dynamics (fluid models). The introduction of "kinetic" equations for modeling these systems revolves around the need to describe instabilities that are not captured by 5 moment models. With in these systems, the goal is to understand and mitigate non-equilibrium effects so as to maximize energy output. There are two key challenges around using kinetic models in this context. The first challenge is the curse of dimensionality. Kinetic models are naturally 6 dimensional plus time, and therefore traditional methods scale as $O(N^6)$. The second challenge is the need for structure and asymptotic preserving methods that permit the bridging of scales. Often there are key physical scale links both in space and time that one would like to step over in most settings but adaptively adjust under certain circumstances.

In this talk I will highlight the need for new mathematical innovation around scale bridging algorithms in fusion energy applications. I will then outline work being carried out by the Center for Hierarchical and Robust Modeling of Non-Equilibrium Transport (CHaRMNET) aimed at addressing the two key fundamental challenges. Finally, I outline highlight our work within CHaRMNET around blended computing as one approach to addressing the curse of dimensionality in a structure preserving context. Blended computing is the systematic hybridization of machine learning with traditional scientific computing. As stability is key in long time predictions, our approach to the design of machine learning surrogates in blended computing is to design surrogates such that they are mathematically consistent with the equations being solved. Here I will talk about this approach in the context of seeking to design scale bridging algorithms to study fuel optimization within capsules used in inertial confinement fusion systems.

MS01: Summation-by-parts: building stable discretizations since 1974 Part I

Organizers: Jason Hicken (RPI), Jesse Chan (Rice)
Time: 9:40 am - 11:10 am, Mon June 17
Abstract: Summation-by-parts (SBP) operators are high order finite difference discretizations that were originally designed to mimic finite-element energy analysis techniques. In recent years, this idea has been generalized to a variety of other spatial discretizations including finite volumes, flux reconstruction, and continuous/discontinuous Galerkin (DG) methods. These generalizations have also been paired with techniques for constructing semi-discretely energy and entropy stable discretizations of nonlinear hyperbolic PDEs. This minisymposium collects talks related to the discretization of PDEs using SBP related methods, as well as the the construction of novel discretizations related to the SBP framework.

1. M Sayyari and Nail Yamaleev (Old Dominion University): Implicit dual time-stepping positivity-preserving entropy stable schemes for the compressible Navier-Stokes equations

   In this talk, we present a generalization of the explicit high-order positivity-preserving entropy stable spectral collocation schemes developed in [J. Upperman & N. K. Yamaleev, J. Sci. Comp., Vols. 94(1) and 95(1), 2023] for the 3-D compressible Navier-Stokes equations to a time implicit formulation. The time derivative is discretized by using the 1st-order implicit backward difference formula (BDF) that is well suited for solving steady state problems considered in this study. To solve the nonlinear system of equations arising from the BDF1 discretization at each time step, a dual time-stepping technique with the explicit 1st-order forward Euler approximation in the pseudo-time is used. This dual time-stepping strategy allows us to combine unconditional stability properties of the implicit time integrator with the positivity and entropy stability properties of the baseline explicit spectral collocation scheme, while providing the design-order of accuracy at the steady state. Numerical results demonstrating efficiency and positivity-preserving properties of the new dual time-stepping schemes are presented for steady viscous flows with strong shock waves and contact discontinuities.

2. Jan Glaubitz (MIT): Beyond polynomials: SBP operators for general approximation spaces

   Solving time-dependent partial differential equations (PDEs) is vital in many fields. Preserving the PDEs' critical structures during discretization enhances the accuracy and robustness of numerical methods, especially for advection-dominated problems. Summation-by-parts (SBP) operators, which mimic integration-by-parts discretely, play a crucial role in this. They facilitate transferring stability estimates from the continuous to the discrete level.

   While traditional SBP operators assume polynomial approximations of PDE solutions, there's an increasing demand for non-polynomial methods. Radial basis function (RBF) schemes and neural network-based approximations are notable examples.

   In this talk, we develop a theory for function-space SBP (FSBP) operators that extend the structure-preserving benefits of polynomial SBP operators to a wider range of function spaces, allowing for more flexibility and applicability.

   This talk is based on joint work with Jan Nordström and Philipp Öffner.

Keywords: Advection-dominated PDEs, stability, summation-by-parts operators, non-polynomial function spaces

3. Anita Gjesteland (University of Waterloo): Injected boundary conditions for the compressible Navier-Stokes equations

Summation-by-parts (SBP) operators are used for numerically approximating the solutions of partial differential equations (PDEs) due to their important stability properties. However, when studying initial-boundary-value problems, the operators must be used in conjunction with stable boundary procedures. The simultaneous approximation term (SAT) has traditionally been used for this purpose in the SBP community, and this technique can be used to prove stability for a wide range of problems.

As an alternative to the SAT, we study here the stability properties for SBP schemes approximating the compressible Navier-Stokes equations where the no-slip condition is imposed using the injection method. That is, the boundary nodes are overwritten with the exact boundary data after each Runge-Kutta stage. The results presented herein are an extension of [1], in that we consider general multidimensional SBP operators as defined in [2] which do not pose any restrictions on the operators' accuracy, and may also be defined on unstructured grids. We present the methodology by considering the linear advection-diffusion equation, and illustrate how the proof carries over to the compressible Navier-Stokes equations.

[1] A. Gjesteland and M. Svärd. Entropy stability for the compressible NavierStokes equations with strong imposition of the no-slip boundary condition. Journal of Computational Physics, 470, 111572, 2022. [2] J. E. Hicken, D. C. Del Rey Fernández and D. W. Zingg. Multidimensional summation-by-parts operators: general theory and application to simplex elements. SIAM Journal on Scientific Computing, Vol. 38, No. 4, 2016.

4. Eric Ching (US Naval Research Laboratory): Positivity-preserving and entropy-bounded discontinuous Galerkin method for the multicomponent, chemically reacting Navier-Stokes equations

This talk presents a positivity-preserving and entropy-bounded discontinuous Galerkin method for the multicomponent, chemically reacting Navier-Stokes equations. To handle stiff chemical reactions, operator splitting is employed, which divides each time step into a transport step and a reaction step. In the transport step, which includes the convective and diffusive operators, entropy boundedness is enforced in a rigorous manner on only the convective contribution to the evolved state, as motivated by the minimum entropy principle satisfied by entropy solutions to the multicomponent Euler equations. To guarantee discrete satisfaction of the minimum entropy principle in the reaction step, we introduce an entropy-stable discontinuous Galerkin method based on diagonal-norm summation-by-parts operators for solving ordinary differential equations. Additional challenges associated with simulating multicomponent, reacting flows in a robust manner will be discussed. The resulting formulation is compatible with curved, multidimensional elements and general quadrature rules with positive weights. Complex reacting flows in two and three dimensions are computed with variable thermodynamics and detailed chemistry, including moving detonation waves and shock/mixing-layer interaction.

MS02: Scientific Machine Learning for Partial Differential Equations Part I

Time: 9:40 am - 11:10 am, Mon June 17
Organizers: Zhongqiang Zhang (WPI), Qiao Zhuang (WPI)
Abstract: Scientific machine learning (SciML) have been widely explored for solving Partial Differential Equations (PDEs) by efficiently combining machine learning techniques with scientific principles and data. In this mini-symposium, we aim to explore underlying mathematical principles of SciML and the applications of SciML in solving PDEs. The topics include stability and error analysis and training strategies for SciML, and architectures of neural networks and more. Additionally, we will address how SciML can be employed to deal with hyperbolic systems, multiscale problems, interface problems, and high-dimensional PDEs.

1. Yanlai Chen (UMass Dartmouth): GPT-PINN and TGPT-PINN: Linear and nonlinear model order reduction toward non-intrusive Meta-learning of parametric PDEs via Physics-Informed Neural Networks

   Physics-Informed Neural Network (PINN) has proven itself a powerful tool to obtain the numerical solutions of nonlinear partial differential equations (PDEs) leveraging the expressivity of deep neural networks and the computing power of modern heterogeneous hardware. However, its training is still time-consuming, especially in the multi-query and real-time simulation settings, and its parameterization often overly excessive.

   In this talk, we present the recently proposed Generative Pre-Trained PINN (GPT-PINN) and the Transformed GPT-PINN (TGPT-PINN). They mitigate both challenges in the setting of parametric PDEs. As a network of networks, GPT-PINN's outer-/meta-network is hyper-reduced with only one hidden layer having significantly reduced number of neurons. Moreover, its activation function at each hidden neuron is a (full) PINN pre-trained at a judiciously selected system configuration. The meta-network adaptively "learns" the parametric dependence of the system and "grows" this hidden layer one neuron at a time. In the end, by encompassing a very small number of networks trained at this set of adaptively-selected parameter values, the meta-network is capable of generating surrogate solutions for the parametric system across the entire parameter domain accurately and efficiently. While GPT-PINN represents a linear model order reduction strategy, TGPT-PINN achieves nonlinear model reduction via the addition of a transformation layer before the pre-trained PINN layer.

2. Zhongqiang Zhang (WPI): Tensor neural networks for high-dimensional Fokker-Planck equations

   We use tensor-neural networks for high-dimensional Fokker-Planck equations, where the solutions are of small scales but not negligible in regions. The use of tensor feedforward networks allows us to efficiently exploit auto-differentiation in major Python packages while using tensor radial basis functions can fully avoid auto-differentiation, which is rather expensive in high dimensions. We demonstrate numerically that the tensor neural networks in physics-informed machine learning are efficient for steady-state Fokker-Planck equations from two to ten dimensions.

3. Khemraj Shukla (Brown): Randomized forward mode of automatic differentiation for optimization algorithms

Here I present a randomized forward mode gradient (RFG) as an alternative to backpropagation. RFG is a random estimator for the gradient that is constructed based on the directional derivative along a random vector. The forward mode automatic differentiation (AD) provides an efficient computation of RFG. The probability distribution of the random vector determines the statistical properties of RFG. Through the second moment analysis, we found that the distribution with the smallest kurtosis yields the smallest expected relative squared error. By replacing gradient with RFG, a class of RFG-based optimization algorithms is obtained. By focusing on gradient descent (GD) and Polyak's heavy ball (PHB) methods, we present a convergence analysis of RFG-based optimization algorithms for quadratic functions. Computational experiments are presented to demonstrate the performance of the proposed algorithms and verify the theoretical findings.

4. Qiao Zhuang (WPI): Two-scale neural networks for partial differential equations with small parameters

We propose a two-scale neural network method for solving PDEs with small parameters using physics-informed neural networks (PINNs). We directly incorporate the small parameters into the architecture of neural networks. The proposed method enables solving PDEs with small parameters in a simple fashion, without adding Fourier features or other computationally taxing searches of truncation parameters. Various numerical examples demonstrate reasonable accuracy in capturing features of large derivatives in the solutions caused by small parameters.

MS03: Summation-by-parts: building stable discretizations since 1974 Part II

Organizers: Jason Hicken (RPI), Jesse Chan (Rice)
Time: 11:25 am - 12:55 pm, Mon June 17

Abstract: Summation-by-parts (SBP) operators are high order finite difference discretizations that were originally designed to mimic finite-element energy analysis techniques. In recent years, this idea has been generalized to a variety of other spatial discretizations including finite volumes, flux reconstruction, and continuous/discontinuous Galerkin (DG) methods. These generalizations have also been paired with techniques for constructing semi-discretely energy and entropy stable discretizations of nonlinear hyperbolic PDEs. This minisymposium collects talks related to the discretization of PDEs using SBP related methods, as well as the the construction of novel discretizations related to the SBP framework.

1. Yulia Peet (ASU): Shock Capturing Schemes in Discontinuous Galerkin Spectral Element Formulation for Euler and Navier-Stokes Equations

   In this talk, we discuss the performance of two shock capturing schemes introduced in a Discontinuous Galerkin Spectral Element Method (DGSEM) as applied to Euler and Navier- Stokes Equations. The developed DGSEM methodology is based on a split formulation of the convective terms and utilizes diagonal norm summation by parts operators, which ensures entropy stability properties. For the discretization of the viscous terms, the Bassi-Rebay (BR1) scheme is employed. For shock capturing, we consider two popular strategies. The first one is based on the entropy viscosity formulation, and the second implements a sub-element order reduction via blending a high-order DG flux with a low-order sub-cell finite-volume flux combined with the second-order reconstruction utilizing a minmod limiter. A shock indicator based on the modified Ducros sensor is proposed for the second approach, which was found to be more suitable for viscous shocked flows than popular alternatives conventionally employed in inviscid flows. The performance of the two shock capturing approaches is compared and the limitations of the presented methodologies are discussed. A number of test cases computed with the developed methodology, featuring weak and strong shocks, shock-boundary layer interaction, and a supersonic turbulent flow over a sphere are discussed.

