Numerical Analysis of Multiphysics Problems
Poster Session Abstracts
Tuesday, February 13, 2024

Nested Iteration and Nonlinear Methods for Liquid Crystal Shape Optimization Applications

Anca Andrei, Tufts University

Anisotropic fluids, such as nematic liquid crystals, can form non-spherical equilibrium shapes known as tactoids. Predicting the shape of these structures as a function of material parameters is challenging and paradigmatic of a broader class of problems that combine shape and order. Here, we develop a discrete shape optimization approach with finite elements to find the configuration of a two-dimensional tactoid using the Landau de Gennes framework and a Q-tensor representation. Efficient solution of the resulting constrained energy minimization problem is achieved using a quasi-Newton and nested iteration algorithm. Numerical validation is performed with benchmark solutions and compared against experimental data and earlier work. We explore physically motivated subproblems, whereby the shape and order are separately held fixed, to explore the role of both and examine material parameter dependence of the convergence. Nested iteration significantly improves both the computational cost and convergence of numerical solutions of these highly deformable materials.

Finite element methods for multicomponent flows

Francis Aznaran, University of Notre Dame

The Onsager framework for linear irreversible thermodynamics provides a thermodynamically consistent model of mass transport in a phase consisting of multiple species, via the Stefan–Maxwell equations, but a complete description of the overall transport problem necessitates also solving the momentum equations for the flow velocity of the medium. We derive a novel nonlinear variational formulation of this coupling, called the (Navier–)Stokes–Onsager–Stefan–Maxwell system, which governs molecular diffusion and convection within a non-ideal, single-phase fluid composed of multiple species, in the regime of low Reynolds number in the steady state. We propose an appropriate Picard linearisation posed in a novel Sobolev space relating to the diffusional driving forces, and prove convergence of a structure-preserving finite element discretisation. This represents some of the first rigorous numerics for the coupling of multicomponent molecular diffusion with compressible convective flow. The broad applicability of our theory is illustrated with simulations of the centrifugal separation of noble gases and the microfluidic mixing of hydrocarbons.

Exploring a Model Heat Exchanger

Sylvie Bronsard, Courant Institute of Mathematical Sciences, New York University

In this poster, I will explore a buoyancy-driven model for a heat exchanger with an incompressible working fluid, and then formulate a compressible-fluid version of the model, with air as the working fluid. The incompressible model equations can be solved numerically
and the results show interesting behavior on two timescales. Work on the compressible-fluid case is currently underway.

Modeling hypothermia with a multiscale model coupling partial differential equations for temperature with ordinary differential equations.

Tyler Fara, Oregon State University

We present a computational model simulating body temperature in extremities subject to extreme cold (hypothermia). The phenomenological description of the problem is that the body responds to hypothermia by vasoconstriction, whereby the body restricts blood flow to the extremity, preserving core body temperature even at the expense of sacrificing tissue in the extremity. Our model includes: (i) a parabolic partial differential equation (PDE) with an energy exchange term modeling blood perfusion through tissue, and this term is derived by multiscale analysis, and (ii) a constrained ODE representing the body's metabolic and vasoconstrictive responses. We approximate the solution to the model with mixed finite element method on Cartesian grids for the PDE with an immersed boundary approach to handle complex geometries.

Exploring traces versus bubbles in the design of robust two-level mixed finite element models Sônia M. Gomes, IMECC-UNICAMP, Campinas, SP, Brazil

Suitable choices of function spaces are crucial for robustness of mixed Finite Element (FE) models of combined physical phenomena. In this direction, the importance of using conforming finite element approx- imations in H1, H(curl), H(div), and L2 forming an exact de Rham complex is well recognized in the area of numerical analysis. The construction of FE exact sequences and the definition of their commuting inter-polants require proper trace spaces, forming lower dimensional exact FE sequences as well. On the other hand, bubble functions, having vanishing traces over element interfaces, play crucial roles in the enforcement of compatibility and accuracy properties. In some cases, it is convenient to have bubble discretization within the elements, more refined than the trace components. These attributes shall be explored with regard to the generality of meshes and of FE local spaces.

InfSupNet for solving high dimensional elliptic PDEs

Xiaokai Huo, Iowa State University

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

Enriched Galerkin Methods for Thermo-Hydraulic-Mechanical Systems

Sanghyun Lee, Florida State Univeresity

This paper proposes a new numerical method for a fully coupled, quasi-static thermo-poroelasticity model in a unified enriched Galerkin (EG) method framework. In our method, the mechanics sub-problem is solved using a locking-free EG method, and the flow and heat sub-problems are solved using a locally conservative EG method. The proposed method offers mass and energy conservation properties with much lower costs than other methods with the same properties, including discontinuous Galerkin methods and mixed finite element methods. The well-posedness and optimal a priori error estimates are carefully derived. Several numerical tests confirm the theoretical optimal convergence rates and the mass and energy conservation properties of the new method.