2. Yimin Lin (Rice): High order entropy stable discontinuous Galerkin spectral element methods through subcell limiting

   Subcell limiting strategies for discontinuous Galerkin spectral element methods do not provably satisfy a semi-discrete cell entropy inequality. In this work, we introduce an extension to the subcell and monolithic convex limiting strategies that satisfies the semi-discrete cell entropy inequality by formulating the limiting factors as solutions to an optimization problem. The optimization problem is efficiently solved using a deterministic greedy algorithm. We also discuss the extension of the proposed subcell limiting strategy to preserve general convex constraints. Numerical experiments confirm that the proposed limiting strategy preserves high-order accuracy for smooth solutions and satisfies the cell entropy inequality.

3. Carolyn Pethrik (McGill): An Assessment of Fully-Discrete Entropy Stable Flux Reconstruction for Turbulent Flows

   Entropy-stable high-order methods add robustness to high-fidelity applications. By providing provable nonlinear stability for arbitrarily long simulation times, entropy-stable methods compare favorably to stabilization methods such as adding artificial

viscosity, using flux limiters, over-integrating the nonlinear flux, or filtering the solution. We use the nonlinearly-stable flux reconstruction scheme (NSFR) of Cicchino et al.[1], and use the relaxation Runge-Kutta method as developed by Ketcheson[2] and Ranocha et al.[3] to formulate a fully-discrete NSFR scheme. The fully discrete NSFR scheme benefits from the increased time step size of flux reconstruction schemes and the robustness of entropy stable methods. The computational cost and applicability to unsteady, turbulent flows are investigated using the TGV test case. We present comparisons of implicit temporal integration to explicit methods, evaluating the feasibility of implicit FD-NSFR for turbulent flows. The presented results highlight that FD-NSFR can improve robustness in viscous simulations. Using implicit temporal integration methods in conjunction with fully-discrete NSFR will enable much larger time step sizes while preserving nonlinear stability properties. Ultimately, the combination could reduce the computational cost of high-fidelity simulations in the aerospace industry.

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[3] Ranocha, H., Sayyari, M., Dalcin, L., Parsani, M., & Ketcheson, D. I. (2020). Relaxation Runge–Kutta methods: Fully discrete explicit entropy-stable schemes for the compressible Euler and Navier–Stokes equations. SIAM Journal on Scientific Computing, 42(2), A612-A638.

4. Akil Narayan (University of Utah): Energy-stable and structure-preserving schemes for the stochastic shallow water equations

The shallow water equations (SWE) are an important set of equations describing fluid flow in a simplified ""shallow water"" setting. These equations are a system of time-dependent, nonlinear hyperbolic balance laws, whose solution can be used to model impact and events resulting from hurricanes and tsunamis. In practice, the environment or initial conditions may be imprecisely known due to incomplete information, or uncertain due to a stochastic model. One effective strategy for propagating this input uncertainty forward through the SWE is the stochastic Galerkin method via polynomial Chaos. An outstanding challenge with numerical methods arising from this approach is that the model may lose important physical structure of the solution. For example, the stochastic Galerkin formulation of the SWE is frequently not a hyperbolic system, and positivity of the water height variable is not guaranteed.

We present novel advances in stochastic Galerkin methods for the SWE system. We show that a known elegant connection in the deterministic case between water height positivity and hyperbolicity of the equations can be extended to the stochastic/uncertain case. We leverage this theoretical connection to develop structure-preserving numerical methods for these equations: Our algorithms ensure positivity of the water height, hyperbolicity of the stochastic Galerkin formulation, and obey the well-balanced property, ensuring stable simulation of certain steady-state solutions. We demonstrate the effectiveness of the algorithm for simulations in one and two spatial dimensions, and describe high order energy conservative and energy stable schemes that are derived from entropy-entropy flux pairs.

MS04: Scientific Machine Learning for Partial Differential Equations Part II

Organizers: Zhongqiang Zhang (WPI), Qiao Zhuang (WPI)
Time: 11:25 am - 12:55 pm, Mon June 17
Abstract: Scientific machine learning (SciML) have been widely explored for solving Partial Differential Equations (PDEs) by efficiently combining machine learning techniques with scientific principles and data. In this mini-symposium, we aim to explore underlying mathematical principles of SciML and the applications of SciML in solving PDEs. The topics include stability and error analysis and training strategies for SciML, and architectures of neural networks and more. Additionally, we will address how SciML can be employed to deal with hyperbolic systems, multiscale problems, interface problems, and high-dimensional PDEs.

1. Zhicheng Wang (Dalian Univ Tech): An artificial viscosity method augmented physics informed neural networks for incompressible flow at high Reynolds number

   Physics-informed neural networks (PINNs) have emerged as a new simulation paradigm for fluid flows and are especially effective for inverse and hybrid problems. However, vanilla PINNs often fail in forward problems, especially at high Reynolds (Re) number flows. Herein, we study systematically the classical lid-driven cavity flow at Re=2,000, 3,000 and 5,000. We observe that vanilla PINNs obtain two classes of solutions, one class that agrees with direct numerical simulations (DNS), and another that is an unstable solution to the Navier-Stokes equations and not physically realizable. We attribute this solution multiplicity to singularities and unbounded vorticity, and we propose regularization methods that restore a unique solution within 1% difference from the DNS solution. In particular, we introduce a parameterized entropy-viscosity method as artificial eddy viscosity and identify suitable parameters that drive the PINNs solution towards the DNS solution. Furthermore, we solve the inverse problem by subsampling the DNS solution, and identify a new eddy viscosity distribution that leads to velocity and pressure fields almost identical to their DNS counterparts. Surprisingly, a single measurement at a random point suffices to obtain a unique PINNs DNS-like solution even without artificial viscosity, which suggests possible pathways in simulating high Reynolds number turbulent flows using vanilla PINNs. In addition, the PINNs with artificial viscosity is extend to solving the mixed/natural convection in a lid-driven cavity up to Re=2000, Pr=3.0 and Ri=0.1, good agreement to the ground truth is achieved.

2. Yeonjong Shin (NCSU): tLaSDI: Thermodynamics-informed latent space dynamics identification

   We present a thermodynamics-informed latent space dynamics identification (tLaSDI) method for learning an intrinsic invariant manifold which comply with the first and second principles of thermodynamics from data. The approach utilizes an autoencoder to provide a nonlinear latent representation and the reconstruction of the high-dimensional data, and the corresponding latent space dynamics are captured using GENERIC formalism informed neural networks (GFINNs). The GFINNs are designed to exactly satisfy the degeneracy condition of the GENERIC formalism, ensuring that the latent space dynamics adhere to fundamental thermodynamics principles. In addition, we develop a novel loss formulation based on rigorous error estimates, which significantly improve the generalization performance.

3. Victor Churchill (Trinity College): Efficient Data-Driven Modeling of PDEs

The flow map learning framework is capable of learning the evolution of unknown ordinary and partial differential equations systems given access to observations of solution vectors. For partially-observed systems, a memory period is required to learn the reduced system. If the solution vector is high-dimensional and a long memory period is required, the model input can become burdensome. E.g., if the solution vector is observed on a 50x50 grid and needs 20 memory steps, then the input will be of dimension 50,000. For neural network based models, a high-dimensional input greatly increases the number of hidden parameters in the model regardless of the complexity of the function being modeled. This in turn requires more data to appropriately learn the hidden parameters without overfitting. In contrast, real world problems frequently require modeling with limited data. Therefore, it is desirable to be able to model complex systems with fewer parameters. This talk will discuss several new approaches to this issue.

4. Anran Jiao (Yale): One-shot learning for solution operators of partial differential equations

Learning and solving governing equations of a physical system, represented by partial differential equations (PDEs), from data is a central challenge in a variety of areas of science and engineering. Current methods require either some prior knowledge (e.g., candidate PDE terms) to discover the PDE form, or they need a large dataset to learn a surrogate model of the PDE solution operator. Here, we propose the first solution operator learning method that only requires one PDE solution, i.e., one-shot learning. We first decompose the entire computational domain into small domains, where we learn a local solution operator, and then we find the solution of a new input function via mesh-based fixed-point iteration (FPI), meshfree local-solution-operator informed neural network (LOINN) or local-solution-operator informed neural network with correction (cLOINN). We tested our method on 7 different PDEs, including linear or nonlinear PDEs, PDEs defined on complex geometries, and PDE systems. Our method demonstrates effectiveness and generalization capabilities across these varied scenarios.

MS05: Advances in the Construction and Use of Summation-by-Parts Operators for Time-Dependent PDEs

Time: 3:10 pm - 4:40 pm, Mon June 17
Organizers: Jan Glaubitz (MIT), Jan Nordstrom (Linköping University)

Abstract: In the numerical solution of partial differential equations (PDEs), the efficiency benefits of higher-order methods are well-known. Their superiority becomes even more pronounced as the error tolerance of a computation tightens. Particularly in computational fluid dynamics, higher-order methods are frequently used for time-dependent problems that demand high resolution. Among the various higher-order spatial discretizations for PDEs, summation-by-parts (SBP) operators combined with weak enforcement of boundary and interface conditions stand out. This minisymposium aims to bring together experts on summation-by-parts operators and numerical PDEs. It seeks to highlight recent advancements, stimulate discussion, and foster new and existing collaborations.

1. David Kopriva (FSU): On the Stability of Discontinuous Galerkin Spectral Element Approximations for Overset Grid Problems for Hyperbolic Systems

   "Overset grid methods accommodate complex geometries by overlapping simpler geometry-fitted grids. Stability of the procedures used to couple the grids has long been a practical and theoretical issue, especially at high order. To date, proofs of stability are not available. One of the difficulties is that the underlying partial differential equations (PDEs) described on the overset domains are not necessarily well-posed, even when characteristic boundary conditions are applied at the grid boundaries. Well-posed PDE formulations for linear systems in one or two space dimensions that use penalties along the overlap boundaries were presented in [1]. Entropy stable formulations were presented in [2].

   The proof of well-posedness of the penalty formulation of the overset domain problem relies on the fact that integration by parts applies to any subdomain. Discrete approximations, e.g. the Discontinuous Galerkin Spectral Element Method (DGSEM), satisfy at best a summation by parts (SBP) property over a fixed domain (e.g. element), so one cannot mimic the proof of well-posedness discretely to show stability. So what can one say about stability? We study this in the context of the DGSEM approximation by deriving energy bounds and the eigenvalue structure. We target the DGSEM because it is of arbitrary (high) order, it satisfies an SBP property, it intrinsically defines interpolations, and it approximates weak forms of the equations.

   We show by way of the energy method that even though the DGSEM is stable for hyperbolic boundary-value problems, and the overset domain problem is well-posed in an appropriate norm, the energy of the approximation is bounded by data only for fixed polynomial order and time. In the absence of dissipation, the coupling of the overlapping domains is itself destabilizing by allowing positive eigenvalues in the discrete system that is integrated in time. These eigenvalues can be stabilized in one space dimension by using the upwind numerical flux. To provide additional dissipation, we introduce a novel penalty method applied at arbitrary points within the overlap region that depends on the difference between the solutions. We present numerical experiments to illustrate the implementation of the well-posed penalty formulation, and show spectral convergence of the approximations when dissipation is applied.

   [1] David A. Kopriva, Jan Nordström and Gregor J. Gassner, ""On the theoretical foundation of overset grid methods for hyperbolic problems: Well-posedness and conservation", Journal of Computational Physics, 448:110732, 2022.

[2] David A. Kopriva, Gregor J. Gassner and Jan Nordström, ""On the theoretical foundation of overset grid methods for hyperbolic problems II: Entropy bounded formulations for nonlinear conservation laws", Journal of Computational Physics, 471:111620, 2022."

2. Jason E. Hicken (RPI): Constructing diagonal-norm summation-by-parts operators on points clouds

   We present an algorithm for building high-order, diagonal-norm, first-derivative summation-by-parts (SBP) operators on point clouds distributed over complex geometries. A Cartesian cut-cell mesh is used to define the sparsity pattern of the operator and to provide quadrature rules, but the mesh is extraneous once the SBP operator has been constructed. Using this temporary mesh, we construct local, cell-based SBP difference operators, which are then assembled into a global operator. The coordinates of the degrees of freedom are optimized to ensure the diagonal mass matrix is positive definite; we propose a low-rank inverse Hessian approximation to find the modified coordinates. We also describe an artificial dissipation operator that complements the first-derivative operator when solving hyperbolic problems. The algorithm is verified and illustrated using numerical experiments.

3. Jesse Chan (Rice): Sparse subcell limiting for multi-dimensional SBP operators on general elements

   Algebraic flux correction methods blend high and low order methods together to ensure that the solution satisfies physical constraints while maintaining conservation and accuracy. For high order summation-by-parts (SBP) operators on tensor product elements, this blending can be done by recasting the high and low order schemes into a "subcell finite volume" formulation. However, this recasting relies heavily on the tensor product structure of the resulting multi-dimensional operators, and cannot be directly extended to more general domains (e.g., simplices).

   In this talk, we will review the construction of low order multi-dimensional SBP operators, use them to construct bounds preserving discretizations on more general elements, and introduce a generalization of the subcell finite volume formulation to simplices based on these low order multi-dimensional SBP operators.

4. Ngoc Cuong Nguyen (MIT): Generative Reduced Order Modeling for Parametrized Partial Differential Equations

   The offline stage of developing reduced-order models (ROMs) for parametrized partial differential equations (PDEs) is crucial, as it involves gathering a comprehensive set of snapshots that capture the underlying PDEs' behavior under various conditions. However, the need to update an existing ROM with additional snapshots poses a significant challenge due to the high computational costs associated with solving the parametrized PDEs anew. This process not only demands extensive computational resources but also considerable time, especially for complex systems with high-dimensional parameter spaces. To address this challenge and mitigate the computational burden, we introduce a generative reduced order modeling (GROM) to enhance the predictive capabilities and accuracy of an existing ROM without generating new snapshots from the full-order model. The main ingredients of our GROM approach include reduced basis approximation, nonlinear lifting operator, Taylor expansion, and proper orthogonal decomposition. We present several numerical examples to illustrate the proposed GROM.

MS06: Design and analysis of machine learning algorithms inspired by traditional numerical methods Part I

Time: 3:10 pm - 4:40 pm, Mon June 17
Organizers: Yanlai Chen (UMass Dartmouth)
Abstract: Machine learning, especially Deep Neural Networks (DNN), has gained increasing attention in the field of numerical methods for differential equation. While many of these DNN-based approaches are perceived to be alternatives to traditional numerical methods such as finite difference, finite element, and spectral methods, these classical approaches have undergone more than half a century of rigorous and systematic development. How do we leverage the best of both worlds? This minisymposium aims to gather experts to discuss novel approaches bridging the classical numerical methods and the more nascent machine learning approaches. We will cover both theoretical and computational aspects of approaches sitting on this interface for solving various PDE models including real-world physical applications.

Talks:

1. Robert Loek Van Heyningen (MIT): Adaptive reduced-order models for high-speed flow via optimal transport

   The simulation of high-speed flow problems with parametrically varying shocks poses challenges for high-fidelity discretization methods and surrogate model construction. We propose an r-adaptive mesh adaptation method to aid in the accurate resolution of flows with strong shocks and the development of reduced-order models of these same flows. Using high-order solutions of the Monge-Ampère equation, grid nodes of a fixed reference mesh are redistributed towards features that require more resolution. When applied to parametrized PDEs, each solution snapshot includes a solution field and a corresponding grid deformation. The mapping defining the grid movement can be used to pull the solution back onto the reference mesh. Here, sharp and local features will be smoothed out and made more globally distributed over the domain, making them more suitable for linear model reduction methods like the proper orthogonal decomposition. Surrogate models can then efficiently be built on the reference mesh for the solution field and grid mappings. The efficiency of this approach is shown for supersonic and hypersonic flows with parametrized boundary conditions.

2. Shuhao Cao (Univ Missouri-Kansas City): Efficient Hybrid Spatio-Temporal Operator Learning

   Recent advancements in operator-type neural networks, such as Fourier Neural Operator (FNO), have shown promising results in approximating the solutions of nonlinear spatio-temporal Partial Differential Equations (PDEs). However, these neural networks often entail considerable training expenses, and may not always achieve the desired accuracy required in many scientific and engineering disciplines. In this paper, we propose a new operator learning framework to address these issues. The proposed paradigm leverages the traditional wisdom from numerical PDE theory, spectral methods, and nonlinear multigrid techniques to refine the pipeline of existing operator neural networks. Numerical experiments on a com-monly used benchmark of 2D Navier-Stokes equations demonstrate significant improvements in both computational time and accuracy, compared to existing FNO variants and traditional numerical approach-es. This is joint work with Francesco Brarda (Emory), Yuanzhe Xi (Emory), and Ruipeng Li (LLNL).

3. Felix Ye (Univ Albany): Robust and fast differentiation for Sinkhorn optimal transport

In shuffled regression problem, the corresponding between input and output data is missing. Such problem is commonly observed in real world situations. The most popular computational framework for this problem is the relaxed smooth bi-level optimization, where the inner optimization is celebrated Sinkhorn algorithms. We developed a robust and fast method to calculate the first and second order derivative of the outer optimization analytically. This approach enables us to apply the Newton's method in the outer optimization and significantly speeds up when the optimization is stiff. We will demonstrate the effectiveness of our algorithm through numerical examples.

4. Wenrui Hao (PSU): Nonlinear scientific computing in machine learning

Machine learning has seen remarkable success in various fields such as image classification, speech recognition, and medical diagnosis. However, this success has also raised intriguing mathematical ques-tions about optimizing algorithms more efficiently and applying machine-learning techniques to address complex mathematical problems. In this talk, I will discuss the neural network model from a nonlinear scientific computing perspective and present recent work on developing a homotopy training algorithm to train neural networks layer-by-layer and node-by-node. I will also showcase the use of neural network discretization for solving nonlinear partial differential equations.

MS07: Advances in Bayesian scientific computing and its applications

Time: 10:30 am - 12:00 pm, Tue Jun 18
Organizers: Tongtong Li (Dartmouth), Jan Glaubitz(MIT)

Abstract: The continued development of high-order numerical methods has made it possible to simulate many mathematical models with high accuracy. Still, in many applications, predictions by these models remain uncertain, with the leading source or errors now being model discrepancies and corrupted input data. Bayesian methodologies, which model the unknown parameters and observations as random variables and endow them with specific probability distributions, stand out in addressing these challenges. The Bayesian approach not only provides additional insights but also enables robust uncertainty quantification in computed solutions and model predictions, enjoying widespread popularity and applications across diverse fields. In practical applications, due to the intricate structure of the underlying system and the variable quality of the observational data – often noisy, indirect, or under-sampled, the fundamental question of effectively utilizing the information from both prior knowledge and observations remains a challenge. This mini-symposium serves as a convergence point for researchers specializing in Bayesian methods and scientific computing, fostering interdisciplinary discussions and exploring intersections with various disciplines. It seeks to highlight recent advancements, stimulate discussion, and foster new and existing collaborations.

1. Mirjeta Pasha (Tufts): Bayesian and Deterministic Methods with Edge-Preserving Priors for Spatio-Temporal Large-Scale Inverse Problems

   Rapidly-growing fields such as data science, uncertainty quantification, and machine learning rely on fast and accurate methods for inverse problems. Three emerging challenges on obtaining relevant solutions to large-scale and data-intensive inverse problems are ill-posedness of the problem, large dimensionality of the parameters, and the complexity of the model constraints. Tackling the immediate challenges that arise from growing model complexities (spatiotemporal measurements) and data-intensive studies (large-scale and high-dimensional measurements collected as time-series), state-of-the-art methods can easily exceed their limits of applicability. For instance, on reconstructing a sequence of time-dependent objects with discontinuity or singularity, e.g. dynamic computerized tomography (CT) images with edges, traditional methods based on Gaussian processes (GP) do not provide satisfactory solutions since they tend to offer over-smooth prior candidates. Edge-preserving constraint has received considerable attention due to the need for reconstructing high-quality and sharp images.

   In this talk we discuss recent advancements on edge-preserving and computationally efficient methods for computing solutions to dynamic inverse problems, where both the quantities of interest and the forward operator change at different time instances. In the first part of the talk, to remedy these difficulties, we apply efficient regularization methods that enforce simultaneous regularization in space and time (such as edge enhancement at each time instant and proximity at consecutive time instants) and achieve this with low computational cost and enhanced accuracy. In the remainder of the talk, we focus on designing spatio-temporal Bayesian Besov priors for computing the MAP estimate and quantifying the uncertainties for large-scale and dynamic inverse problems. Numerical examples from a wide range of applications are used to illustrate the effectiveness of the described methods. (This talk is mainly

based on two manuscripts. The first is joint work with Arvind Saibaba, Silvia Gazzola, Malena Espanol, and Eric de Sturler. The second is joint work with Shiwei Lan and Shuyi Li).

2. Mathieu Le Provost (MIT): Preserving linear invariants in ensemble filtering methods

Formulating dynamical models for physical phenomena is essential for understanding the interplay between the different mechanisms, predicting the evolution of physical states, and developing effective control strategies. However, a dynamical model alone is often insufficient to address these fundamental tasks, as it suffers from model errors and uncertainties. One common remedy is to rely on data assimilation, where the state estimate is updated with observations of the true system. Ensemble filters sequentially assimilate observations by updating a set of samples over time. They operate in two steps: a forecast step that propagates each sample through the dynamical model and an analysis step that updates the samples with incoming observations. For accurate and robust predictions of dynamical systems, discrete solutions must preserve their critical invariants. While modern numerical solvers satisfy these invariants, existing invariant-preserving analysis steps are limited to Gaussian settings and are often not compatible with classical regularization techniques of ensemble filters, e.g., inflation and covariance tapering. The present work focuses on preserving linear invariants, such as mass, stoichiometric balance of chemical species, and electrical charges. Using tools from measure transport theory (Spantini et al., 2022, SIAM Review), we introduce a generic class of nonlinear ensemble filters that automatically preserve desired linear invariants in non-Gaussian filtering problems. By specializing this framework to the Gaussian setting, we recover a constrained formulation of the Kalman filter. Then, we show how to combine existing regularization techniques for the ensemble Kalman filter (Evensen, 1994, J. Geophys. Res.) with the preservation of the linear invariants. Finally, we assess the benefits of preserving linear invariants for the ensemble Kalman filter and nonlinear ensemble filters.

3. Abhishek Balakrishna (Univ South Calif): A regularity criterion for the 3D Navier-Stokes equations based on finitely many observations

Data assimilation is a technique that combines observational data with a given model to improve the model's accuracy. We first discuss the application of a particular data assimilation technique (AOT algorithms) to the 3-D Navier-Stokes equation (3D NSE); we then describe how a data assimilated solution approximates the true solution. Then we observe the data assimilated solution is, in fact, regular (i.e., a strong solution) when the observed data satisfies a condition we present for only a finite collection of data. This result suggests a connection between our condition and the regularity of solutions to the actual 3D NSE. We pursue this line of inquiry to confirm this hypothesis, and formulate such a regularity criterion for the 3D NSE purely in terms of finitely-observed data.

4. Chenyi Fei (MIT): Bayesian inference of biological dynamics

Biological dynamics, spanning from the molecular to the ecosystem level, are fundamental to all life processes. Recent advancements in imaging technologies have enabled long-term tracking of biological dynamics at the single-cell level. These measurements not only deepen our understanding of many biological processes but also open opportunities for developing quantitative models. In this talk, I will present a data-driven framework that combines basis-function representations with sparse Bayesian inference to learn stochastic-differential-equation (SDE) models for various biological dynamics. I will demonstrate the broad applicability of

our framework to various biological time-series data, highlighting the novel insights it brings to understanding unicellular division, mosquito flight, mice limb control, and starfish embryo aggregation.

MS08: Next-generation solvers using fast and high-order accurate integral equation methods

Time: 10:30 am - 12:00 pm, Tue Jun 18
Organizers: Thomas G. Anderson (Rice)

Abstract: Integral equation methods have historically faced multiple challenges that stymie broader adoption: (1) the need for delicate singular quadratures (2) efficient application of dense operators and the need for fast direct solvers (3) limitations for volumetric and nonlinear problems, and (4) a limited software ecosystem. This minisymposium will feature progress on many of these problems, including real-world scientific and engineering applications.

1. David Krantz (KTH): Accurate approximation of layer potentials evaluated near axisymmetric surfaces

   Layer potentials represent solutions to partial differential equations in an integral equation formulation. When numerically evaluating layer potentials at target points close to the domain boundary, specialized quadrature techniques are required for accuracy because of the rapid variations in the integrand. With the goal of efficiently achieving results within a specified error tolerance, we introduce an adaptive quadrature method with automatic parameter adjustment, facilitated through error estimation. This approach is tailored for axisymmetric surfaces, employing a trapezoidal rule in the azimuthal angle and a Gauss-Legendre quadrature rule in the polar angle. Notably, while each surface must be axisymmetric, the integrand need not be, thus enabling application to complex geometries featuring multiple axisymmetric shapes. The adaptive quadrature method utilizes so-called interpolatory semi-analytical quadrature in conjunction with a singularity swap technique in the azimuthal angle. In the polar angle, such a technique is utilized as needed, depending on the integral kernel, in combination with an adaptive subdivision of the integration interval.

   Estimates for both quadrature and interpolation errors are derived by complex analysis to complement existing error estimates. For each evaluation point close to the surface, an error estimate is used to determine if the special quadrature method is needed to meet the error tolerance, and if so, to perform the adaptive panel subdivision, and in some instances, to decide on which approach should be utilized to evaluate a certain quantity. Numerical examples are presented to elucidate the method's efficacy.

2. Oscar Bruno (Caltech): Frequency- and Time-domain Green function methods for electromagnetic simulation, optimization, and design

   We present a family of numerical methods for the solution of Maxwell's equations, with application to simulation, optimization, and design. In particular, a novel rectangular-polar integral equation solver is mentioned which can produce solutions to the time harmonic Maxwell's equations, with high order accuracy, for general 2D and 3D structures, with an extension to time domain problems on the basis of a time re-centering synthesis technique. An effective integral equation acceleration method, the IFGF method (Interpolated Factored Green Function), is used, which evaluates the action of Green function-based integral operators for an -point surface discretization at a computational cost of $O(N \log(N))$ operations without recourse to the FFT – thus, lending itself to effective distributed memory parallelization. Computational illustrations include applications to photonic optimization and design.

3. Eduardo Corona (Univ Colorado Boulder): Fast algorithms for Stokesian rigid body suspensions

   A wide range of applications in science and industry, from the study of cell mechanics to smart material design involve understanding how "soft matter" works, and more specifically, the study and simulation of viscous fluid suspensions. In this talk, we will discuss recent developments on our framework using boundary integral methods to simulate dense rigid body suspensions, including work on fast algorithms for singular and near singular evaluation of integral operators on spheroidal suspensions and work in optimization solvers for contact resolution.

4. Thomas G. Anderson (Rice): Fast, provably high-order accurate methods for volume integral operators

   Volume integral operators (VIOs) are fundamental tools for solving volumetric problems with integral equation methods, including wave scattering problems in inhomogeneous media. We will discuss a treatment using Green's third identity and a local polynomial interpolant of the density function that transforms a VIO into regularized VIOs (as well as layer potentials, and a polynomial PDE solution): the (globally!) regularized operators can be evaluated to provably high-order accuracy using entirely generic volumetric quadrature and can make efficient use of fast algorithms. Detailed error and stability analysis is provided in two dimensions for this regularizing effect, including connections to quadrature of functions of limited regularity at isolated points, and the guarantees will provide a point of contrast with the "locally-corrected" (near-)singular correction methods in widespread use.

MS09: Matrix-free Methods for Advanced High-Fidelity Simulations

Time: 2:20 pm - 3:50 pm, Tue Jun 18
Organizers: Yohann Dudouit (LLNL)

Abstract: The advent of matrix-free methods has marked a significant milestone in computational simulations, offering substantial improvements in performance and memory efficiency. These methods, eschewing the traditional assembly of large sparse matrices, are pivotal in large-scale, high-fidelity simulations in various scientific and engineering fields. This mini-symposium is dedicated to exploring the cutting-edge developments in matrix-free methods, with a focus on addressing both their advantages and challenges. It aims to create a collaborative platform for researchers to discuss innovations in matrix-free preconditioners and solvers, and to showcase their practical applications in high-fidelity physics simulations. The mini-symposium will include:

- Presentations on the latest advancements in matrix-free algorithms, emphasizing their performance and memory efficiency.

- Discussions on the challenges of developing suitable preconditioners and solvers for matrix-free methods, sharing solutions and best practices.

- Case studies highlighting the application of matrix-free methods in complex simulations, demonstrating their advantages and addressing their limitations.

1. Yohann Dudouit (LLNL): Overcoming the Curse of Dimensionality: Matrix-Free, High-Order Discontinuous Galerkin Methods for Advection-Diffusion in Phase Space

   The challenge of solving high-dimensional physics problems, such as advection-diffusion in phase space, necessitates computational strategies that effectively mitigate the curse of dimensionality. Following the steps of the Center for Efficient Exascale Discretizations (CEED) project, the matrix-free, high-order Discontinuous Galerkin (DG) approach presented in this talk offers a powerful solution. It provides potential speedups in computational efficiency on the order of p^d , where p represents the polynomial order of the discretization, and d denotes the dimensionality of the space, when compared to traditional sparse matrix approaches. This methodology significantly reduces data movement, a critical factor in enhancing scalability on high-performance computing architectures. By directly addressing these problems in high dimensions, our approach contributes to the reduction of typical numerical artifacts, such as ray effects, which are often show stoppers in traditional simulations. This capability enables the use of deterministic methods in domains where Monte Carlo methods are typically preferred. In this talk, we will explain how we have constructed our high-dimension, high-order, matrix-free, discontinuous Galerkin method and present encouraging performance results.

2. Tim Warburton (Virginia Tech): GPU optimization of an implicitly time-stepped high-order finite element wave solver

   "It is quite common in the literature to pair an explicit time integrator with a high-order finite element spatial discretization when solving the acoustic wave equation. In this scenario the time step restriction is $dt \leq C_{TS} \frac{h}{N^2}$ where C_{TS} is a constant depending on the time-stepping method, h is the smallest element size, N is the polynomial degree. In this talk we will compare the relative

performance of high-order explicit Runge-Kutta and implicit Runge-Kutta Nystr"om time integrators [6] when paired with high-order nodal continuous or discontinuous spatial discretizations. I will present computational results demonstrating that the implicit time-stepping treatment can be advantageous on the GPU if we use highly optimized matrix-free linear solvers combined with a multigrid preconditioner [5], effective initial guess algorithms [3], [2] and aggressive stopping conditions [1], [4].

[1] Mario Arioli, Daniel Loghin, and Andy J Wathen. Stopping criteria for iterations in finite element methods. Numerische Mathematik, 99:381–410, 2005.

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3. Yu-Hsiang Lan (UIUC): Low-Order Preconditioning for SEM-Based Advection-Diffusion Problems

Simulating steady state solutions for advection-diffusion has been of great interest to engineers in order to bypass long transients in thermal fluids applications in complicated domains. The steady advection-diffusion equation is the main system for conjugate heat transfer and for the linearized incompressible Navier-Stokes equations. One challenge to developing a preconditioner of such problems is the boundary layer caused by small diffusivity which raises extra stability issues.

In this work, we deploy a low-order preconditioner for the steady advection diffusion operator based on the existing collocation points of the spectral element method (SEM). It is feasible to construct the full preconditioner since the number of nonzeros of the low-order matrix in d space dimensions is only $O(N^d)$ rather than $O(N^{2d})$ for the Nth-order SEM matrix (which is not formed). In the low-order formulation, the convective term is dealiased with a 3-point Gauss rule in order to ensure skew-symmetry. Several local reordering strategies are discussed to reduce the fill of the LU or ILU solver. The solver combines the polynomial preconditioner to further reduce the iteration numbers and computational time. We provide numerical results for parameter studies and compare our solver with traditional time advancing schemes for benchmark cases from nuclear engineering applications.

4. Jihun Han (Dartmouth): A stochastic approach for solving PDEs: multiscale problems and perforated domain problems

A wide range of applications in science and engineering involve a PDE model in a domain with perforations, such as perforated metals or air filters. Solving such perforated domain problems suffers from computational challenges related to resolving the scale imposed by the geometries of perforations. We propose a neural network-based mesh-free approach for perforated domain problems. The method is robust and efficient in capturing various configuration scales, including the averaged macroscopic behavior

of the solution that involves a multiscale nature induced by small perforations. The new approach incorporates the derivative-free loss method that uses a stochastic representation or the Feynman-Kac formulation. In particular, we implement the Neumann boundary condition for the derivative-free loss method to handle the interface between the domain and perforations. A suite of stringent numerical tests is provided to support the proposed method's efficacy in handling various perforation scales.

This is joint work with Yoonsang Lee at Dartmouth College.

MS10: Design and analysis of machine learning algorithms inspired by traditional numerical methods Part II

Time: 2:20 pm - 3:50 pm, Tue Jun 18
Organizers: Yanlai Chen (UMass Dartmouth)
Abstract: Machine learning, especially Deep Neural Networks (DNN), has gained increasing attention in the field of numerical methods for differential equation. While many of these DNN-based approaches are perceived to be alternatives to traditional numerical methods such as finite difference, finite element, and spectral methods, these classical approaches have undergone more than half a century of rigorous and systematic development. How do we leverage the best of both worlds? This minisymposium aims to gather experts to discuss novel approaches bridging the classical numerical methods and the more nascent machine learning approaches. We will cover both theoretical and computational aspects of approaches sitting on this interface for solving various PDE models including real-world physical applications.

1. Donsub Rim (Washington Univ St Louis): Low Rank Neural Representation (LRNR) for model reduction of nonlinear conservation laws

   Model reduction for hyperbolic PDEs using classical techniques is difficult due to the slow decay in the Kolmogorov n-width, making it necessary to explore new forms of approximation. We will discuss a new approach using deep neural networks endowed with a particular low-rank structure which we call Low Rank Neural Representation (LRNR). A LRNR is a family of implicit neural representation in which the weights and biases belong to linear spaces of small dimensions. We will show that entropy solutions to scalar conservation laws can be represented efficiently by such a representation. Numerical examples il-lustrating the efficacy of the neural network will be shown, and we will also discuss applications of LRNRs regarding the so-called failure modes of Physics Informed Neural Networks (PINNs).

2. Yue Yu (Lehigh University): Projection method for causal discovery

   Automatic discovery of directed acyclic graph (DAG) structure is important in many causal inference tasks. However, learning a DAG from observed samples of an unknown joint distribution is generally a challenging combinatorial problem. A recent breakthrough formulates the problem as a continuous optimization with a structural constraint that ensures acyclicity constraint (NOTEARS [1]), which enables a suite of continuous optimization techniques to be used for DAG learning problems.

   In this talk, we take a step further to propose new continuous optimization algorithms without acyclicity constraints to improve the continuous optimization-based DAG learning framework on both efficiency and accuracy. We first show that the weighted adjacency matrix of a DAG can be represented as the Hadamard product of a skew-symmetric matrix and the gradient of a potential function on graph vertices, and vice versa. As such, a DAG can be seen as a weighted curl-free graph, and each (possibly cyclic) graph can be written as the summation of an acyclic component and the remaining component, using the Helmholtz-Hodge decomposition. Based on that, a fast projection method, DAG-NoCurl, is developed to formulate DAG learning as a continuous optimization approach without constraints [2]. Experimental studies on benchmark datasets demonstrate that our method provides comparable accuracy but better efficiency, often by more than one order of magnitude. To further improve the accuracy, we combine DAG-NoCurl

with a variational autoencoder structure parameterized by a graph neural network architecture [3], to capture complex nonlinear mappings and data types. We demonstrate that the proposed method is capable of handling datasets with either continuous or discrete variables, and it learns more accurate graphs for samples with more complex distributions.

References: [1] Zheng, X., Aragam, B., Ravikumar, P., Xing, E. P. DAGs with NO TEARS: Continuous Optimization for Structure Learning. Advances in Neural Information Processing Systems (NeurIPS), 2018.

[2] Yu, Y., Gao, T., Yin, N., Ji, Q. DAGs with No Curl: An Efficient DAG Structure Learning Approach. In International Conference on Machine Learning (pp. 12156-12166). PMLR., 2021

[3] Yu, Y., Chen, J., Gao, T., Yu, M. DAG-GNN: DAG structure learning with graph neural networks. In International Conference on Machine Learning (pp. 7154-7163). PMLR. 2019

3. Jonathan Siegel (TAMU): Approximation Rates for Shallow ReLU^k Neural Networks on Sobolev and Besov Spaces

   Shallow ReLU^k neural networks, also known as ridge splines, are an important and well-studied ap-proximation method in machine learning. Nonetheless, there remain interesting and important open ques-tions concerning their precise approximation properties. In this talk, we will consider the problem of how efficiently shallow ReLU^k neural networks can approximate functions from the Sobolev space $W^s(L_q)$ with error measured in the L_p norm. In particular, we will present recent progress which provides a complete solution to this problem in the linear regime where $p \leq q$. We will also discuss the extension to Besov spaces and the difficulties in resolving the non-linear regime where $p > q$, which remains an intriguing open problem.

4. Panos Stinis (PNNL): Multifidelity Scientific Machine Learning

   In many applications across science and engineering it is common to have access to disparate types of da-ta or models with different levels of fidelity. In general, low-fidelity data are easier to obtain in greater quantities, but it may be too inaccurate or not dense enough to accurately train a machine learning model. High-fidelity data is costly to obtain, so there may not be sufficient data to use in training, however, it is more accurate. A small amount of high-fidelity data, such as from measurements or simulations, com-bined with low fidelity data, can improve predictions when used together. The important step in such con-structions is the representation of the correlations between the low- and high-fidelity data. In this talk, we will present two frameworks for multifidelity machine learning. The first one puts particular emphasis on operator learning, building on the Deep Operator Network (DeepONet). The second one is inspired by the concept of model reduction. We will present the main constructions along with applications to closure for multiscale systems and continual learning. Moreover, we will discuss how multifidelity approaches fit in a broader framework which includes ideas from deep learning, stochastic processes, numerical meth-ods, computability theory and renormalization of complex systems.

MS11: Recent Advances in Finite Element Methods for Flow Problems

Time: 9:40 am - 11:10 am, Wed Jun 19
Organizers: Zheng Sun (Univ Alabama), Ziyao Xu (Univ Notre Dame)
Abstract: Finite element methods have emerged as pivotal tools for addressing complex flow problems across diverse domains. Our minisymposium, "Recent Advances in Finite Element Methods for Flow Problems," aims to bring together researchers, experts, and enthusiasts to explore cutting-edge developments in the field of computational fluid dynamics with finite element methods. The talks will encompass both computational and analytical dimensions, providing perspectives on recent advancements in the field. With a special focus on the development of discontinuous Galerkin methods, the minisymposium aims to delve into the intricacies of this versatile approach. Researchers will share insights into the application and analysis of discontinuous Galerkin methods, showcasing their efficacy in tackling challenging flow problems. Additionally, the event will touch upon other finite element methods, offering a well-rounded exploration of the field's recent progress.

1. Yang Yang (Michigan Tech Univ): A reinterpreted discrete fracture model for Darcy-Forchheimer flow in fractured porous media

    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.

2. Ziyao Xu (University of Alabama): An interior penalty discontinuous Galerkin (IDPG) method for an interface model of flows in fractured media

    Flow and transport in cracked rocks are of great interest in many scientific and engineering applications. In the context of subsurface flow, fractures can act either as highly permeable, flow-preferential channels or as low-permeability, flow-blocking barriers; both have a tiny lateral dimension but a significant impact on the hydraulic properties of rocks. In this talk, we present and analyze an interior penalty discontinuous Galerkin (IPDG) method for an interface model of flows in fractured media. Unlike existing works on discontinuous Galerkin discrete fracture models based on interface models, our method does not introduce additional equations and degrees of freedom to account for the flows on fracture interfaces, thus it is more efficient. In particular, the modeling

of low-permeability barriers is even cost-free. The stability and optimal h-p error estimates are established for the proposed IPDG method. Numerical experiments based on published benchmarks are performed to validate the theoretical analysis and demonstrate the good performance of the method. Extensions to two-phase flow are also investigated and presented.

3. Raven Shane Johnson (Rice): High order entropy stable methods for blood flow simulations

The blood flow equations are a 1D nonlinear hyperbolic system which serves as a reduced model of arterial blood flow. We are interested in constructing entropy stable discontinuous Galerkin (DG) methods for this system, which enforce a semi-discrete cell entropy inequality while retaining high order accuracy. An entropy stable method for the blood flow equations was introduced by Burger, Valbuena, and Vega [(2023). Numer. Methods Partial Differ. Eq.. 39, 2491–2509] using primitive variables. We propose an entropy stable DG method for the blood flow equations based on conservative variables, based on a new condition for entropy stability introduced in Chan, Shukla, et al. [(2024). Journal of Computational Physics, 112876] that eases the analysis of non-conservative terms in the 1D blood flow equations.

4. Lu Zhang (Rice): An energy-based discontinuous Galerkin method for stochastic wave equations in second-order form

In this talk, we present an energy-based discontinuous Galerkin method to approximate stochastic wave equations in second-order form, which is an efficient high-order scheme. We study the stability for the proposed semidiscrete DG methods. Error estimates in the energy norm for certain numerical fluxes are obtained for smooth solutions. Numerical experiments are performed to confirm the analytical results.

MS12: High-order methods for computational relativity

Time: 9:40 am - 11:10 am, Wed Jun 19
Organizers: Vijay Varma (UMass Dartmouth)

Abstract: Higher order methods like spectral methods have played a central role in numerical relativity simulations of black hole mergers. The gravitational wave signals extracted from the simulations have provided the most accurate predictions for the signals observed by detectors like LIGO. However, to keep up with the demands of future detectors like LISA in space, there is a need for at least an order of magnitude improvement in simulation accuracy over the next decade. This mini-symposium will cover the latest developments in numerical relativity aiming to address this need, from high-accuracy simulations of black hole and neutron star mergers to accurate gravitational waveform extraction methods.

1. Geoffrey Lovelace (Calif State Univ Fullerton): Simulating binary black holes with higher order methods using SpECTRE

   Binary black holes are among the most important sources of gravitational waves. Learning as much as possible from gravitational-wave observations of binary black holes requires accurate models of the expected waves—and these models require numerical relativity. A new generation of gravitational-wave observatories, including Cosmic Explorer, Einstein Telescope, and the Laser Interferometer Space Antenna, will be so sensitive that numerical-relativity models will need to achieve an order of magnitude increase in accuracy; otherwise, limitations in our models will limit how much we can learn from the next-generation detectors' observations. SpECTRE is a next-generation numerical-relativity code under active development that seeks to achieve the high accuracy that future detectors will require through combining a discontinuous-Galerkin method with task-based parallelism. In this talk, I will discuss SpECTRE's recent progress toward simulating merging black holes, including SpECTRE's first complete calculation of black holes as they spiral together, merge, and ring down to a final, stationary black hole.

2. Keefe Mitman (Caltech): Extracting physics from black hole simulations with Cauchy-characteristic evolution

   Evolving Einstein's equations from some finite volume region to the asymptotic boundary of spacetime—future null infinity—using spectral methods offers a robust and efficient means for providing accurate solutions to GR. In this talk, I will present a means for performing such an evolution using a technique called Cauchy-characteristic evolution (CCE). I will show that, with CCE, not only can one obtain more accurate gravitational wave solutions to important astrophysical phenomena, such as the merging of black holes, but one can also resolve key physics—like memory effects—that other waveform extraction schemes cannot. This highlights the fact that, for future gravitational wave observations, using waveforms computed with CCE, or similar computational methods, will be absolutely vital for testing Einstein's theory of GR and probing the astrophysical content of our Universe.

3. Sizheng Ma (Perimeter Institute): Higher order boundary conditions in numerical relativity through Cauchy-characteristic matching

   Two major approaches are used when numerically solving the Einstein field equations. The first one is to use spatial Cauchy slices and treat the system as a standard Cauchy initial value problem. Characteristic evolution serves as the second approach, which evolves spacetime based on null hypersurfaces. The Cauchy formulation is well-suited for strong gravitational fields, yet extending

it to the wave zone increases computational expense. Conversely, the Characteristic approach demonstrates efficiency in the wave zone but encounters limitations near binary systems due to the caustics of null surfaces. By combining those two techniques — simulating the inner region with Cauchy evolution and the outer region with characteristic evolution, Cauchy-Characteristic matching (CCM) enables us to take advantage of both methods. In this talk, I present our recent implementation of CCM based on a numerical relativity code SpECTRE. I also discuss how CCM improves the accuracy of Cauchy boundary conditions — a benefit that allows us to evolve less of the wave zone in the Cauchy code without losing precision.

4. Francois Foucart (Univ New Hampshire): Simulating binary neutron star mergers with mixed Discontinuous Galerkin - Finite Volume methods

Discontinuous Galerkin (DG) methods offer the potential for high-order, scalable evolutions of colliding black holes and neutron stars. In the presence of neutron stars, however, shocks and surface discontinuities have limited our ability to carry out stable and accurate evolutions of these systems with DG methods. In this talk, I will present our recent extension, within the Spectre code, of a mixed DG-finite volume (FV) scheme in which FV elements replace DG elements when the solution is no longer sufficiently smooth. I will show that this allowed us to perform the first simulations of a binary neutron star inspiral and merger using a DG code, and I will discuss the accuracy and performance of the Spectre code for these evolutions.

MS13: Highly Accurate Machine Learning Methods for Solving PDEs

Time: 11:25 am - 12:55 pm, Wed Jun 19
Organizers: Keenan Eikenberry (Dartmouth), Lizuo Liu (Dartmouth), Tongtong Li (Dartmouth)
Abstract: This mini-symposium explores the intersection of machine learning and computational mathematics for solving Partial Differential Equations (PDEs). We will showcase recent advancements in this field. Discussions will focus on challenges, opportunities, and the development of reliable methodologies, fostering collaboration to enhance accuracy and efficiency in modeling complex physical systems.

Talks:

1. Wei Zhu (UMass Amherst): Data-driven discovery of independent conservation laws through neural deflation

   We introduce a methodology for seeking conservation laws within a Hamiltonian dynamical system, which we term "neural deflation." Inspired by deflation methods for steady states of dynamical systems, we propose to iteratively train a number of neural networks to minimize a regularized loss function accounting for the necessity of conserved quantities to be in involution and enforcing functional independence thereof consistently in the infinite-sample limit. The method is applied to a series of integrable and nonintegrable lattice differential-difference equations. In the former, the predicted number of conservation laws extensively grows with the number of degrees of freedom, while for the latter, it generically stops at a threshold related to the number of conserved quantities in the system. This data-driven tool could prove valuable in assessing a model's conserved quantities and its potential integrability.

2. Zezheng Song (Univ Maryland): A Finite Expression Method for Solving High-Dimensional Committor Problems

   " Transition path theory (TPT) is a mathematical framework for quantifying rare transition events between a pair of selected metastable states A and B. Central to TPT is the committor function, which describes the probability to hit the metastable state B prior to A from any given starting point of the phase space. Once the committor is computed, the transition channels and the transition rate can be readily found. The committor is the solution to the backward Kolmogorov equation with appropriate boundary conditions. However, solving it is a challenging task in high dimensions due to the need to mesh a whole region of the ambient space. In this work, we explore the finite expression method (FEX, Liang and Yang (2022)) as a tool for computing the committor. FEX approximates the committor by an algebraic expression involving a fixed finite number of nonlinear functions and binary arithmetic operations. The optimal nonlinear functions, the binary operations, and the numerical coefficients in the expression template are found via reinforcement learning. The FEX-based committor solver is tested on several high-dimensional benchmark problems. It gives comparable or better results than neural network-based solvers. Most importantly, FEX is capable of correctly identifying the algebraic structure of the solution which allows one to reduce the committor problem to a low-dimensional one and find the committor with any desired accuracy."

3. Shikai Fang (Univ Utah): Solving High Frequency and Multi-Scale PDEs with Gaussian Processes

   Machine learning based solvers have garnered much attention in physical simulation and scientific computing, with a prominent example, physics-informed neural networks (PINNs). However, PINNs often struggle to solve high-frequency and multi-scale

PDEs, which can be due to the spectral bias during neural network training. To address this problem, we resort to the Gaussian process (GP) framework. To flexibly capture the dominant frequencies, we model the power spectrum of the PDE solution with a student mixture or Gaussian mixture. We then apply inverse Fourier transform to obtain the covariance function (according to the Wiener-Khinchin theorem). The covariance derived from the Gaussian mixture spectrum corresponds to the known spectral mixture kernel. We are the first to discover its rationale and effectiveness for PDE solving. Next, we estimate the mixture weights in the log domain, which we show is equivalent to placing a Jeffreys prior. It automatically induces sparsity, prunes excessive frequencies, and adjusts the remaining toward the ground truth. Third, to enable efficient and scalable computation on massive collocation points, which are critical to capture high frequencies, we place the collocation points on a grid, and multiply our covariance function at each input dimension. We use the GP conditional mean to predict the solution and its derivatives so as to fit the boundary condition and the equation itself. As a result, we can derive a Kronecker product structure in the covariance matrix. We use Kronecker product properties and multilinear algebra to greatly promote computational efficiency and scalability, without any low-rank approximations. We show the advantage of our method in systematic experiments.

4. Lizuo Liu (Dartmouth): DeepPropNet - A Recursive Deep Neural Network Propagator for Learning Evolutionary PDE Operators

"In this work, we propose a deep neural network ap- proximation to the evolution operator for time dependent PDE sys- tems over long time period by recursively using one single neural network propagator, in the form of POD-DeepONet with built-in causality feature, for a small time interval. The trained DeepProp- Net of moderate size is shown to give accurate prediction of wave solutions over the whole time interval."

Contributed Talks Session 01

Time: 11:25 am - 12:55 pm, Mon Jun 17

1. Tom Hagstrom (SMU): Spectrally convergent local algorithms for nonlocal problems

   Nonlocal operators, in particular space-time integral operators, arise in various applications. A primary example is the radiation boundary condition needed to truncate an unbounded domain to a finite one to enable numerical solutions, as well as closely-related operators for unidirectional propagation. In this work we show how to leverage results from rational function approximation theory, in particular results on optimal approximations to Markov functions, to construct spectrally-convergent local algorithms for evaluating such operators. For an important class of problems - systems equivalent to the scalar wave equation, such as acoustics or Maxwell's equations in homogeneous, isotropic media, we will explain the construction, analysis, and implementation of our complete radiation boundary conditions, which are in a certain sense optimal. We will also discuss other applications of these approximation methods, as well as the fundamental barriers to extending the successful methods to other systems.

2. Yann-Meing Law (Cal State Long Beach): A Hermite Method for Nonlinear Dispersive Maxwell's Equations

   Hermite methods are high-order methods, especially well-suited for linear hyperbolic problems, that rely on a Hermite interpolation procedure in space and a local time-stepping method to evolve the data in time [1]. In [3], Hagstrom proposed dissipative and conservative Hermite methods of arbitrary order for Maxwell's equations in linear dispersive media described by generalized Lorentz models. The dissipative Hermite method evolves the spatial derivatives of the electromagnetic fields through order m to achieve a 2m + 1 order method. Moreover, the time-step size needs to satisfy a stability condition that depends only on the maximum wave speed and is independent of the order.

   In this talk, we propose a dissipative Hermite method for nonlinear optics problems. We consider Kerr-type nonlinear media modeled by Maxwell's equations with auxiliary differential equations describing the linear and nonlinear responses of the underlying media. The method relies on a recursion relation for the system of ordinary differential equations required to evolve the Hermite polynomial coefficients in time. The fifth-order Runge-Kutta method is used as the local time-stepping method. The method is free of any nonlinear algebraic solver and requires solving small local linear systems of equations for which the dimension is independent of the order. Note that p-adaptivity described in [2] is straightforward in this setting. Numerical examples in 1-D and 2-D are performed and the expected convergence order is observed for reasonable values of m.

   References [1] J. Goodrich, T. Hagstrom, and J. Lorenz. Hermite methods for hyperbolic initial-boundary value problems. Math. Comp., 75:595–630, 2005. [2] R. Chen and T. Hagstrom. P-adaptive Hermite methods for initial value problems. ESAIM:M2AN, 46:545- 557, 2012. [3] T. Hagstrom. Hermite Methods for Electromagnetic Waves in Dispersive Media 2019 International Applied Computational Electromagnetics Society Symposium (ACES), 1-2, 2019.

3. Andreas Buttenschoen (Univ Mass Amherst): Graph-theoretic preconditioners for centre-based tissue models

   Center-based models of multicellular systems are a type of agent-based models used to simulate cell and tissue phenomena. In recent years they have become an indispensable tool in biomedical research. In center-based models cells are approximated as elastic

spheres, capsules or ellipsoids. A typical simulation step contains the following major steps: (1) collision detection i.e. determining each cell's neighbors; (2) resolving all cell-cell forces; (3) solving the over damped equation of motion; and finally (4) integrating the systems differential equations. Profiling shows that the majority of computational time is spent solving the equation of motion a large sparse linear system. Good preconditioners are known to reduce the required iteration count and thus computational cost. This motivates us to develop a graph theoretic matrix-free preconditioning scheme using information available when solving center-based models. Initial results suggests an iteration reduction of more than 50%.

4. Bowei Wu (Univ Mass Lowell): Simple quadrature for near-singular integral operators

Near-singular integrals frequently arise in fluid dynamics, material science, and many other scientific applications, where close fluid-structure interactions are common. Numerical approximation of near-singular integrals thus has practical importance. Approximating near- singular integrals using regular quadrature methods is in general inefficient and expensive. But more efficient quadrature rules can be developed by modifying regular quadrature rules using an error correction approach. We introduce new generalized Euler-Maclaurin formulas that are tailored to a family of near-singular functions. High-order accurate modified Trapezoidal quadrature rules are then derived based on these formulas.

Contributed Talks Session 02

Time: 3:10 pm - 4:40 pm, Mon Jun 17

1. Rick Archibald (ORNL): Federated Machine Learning for Experimental Facilities

   The US Department of Energy (DOE) makes substantial investments in the production and collection of massive amounts of scientific data through supporting the user facilities and scientific software. The high-performance computing (HPC) resources supported by the Office of Advanced Scientific Computing Research (ASCR) provide an ideal platform for applying scientific machine learning (SciML) on these massive data to accelerate scientific discoveries. However, an efficient, scalable, federated algorithm is necessary to apply SciML to distributed data produced at scientific user facilities. There is a push at Oak Ridge National Laboratory (ORNL) to develop the next generation of smart laboratories (https://www.ornl.gov/intersect), locally developing connections between experimental and computational facilities at ORNL. This talk will focus on recent efforts by IBM/INTERSECT/ORNL/REDHAT/SLAC to connect experimental facilities at different laboratories using federated learning.

2. Svetlana Tokareva (LANL): Structure-preserving matrix-free finite element method

   We present a three-dimensional matrix-free finite element method (MF-FEM) which provides an explicit and arbitrary high order approximation of the smooth solutions of the advection-diffusion partial differential equations both in space and time. The scheme allows for an efficient diagonalization of the mass matrix without any loss of accuracy. This is achieved by coupling the MF-FEM formulation with a Deferred Correction (DeC) type method for the discretization in time. We will first focus on the staggered grid MF-FEM (SG MF-FEM) scheme for the Lagrangian hydrodynamics. In Lagrangian formulation, the equations are written in a moving reference frame with respect to velocity and internal energy. We will discuss the structure-preserving properties of our scheme, in particular, local conservation of the total energy by means of simple force correction in the momentum update equation. Next, we will present a high-order MF-FEM scheme for the shallow water equations and show that our scheme is well-balanced with a proper choice of numerical quadratures and stabilization operators. The MF-FEM implementation is part of the Fierro computational mechanics code which leverages the immense utility of the MATAR C++ library, providing a seamless integration of the Kokkos Performance Portability EcoSystem with MPI for distributed computing.

3. Brian Helenbrook (Clarkson Univ): Can High-Order Convergence Be Obtained for Practical Problems in Engineering?

   With all of the interest in high-order methods, it is still not clear whether these methods have an advantage over their low-order counterparts for practical problems. In this talk, high-order hp-finite element moving mesh formulations for problems with moving boundaries and discontinuous solutions will be discussed. In particular, the attainable order of accuracy will be examined for several practical applications. These applications include ducted wind turbines where the rotor is modeled with an actuator disc, solidification of silicon with a moving free-surface and solidification front, and re-entry vehicles with a bow shock where the bow shock is tracked by the moving mesh. In all of these cases the solutions have non-smooth behaviors which makes obtaining design order of accuracy difficult / impossible. We examine whether high-order accurate schemes are still advantageous for these types of problems for both uniform mesh refinement approaches and adaptive meshing. We then investigate coordinate transforms that allow high-order methods to obtain optimal accuracy even for problems with singularities.

4. Catherine Mavriplis (Univ Ottawa): Implementing Immersed Boundaries in Continuous and Discontinuous Spectral Element Methods with hp-Adaptivity

While high order spectral element methods provide geometrical flexibility over global spectral methods, the treatment of curved or complex geometries remains challenging. Curved boundaries can be treated with high order polynomial representation or high order mappings, but subsequent grid generation is more complex than using straightforward Cartesian grids. We discuss the introduction of immersed boundaries, allowing for simple Cartesian grids for practicality, while including automatic grid adaptation to refine the mesh around the immersed boundaries and other regions where the solution varies rapidly. The immersed boundary is introduced through a volume penalization technique and the performance of the method is evaluated in both continuous and discontinuous Galerkin spectral element solvers with hp-adaptivity. The continuous spectral element method requires more adaptivity to compensate for the sudden introduction of an immersed boundary, while the discontinuous method is more forgiving since a flux condition obviates the need for continuity. Viscosity aids in the adaptation to the immersed boundary. For low viscosity cases, an artificial viscosity can be introduced near the immersed boundary when adaptivity alone is not sufficient to resolve the sudden change. We will evaluate the trade-offs between these approaches. Test cases will be given comparing the immersed boundary method to high order polynomial representation and high order mapping techniques. In particular, the acoustic scattering off a circular cylinder will be modeled using curvilinear mapping from a Cartesian grid and using the immersed boundary method on a regular rectangular Cartesian grid.

Contributed Talks Session 03

Time: 10:30 am - 12:00 pm, Tue Jun 18

1. Shanyin Tong (Columbia): Policy iteration method for inverse mean field games

   Mean-field games study the Nash Equilibrium in a non-cooperative game with infinitely many agents, they have a wide range of applications in engineering, economics, and finance. The coupling structure of the forward-backward equations of MFG raises specific difficulties in finding solutions to MFG, and makes it even more challenging to solve its inverse problem. In this talk, we will introduce a policy iteration method for solving inverse MFG, giving partial data of value functions and recovering the potential or obstacle function in the environment. The method takes ideas from policy iterations for forward MFG and separates the inversion step as solving a linear inverse problem, which substantially simplifies the problems and results in an efficient algorithm. We will use several numerical examples to demonstrate the accuracy and efficiency of the proposed method, and also discuss its convergence.

2. Ben Southworth (LANL): High-order time integration for nonlinearly partitioned multiphysics

   In multiscale and multiphysics simulation, a predominant challenge is the accurate coupling of physics of different scales, stiffnesses, and dimensionalities. The underlying problems are usually time dependent, making the time integration scheme a fundamental component of the accuracy. Remarkably, most large-scale multiscale or multiphysics codes use a first-order operator split or (semi-)implicit integration scheme. Such approaches often yield poor accuracy, and can also have poor computational efficiency. There are technical reasons that more advanced and higher order time integration schemes have not been adopted however. One major challenge in realistic multiphysics is the nonlinear coupling of different scales or stiffnesses. Here I present a new class of nonlinearly partitioned Runge-Kutta (NPRK) methods that facilitate high-order integration of arbitrary nonlinear partitions of ODEs. Order conditions for an arbitrary number of partitions are derived via a novel edge-colored rooted-tree analysis. I then demonstrate NPRK methods on novel nonlinearly partitioned formulations of thermal radiative transfer and radiation hydrodynamics, demonstrating orders of magnitude improvement in wallclock time and accuracy compared with current standard (semi-)implicit and operator split approaches, respectively.

3. Tongtong Li (Dartmouth): A structurally informed data assimilation approach for discontinuous state variables

   Data assimilation is a scientific process that combines available observations with numerical simulations to obtain statistically accurate and reliable state representations in dynamical systems. However, it is well known that the commonly used Gaussian distribution assumption introduces biases for state variables that admit discontinuous profiles, which are prevalent in nonlinear partial differential equations. In this talk, we focus on the design of a new structurally informed prior that exploits statistical information from the simulated state variables. In particular, we construct a new weighting matrix based on the second moment of the gradient information of the state variable to replace the prior covariance matrix used for model/data compromise in the data assimilation framework. We further adapt our weighting matrix to include information in discontinuity regions via a clustering technique. Our numerical experiments demonstrate that this new approach yields more accurate estimates than those obtained using ensemble transform Kalman filter (ETKF) on shallow water equations.

4. Duk-Soon Oh (Chungnam Nat Univ): New Analysis of Overlapping Schwarz Methods for Vector Field Problems in Three Dimensions with Generally Shaped Domains

   In this talk, we introduce an alternative approach to analyzing overlapping Schwarz methods for vector field problems in three dimensions. The theory is based on new regular decompositions that are robust to the topology of the domain or the subdomains. Enhanced estimates for the condition numbers of the preconditioned linear system are derived, dependent linearly on the relative overlap between the overlapping subdomains.

Contributed Talks Session 04

Time: 9:40 am - 11:10 am, Wed Jun 19

1. Gustaaf Jacobs (SDSU): High-order Lagrangian algorithms for Liouville models

   Eulerian-Lagrangian models describe fluid flow and particle dynamics in the Eulerian and Lagrangian frameworks, respectively. In chaotic systems the particle dynamics are stochastic because the suspended particles are subjected to random forces. We use a polynomial chaos expansion (PCE), rather than a postulated constitutive law, to capture structural and parametric uncertainties in the particles' forcing. The stochastic particle dynamics is described by a joint probability density function (PDF) of a particle's position and velocity and random coefficients in the PCE. We deploy the method of distributions (MoD) to derive a deterministic (Liouville-type) partial-differential equation for this PDF. We reformulate this PDF equation in a Lagrangian form, obtaining PDF flow maps and tracing events and their probability in the phase space. That is accomplished via a new high-order spectral scheme, which traces, marginalizes and computes moments of the high-dimensional joint PDF on conformally mapped hypercubes and comports with high-order carrier-phase solvers. Our approach has lower computational cost than either high-order Eulerian solvers or Monte Carlo methods, is not subjected to a CFL condition, does not suffer from Gibbs oscillations and does not require (order-reducing) filtering and regularization techniques. These features are demonstrated on several test cases.

2. Catherine Mavriplis (Univ Ottawa): A Parallel hp-Adaptive Discontinuous Galerkin Spectral Element Method Solver for Acoustic Problems in Curvilinear Geometries with Dynamic Load Balancing

   hp-adaptive meshes help mitigate the computational cost of high order spectral element methods by refining the areas in the computational domain that require higher resolution for complex solutions. h-adaptivity either splits or coarsens elements, while p-adaptivity increases or decreases the polynomial order of the solution within an element. The dynamic nature of the hp-adaptive process requires frequent load balancing in high performance computing environments to efficiently redistribute resources across a computing cluster. This talk will present a parallel hp-adaptive discontinuous Galerkin spectral element method solver for acoustic problems in curvilinear geometries with dynamic load balancing based on a Hilbert space-filling curve algorithm. Acoustic scattering cases in a semi-annulus, above a wavy boundary, and in a curved channel, will be presented. Strong and weak scaling tests will be presented for these cases.

3. Jonah A Reeger (Air Force Insititute of Technology): Local Adaptivity in Kernel Methods

   Building on the successes of local kernel methods for approximating the solutions to partial differential equations (PDE) and the evaluation of definite integrals (quadrature/cubature), a local estimate of the error in such approximations has recently been developed. This estimate is useful for determining locations in the solution domain where increased node density (equivalently, reduction in the spacing between nodes) can decrease the error in the solution. Such methods are necessary or desirable when approximating solutions to PDE (or in the case of quadrature/cubature), where the initial data and subsequent solution (or integrand) exhibit localized features that require significant refinement to resolve and where uniform increases in the density of nodes across the entire computational domain is not possible or too burdensome. This talk will describe the error estimate and an

adaptive procedure for adding nodes to the domain for both the approximation of derivatives and the approximate evaluation of definite integrals. Computational experiments will also be presented demonstrating close agreement between the error estimate and actual absolute error in the approximation.

4. Ngoc Cuong Nguyen (MIT): Discontinuous Galerkin Methods for Hypersonic Flows

In recent years, high-order discontinuous Galerkin (DG) methods have emerged as an attractive approach for numerical simulations of compressible flows. We present an overview of the recent development of DG methods for compressible flows with particular focus on hypersononic flows. We describe various shock capturing methods to deal with strong shock waves in hypersonic flows. We discuss r-adaptivity techniques to refine meshes for hypersonic boundary layers. We present a few examples to demonstrate the ability of high-order DG methods to provide accurate solutions of hypersonic laminar flows. Furthermore, we present direct numerical simulations of hypersonic transitional flow past a flared cone at Reynolds number 10.8×10^6, and hypersonic transitional shock wave boundary layer interaction flow over a flat plate at Reynolds number 3.97×10^6. These simulations run entirely on hundreds of graphics processing units (GPUs) and demonstrate the ability of DG methods to directly resolve hypersonic transitional flows, even at high Reynolds numbers, without relying on transition or turbulence models.

Contributed Talks Session 05

Time: 11:25 am - 12:55 pm, Wed Jun 19

1. Zheng Sun (University of Alabama): The Runge–Kutta Discontinuous Galerkin Method with Stage-Dependent Polynomial Spaces for Hyperbolic Conservation Laws

   In this talk, 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 P^k and P^{k-1} piecewise polynomial spaces, are used at different RK stages. The resulting method is referred to as the sdRKDG method. It features fewer floating-point operations and may achieve larger time step sizes. For problems without sonic points, we observe optimal convergence for all the sdRKDG schemes; and for problems with sonic points, we observe that a subset of the sdRKDG schemes remains optimal. 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, for problems including two-dimensional Euler equations for gas dynamics, are provided to demonstrate the performance of the new method.

2. Bosu Choi (Dartmouth College): Enhanced data assimilation based on the energy spectrum of nonlinear chaotic dynamics

   Kolmogorov's turbulence theory focuses on the statistical characteristics of turbulence, particularly on the energy spectrum within the turbulent cascade range. Conversely, the Khinchin-Kolmogorov theorem establishes a connection by identifying that the Fourier transform of the correlation function represents the energy spectrum of translation-invariant dynamics. These theoretical foundations enable us to estimate the correlation function of chaotic yet stationary processes based on their energy spectrum. In this study, we explore utilizing this statistical information to improve the prior covariance estimation and thereby reconstruct dynamics from limited observations with higher accuracy. Specifically, we enhance the performance of data assimilation methods by incorporating a solution-statistics-based prior rather than solely relying on a Gaussian prior. Our approach's robustness and effectiveness are demonstrated through a series of numerical tests using the Lorenz 96 model, commonly employed to simulate turbulent flows characterized by its stationary and translation-invariant dynamics. This is joint work with Yoonsang Lee at Dartmouth College.

3. Phil Roe (University of Michigan): Stencils and Representations that Promote High-Order Accuracy

   Heuristic considerations and analysis of special cases such as one-dimensional advection suggest that accuracy is best served by stencils that center as narrowly as possible on the exact domain of dependence, and are fully explicit. We consider adding more more information to the narrowest possible stencils and arrive at Hermitian schemes of odd-order accuracy having the form

   $$\mathbf{u}^{n+1} = \mathbf{PERu}^n$$

   where $\mathbf{R}$ is a reconstruction from discrete to continuous data, $\mathbf{E}$ is an exact or approximate evolution operator, and $\mathbf{P}$ projects back into the discrete space. In higher dimensions this encourages the use of simplicial grids. If the additional information is placed on

element boundaries it has twice the value. The operator **E** is available in multiple dimensions for several common problems. This method allows a collapsing cylindrical shockwave to be followed down to a very small radius.

4. Iman Samani (University of Michigan): Fifth-order Active Flux Methods for Wave Propagation

We introduce a new finite element on triangles. The degrees of freedom are the point values at vertices and midpoints (6 values), the gradients at vertices (6 values) and at each vertex the gradient toward the centroid (3 values) These 15 values support a quartic reconstruction. Some two-dimensional linear wave propagation problems admit exact solutions as integrals of the initial data. By exactly integrating the approximate (quartic) data we find fifth-order approx- imations to the point updates. The method is conservative, mutidimensional, and easy to implement. It applies at boundaries. Results will be shown for acoustics and elastodynamics. The three-dimensional extension can be made but has not yet been implemented.

Poster presentation

- Roberto Aaron (University of Notre Dame): A hybrid shock fitting-capturing method for high-speed flows

  High-Order Implicit Shock Tracking (HOIST) is a class of methods that computes the solution of a conservation law and the nodal coordinates of the shock aligned mesh through the formulation of a PDE-constrained optimization problem. The PDE constraint uses a DG discretization with conservation, stability and high-order accuracy properties. A sequential quadratic programming method is used to converge simultaneously the DG solution and the nodal coordinates, which avoids nonlinear stability issues due to a non-aligned mesh. The method allows high-order approximations of high speed flows without requiring extensive mesh refinement in non-smooth regions. Curved interfaces are tracked to high-order accuracy by the use of high-order elements to generate curved elements. This work presents a new methodology that integrates shock capturing and shock tracking to leverage the advantages of each. Strong bow shocks will be fully tracked because they play a critical role in the prediction of aerodynamic forces and can be readily fit with the grid using modern shock tracking techniques. Weaker secondary shocks that have proven more difficult (and less critical) to fit will be captured using artificial viscosity.

- Byeong-Ho Bahn (University of Massachusetts Amherst): Semilinear elliptic eigenvalue problem: Parametric analyticity and the uncertainty quantification

  In this talk, we will discuss parametric semilinear elliptic eigenvalue problem. For last few decades, parametric elliptic problem has received tremendous attentions. Even if its ubiquity, the eigenvalue problem has only studied recently. Also, the problems are only focused on linear case. In this study, to the best of our knowledge, we first attempt semilinear eigenvalue problem. A special case of our problem would be Gross Pitaevskii equation which describes super-fluidity and super-conductivity with random potential function. The main obstacle was showing analyticity of the ground state because the mixed derivative of them has no meaning without the analyticity. This obstacle is resolved by using implicit function theorem and multidimensional complex analysis. With careful analysis, we obtain the bound of mixed derivatives. With this bound, we suggest a method of uncertainty quantification for the ground state.

- Andrey Brinsko (University of Massachusetts Amherst): Computation of Nonlinear Sound Waves

  We compute globally defined, space and time periodic classical solutions of the 3 x 3 compressible Euler equations in one space dimension. A solution of a linear wave equation is put through the nonlinear evolution described by the Euler equations via a mixed spectral finite-difference method. A Newton type method is used to find a perturbation of the original solution that more closely satisfies the Euler equations. Iteratively applying this method until a desired accuracy is reached, the tile the solution was computed on covers the plane with a smooth, periodic solution. Transforming from the material variable used in computation to the spatial variable, we investigate the acoustics of the computed solution.

- Ziyu Chen (University of Massachusetts Amherst): Symmetry-Preserving Machine Learning: from the view of sample complexity

  Symmetry is ubiquitous in machine learning (ML) and scientific computing, with compelling implications for model development. ML models that preserve group symmetry have shown marked improvements in learning tasks with inherent group structures,

especially when faced with limited data. This talk will explore our recent and ongoing work toward understanding the gain of equivariant models. Specifically, I will talk about how group symmetry can help reduce the sample cost of generative models. By developing variational representations of probability divergence with embedded symmetry, I will share both theoretical insights and empirical findings, in a way explaining why symmetry-preserving generative models can generate good samples with limited training data.

- Nicolas Christensen (University of Illinois at Urbana-Champaign): Dispersion Properties of the Spectral Element Method

  We examine the dispersion properties of the spectral element method (SEM) for advection and advection-diffusion on a 1D periodic-domain model problem in both the well-resolved (asymptotic) limit and the marginally resolved (pre-asymptotic) limit. The study considers a broad range of wave-numbers, element counts, and local polynomial orders and includes Bloch-wave analysis of the dispersion properties. We observe high-order SEM requires fewer points-per-wavelength (PPW) to attain engineering tolerances with long time-integration and that Gottlieb's PPW $\gtrsim 5$ heuristic for engineering tolerances remains valid over many polynomial orders and element counts. Comparing use of exact quadrature on the Gauss-Legendre points and inexact quadrature (i.e., with a diagonal mass matrix) on the GLL points, we observe inexact quadrature is not significantly detrimental to solution accuracies at high polynomial orders. At high polynomial orders, both approaches exhibit error spikes near certain values of PPW, disrupting the convergence behavior. We show these spikes are caused by previously observed gaps in the eigenvalue spectrum of the discrete operators, resulting in unrepresentable wave-speeds. We demonstrate that diffusive mechanisms, effected either using upwinding within a high-order DG formulation or via a direct filtering approach, can largely mitigate these error spikes. Two dimensional model problems further illustrate the effectiveness of this mitigation strategy.

- Jaryd Domine (Southern Methodist University: Waves in black hole geometries: An energy-based discontinuous Galerkin method

  We are interested in the behavior of waves in the vicinity of black holes, highlighting here the special case of a scalar wave equation in the Kerr metric (that of a rotating, uncharged black hole). We present an energy-based discontinuous Galerkin method (EDG-GR) for the simulation of waves in black hole geometries, a proof-of-concept for the use of DG methods in numerical relativity. Our method distinguishes itself in that (1) It is localized, with minimal talking between elements, making it efficient and parallelizable; (2) Accurate radiation conditions allow us to simulate over a smaller region while preserving accuracy, and (3) Our uncommon choice of a first-order time, second-order space (FOTSOS) form greatly reduces the number of variables we must evolve.

  This work has applications to Extreme Mass Ratio (EMR) simulations – which are computationally expensive and require high resolution – and other prominent problems like back reaction, self-force, and the inverse problem of describing the black hole from observations. Future work will incorporate more complex spacetime metrics and wave equations, i.e. the Teukolsky equation and the full EFE.

- Huijing Dong (University of Notre Dame): A p-adaptive implicit shock tracking method for high-speed viscous flows

  Shock tracking or shock fitting, where the computational mesh is moved to align mesh element faces with discontinuities, represents them perfectly with the inter-element jump in the solution basis without requiring additional stabilization when addressing shocks. In our previous work, we introduced an implicit shock tracking framework that discretizes conservation laws on a mesh without

knowledge of discontinuities and solves a PDE-constrained optimization problem over the discrete solution variables and nodal coordinates of the mesh. A Discontinuous Galerkin (DG) discretization of the governing equation is applied and implicit tracking is formulated as an optimization problem constrained by the DG residual to endow the method with desirable properties of DG: consistency, conservation, and stability. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and flow solution to their optimal values. In this talk, we present a p-adaptive implicit shock tracking method aimed at solving steady and unsteady high-speed viscous flows. The polynomial degree is adapted used an indicator based on the enriched residual, which tends to increase the polynomial degree within shocks and boundary layers. A series of shock-dominated numerical experiments demonstrate the potential of the method to efficiently produce accurate solutions to these challenging problems.

- David Gillcrist (University of Massachusetts Dartmouth): Inverse Analysis and Calibration of Physical Models: An Approached Based on Greedy Kaczmarz Multi-Fidelity Surrogates and Aggregated Directional Statistics

  Advances in surrogate modeling have allowed for highly accurate Polynomial Chaos (PC) expansions to be constructed for physical models ranging from mild to major complexity in their respective parameter spaces. Multi-fidelity techniques in uncertainty quantification have been employed to efficiently capture the variations in the outputs of models given reasonable perturbations in these parameters. Recently, a greedy Kaczmarz algorithm (GKA) has been used to cheaply construct surrogate models that greatly outperform the previous least square approaches that demand 2-3 times the number of samples than the coefficients in the PC expansion.

  In this research we look at the utility of GKA–produced surrogate models in solving parameter estimation problems (inverse problems typically solved using statistical least squares methods). We present a generalized approach to solving two-dimensional parameter estimations for an underground aquifer modeled using the borehole function and the source localization of a contaminant in a river when modeled by an advection-diffusion-reaction equation.

  For each model, an array of surrogates is constructed to capture the variation in outputs, corresponding to hypothetical in situ detector apparatuses, at these detectors concerning the primary models' parameter spaces. Using global sensitivity analysis and directional statistical techniques we examine the optimal combination of the surrogates to perform the estimations. Various cost values for these surrogate combinations are used to judge the quality of the particular surrogates used to achieve the estimations.

- Sining Gong (Michigan State University): A Fully-implicit High order Strong Stability Preserving Method with Asymptotic-Preserving Property

  Recent work by Christlieb, Gong, Gottlieb, and Grant has led to the development of a novel family of fully-implicit, high-order, unconditionally strong stability-preserving (SSP) multi-derivative Runge–Kutta schemes designed for equations containing stiff terms. This approach has been validated to possess the asymptotic-preserving property, which preserves the asymptotic limit of the equation and the scheme automatically reduces to a high order time discretization for the limiting system. Additionally, the inherent contractivity of the SSP method ensures the uniqueness of solutions in the stage equations of the implicit Runge-Kutta method. David I. Ketcheson has demonstrated the existence of a second-order unconditionally SSP Runge–Kutta method that

incorporates downwind conditions. Our research, however, reveals that employing this method directly, even when integrating the backward derivative condition suggested by Christlieb et al., fails to work. Instead, by leveraging this idea with the downwind conditions and integrating it with additive Runge–Kutta methods, we have developed a new family of second-order SSP methods that eliminate time-step limitations for various problems, including the Broadwell model, the radiative transport equation, and the Bhatnagar-Gross-Krook (BGK) kinetic equation. In this talk, we provide a summery of the key theorems and present the corresponding numerical results associated with the models. The authors would like to thank the Department of Energy for their support of this research.

- Russell Hankey (Clarkson University): The Spectral Difference with Divergence Cleaning Method for Solutions of Kinematic Dynamo Problems

"The Spectral Difference with Divergence Cleaning (SDDC) method has been used to successfully model a number of nonlinear MHD problems [1,2]. The spectral difference method is a versatile high order method that can be used for unstructured grids and can be massively parallelized. In this study, the SDDC method is applied for solving two kinematic dynamo problems. The first kinematic dynamo problem was solved in a cubic box with all periodic boundary conditions. The SDDC method will be verified to capture the "Cigar" structures published in the literature [3]. The second kinematic dynamo problem adopts a spherical shell geometry and non-penetrative and stress-free boundary conditions [4]. The SDDC method will be employed to predict Sunspot cycles [5].

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- Yajie Ji (Shanghai Jiao Tong University): MCMS-RBM: Efficient transition pathway identification for crystals and quasicrystals via the Multi-Component Multi-State Reduced Basis Method

Traditional numerical methods encounter difficulties when applied to quasicrystals. The projection method is a prominent solver by transforming them into higher-dimensional periodic structures. However, this approach presents computational limitations,

particularly when dealing with the phase field model (e.g. Lifshitz-Petrich(LP) model) with many candidate quasicrystals and crystals for a wide range of parameters. In this talk, I will introduce a Multi-Component Multi-State Reduced Basis Method (MCMS-RBM) as a generic framework for reduced order modeling for parametric problems whose solution has multiple states across the parameter domain. A series of numerical tests for LP model demonstrate the stability, effectiveness, and efficiency of this numerical method. Specifically, in a parallel environment, using the reduced basis method to generate a delicate phase diagram takes only about three hours.

- Dohyun Kim (Brown University): A Projected Mirror Descent for Topology Optimization

  "In this presentation, we explore the application of a mirror descent approach to topology optimization. The mirror descent method, a generalized form of gradient descent, diverges from the traditional approach by replacing the quadratic Euclidean norm term with a Bregman divergence. Specifically, we leverage the Fermi-Dirac entropy as a Bregman divergence, a choice naturally derived from the bound constraint of the design variable.

  This divergence selection is particularly relevant as it facilitates a natural projection for the volume correction, effectively enforcing the volume constraint. The resulting projected mirror descent method seamlessly generates a sequence of bound-preserving design variables, even when employing high-order finite element approximations without additional treatment.

  To enhance the method's performance, we also propose an adaptive step size rule, incorporating the generalized Barzilai-Borwein method in conjunction with an Armijo-type backtracking line search algorithm. The efficacy of the proposed approach is demonstrated through several numerical examples, including applications to compliant mechanisms. Our results include comprehensive comparisons with other standard algorithms, showcasing the advantages and capabilities of the mirror descent method in the context of topology optimization."

- Shawn Koohy (University of Massachusetts Dartmouth): GPT-PINN: Generative Pre-Trained Physics-Informed Neural Networks toward non-intrusive Meta-learning of parametric PDEs

  "Physics-Informed Neural Networks (PINNs) have proven to be a powerful tool for obtaining the numerical solutions of nonlinear partial differential equations (PDEs) leveraging the expressivity of deep neural networks and the computing power of modern hardware. However, their training is still time-consuming, espe- cially in the multi-query and real-time simulation settings, and its parameterization is often overly excessive. We propose the Generative Pre-Trained PINN (GPT-PINN) to mitigate both challenges in the setting of parametric PDEs. GPT-PINN is a hyper-reduced network that generates surrogate solutions of a parametric system across the entire parameter domain accurately and efficiently by means of adaptive sampling."

- Nicholas Krupansky (Michigan State University): Surrogate Models using Neural Networks for Moment Equations

  We present recent work in machine learning surrogate models in the Boltzmann-BGK moment equations. For the so-called moment closure problem, we show a hyperbolicity preserving neural network closures to the BGK equation, trained with HME and DVM derived moments, with predictive capability beyond training times. We also present newer work on machine learning applied to the boundary conditions for the moment equations of the BGK equation. Typical methods for treating the Maxwellian boundary

conditions for the BGK equation require information about the underlying velocity distribution function, where we apply neural networks to treat the boundary condition from the moment equations directly.

- David Masse (University of Massachusetts Amherst): Mesoscale modeling of an Active Colloid's Motion

  It has been demonstrated in molecular dynamics simulations that colloids endowed with various physical properties can achieve enhanced diffusion, where localized particle-bath interactions cause the particle to diffuse faster than a simple particle in the bath. Such simulations remain computationally costly, and so a mesoscale model demonstrating the same behavior is sought, allowing for more, and more complex, simulations. Here we present such a model for the isotropic colloids studied by Decayeux et al., which achieve enhanced diffusion via phase transitions. Our model makes novel use of the Cahn-Hilliard equation as a means to promote phase separation near the colloid. Results of the implementation of this model are presented, along with comparisons to the molecular dynamics model used in the literature.

- Kimberly Matsuda (Rensselaer Polytechnic Institute): High-Order Asymptotic Preserving IMEX-BDF-DG Schemes for Linear Kinetic Transport Equations

  Kinetic transport equations (KTE) are used to model phenomena such as radiative transfer and neutron transport. Here, we consider a linear KTE under a diffusive scaling that converges to a diffusion equation as the Knudsen number epsilon goes to 0. One challenge in solving the KTE is that it is multiscale in epsilon. Also, the KTE becomes stiff when epsilon is much smaller than 1. Further, our goal is to develop high-order asymptotic preserving schemes to solve the KTE for a broad range of epsilon and assess their accuracy and stability. Our schemes use implicit-explicit-BDF methods combined with discontinuous Galerkin methods and the discrete ordinates method. We use Fourier analysis to determine the stability of the schemes. We further apply these schemes to various numerical examples to demonstrate their accuracy.

- Jean-Louis Mervin (University of Mauritius): Application of Second-Order Finite Volume Method to New Quasi-Hydrostatics Thermal Rotating Shallow Water Equations

  The new geophysical model, namely, the quasi-hydrostatics thermal rotating shallow water equations is spatially discretized with second-order finite volume method to analyze numerically weather disturbances. Results computed with the second-order finite volume method show significant differences when compared to the spectral method.

- Charles Naudet (University of Notre Dame): High-Order Implicit Shock Tracking for time-dependent flows

  Shock tracking aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter- element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or exten- sive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features. High-Order Implicit Shock Tracking (HOIST) recasts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an

error- based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conser- vation, stability, and high-order accuracy. By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh [1] . In this work, the HOIST method is further extended to simulate time-dependent, inviscid flows for higher dimensions. We use a space-time formulation of the governing equations and perform shock tracking over a space-time slab [2]. In the two-dimensional space and time setting we generate a three- dimensional mesh by extruding a spatial mesh of quadrilateral elements into hexahedral elements. We also introduce robustness measures for hexahedral element collapses, as well as a method to leverage information from previous time-slabs to improve the initial guess for our mesh on the current slab.

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- Zezheng Song (University of Maryland, College Park): A Finite Expression Method for Solving High-Dimensional Committor Problems

  Transition path theory (TPT) is a mathematical framework for quantifying rare transition events between a pair of selected metastable states A and B. Central to TPT is the committor function, which describes the probability to hit the metastable state B prior to A from any given starting point of the phase space. Once the committor is computed, the transition channels and the transition rate can be readily found. The committor is the solution to the backward Kolmogorov equation with appropriate boundary conditions. However, solving it is a challenging task in high dimensions due to the need to mesh a whole region of the ambient space. In this work, we explore the finite expression method (FEX, Liang and Yang (2022)) as a tool for computing the committor. FEX approximates the committor by an algebraic expression involving a fixed finite number of nonlinear functions and binary arithmetic operations. The optimal nonlinear functions, the binary operations, and the numerical coefficients in the expression template are found via reinforcement learning. The FEX-based committor solver is tested on several high-dimensional benchmark problems. It gives comparable or better results than neural network-based solvers. Most importantly, FEX is capable of correctly identifying the algebraic structure of the solution which allows one to reduce the committor problem to a low-dimensional one and find the committor with any desired accuracy.

- Manas Vishal (University of Massachusetts Dartmouth): Towards exponentially-convergent simulations of extreme-mass-ratio inspirals: A time-domain solver for the Teukolsky equation with singular source terms

  Laser Interferometer Space Antenna (LISA), a future space-borne gravitational wave detector, is primarily sensitive to Extreme Mass Ratio Inspirals (EMRIs), which are black hole mergers with a mass ratio greater than 100,000. We require an extremely precise

template wave bank for the matched filtering procedure. In this talk, I will discuss about a Discontinuous Galerkin (DG) technique for gravitational wave simulations of EMRI systems. The Teukolsky equation, which governs the behavior of EMRIs, is first reduced to a set of coupled 1+1D wave equations with a delta source term that functions as the secondary black hole in an EMRI system. Our DG approach, in contrast to previous numerical schemes, can precisely incorporate the smaller black hole's point particle behavior in the form of a delta function. Compared to previous methods, our efficient method produces very accurate waveform due to the scheme's spectral (super)convergence property and exact treatment of the Dirac delta function that models the smaller black hole. Our time domain solver now includes hyperboloidal layers, which allow us to extract the solution at null infinity. We verify our computation by calculating Kerr and Schwarzschild energy fluxes from circular orbits at null infinity and Price tail power laws.

- Taorui Wang (Worcester Polytechnic Institute): Detecting the Structure of high dimensional Fokker Planck Equation's Solution by Radial Basis Function Based Tensor Network

  The Fokker-Planck equation, crucial in physics and finance, challenges solvers in high-dimensional, unbounded domains. This poster presents an innovative tensor network-RBF approach to accurately represent the solution within a truncated domain. By combining tensors with multiple RBFs, our method efficiently isolates high-probability solution regions, overcoming the Fokker-Planck equation's computational hurdles through a gradient-based optimizer. This advancement effectively tackles new high-dimensional steady state Fokker-Planck equation benchmarks.

- Stephen White (Michigan State University): A Family of Gauge Conserving Methods

  Recent work by Christlieb, Sands, and White has developed a new particle-in-cell method for the Vlasov-Maxwell system, casting the electromagnetic fields and the equations of motion for the particles in terms of scalar and vector potentials through a Hamiltonian formulation using the Lorenz gauge. This particle-in-cell method was proved to have the desirable property of conserving charge if and only if it satisfied the Lorenz gauge condition. Additionally, it has been shown that the satisfaction of the gauge condition entails the satisfaction of Gauss' Law. We now generalize this property to a family of methods, both to arbitrary order Backward Difference Formulation and s-step Diagonally Implicit Runge Kutta schemes, presenting both the theorems proving these properties and the numerical results. The author would like to thank the department of energy for their support of this work.