Automated construction of effective potential via algorithmic implicit bias
Xingjie Helen Li, University of North Carolina Charlotte

We introduce a novel approach for decomposing and learning every scale of a given multiscale objective function in multi-dimensional space. This approach leverages a recently demonstrated implicit bias of the optimization method of gradient descent, which enables the automatic generation of data that nearly follow Gibbs distribution with an effective potential at any desired scale.

One application of this automated effective potential modeling is to construct reduced-order models. For instance, a deterministic surrogate Hamiltonian model can be developed to substantially soften the stiffness that bottlenecks the simulation, while maintaining the accuracy of phase portraits at the scale of interest. Similarly, a stochastic surrogate model
can be constructed at a desired scale, such that both its equilibrium and out-of-equilibrium behaviors (characterized by auto-correlation function and mean path) align with those of a damped mechanical system with the original multiscale function being its potential.
The robustness and efficiency of our proposed approach in multi-dimensional scenarios have been demonstrated through a series of numerical experiments. A by-product of our development is a method for anisotropic noise estimation and calibration. More precisely, Langevin model of stochastic mechanical systems may not have isotropic noise in practice, and we provide a systematic algorithm to quantify its covariance matrix without directly measuring the noise. In this case, the system may not admit closed form expression of its invariant distribution either, but with this tool, we can design friction matrix appropriately to calibrate the system so that its invariant distribution has a closed form expression of Gibbs.

This is a joint work with Dr. Molei Tao from Georgia Institute of Technology.

Sensitivity to different assumptions in a permafrost model responding to surface temperature variations
Praveeni Mathangadeera, Oregon State University

We start with a one-dimensional finite difference model of phase change in permafrost soil defined in [Bigler, Peszynska, Vohra, 2022]. This computational model requires careful handling of nonlinear relationships. We also use data and constitutive parameters from [Ling, Zhang'2003] which require extensions of this model; we also use daily temperature data from databases in the Arctic. To introduce these elements, we add to our computational model a new possibility of sequential rather than implicit treatment of nonlinearities. Next, we evaluate the response of the model depending on which assumptions are made. In particular, we allow presence of a snow layer which influences the top boundary condition for the model; and we study the effects of snow thermal conductivity, volumetric heat capacity, and albedo.

The Runge–Kutta discontinuous Galerkin method with compact stencils for hyperbolic conservation laws
Zheng Sun, The University of Alabama

We develop a new type of Runge--Kutta (RK) discontinuous Galerkin (DG) method for solving hyperbolic conservation laws. Compared with the original RKDG method, the new method features improved compactness and allows simple boundary treatment. The key idea is to hybridize two different spatial operators in an explicit RK scheme, utilizing local projected derivatives for inner RK stages and the usual DG spatial discretization for the final stage only. Limiters are applied only at the final stage for the control of spurious oscillations. We also explore the connections between our method and Lax--Wendroff DG schemes and ADER-DG schemes. Numerical examples are given to demonstrate the performance of the cRKDG method.

Accelerating and enabling convergence of nonlinear solvers for Navier-Stokes equations by continuous data assimilation
Duygu Vargun, ORNL

This study considers improving the Picard and Newton iterative solvers for the Navier- Stokes equations in the setting where data measurements or solution observations are available. We construct adapted iterations that use continuous data assimilation (CDA) style nudging to incorporate the known solution data into the solvers. For CDA-Picard, we prove the method has an improved convergence rate compared to usual Picard, and the rate improves as more measurement data is incorporated. We also prove that CDA-Picard is contractive for larger Reynolds numbers than usual Picard, and the more measurement data that is incorporated the larger the Reynolds number can be with CDA-Picard still being contractive. For CDA- Newton, we prove that the domain of convergence, with respect to both the initial guess and the Reynolds number, increases as the amount of measurement data is increased. Additionally, for both methods we show that CDA can be implemented as direct enforcement of measurement data into the solution. Numerical results for common benchmark Navier-Stokes tests illustrate the theory.

Operator learning for hyperbolic partial differential equations
Chris Wang, Cornell University

We construct the first rigorously justified probabilistic algorithm for recovering the solution operator of a hyperbolic partial differential equation (PDE) in two variables from input-output training pairs. The primary challenge of recovering the solution operator of hyperbolic PDEs is the presence of characteristics, along which the associated Green's function is discontinuous. Therefore, a central component of our algorithm is a rank detection scheme that identifies the approximate location of the characteristics. By combining the randomized singular value decomposition with an adaptive hierarchical partition of the domain, we construct an approximant to the solution operator using $O(\epsilon^{-7}\log(\epsilon^{-1}))$ input-output pairs with relative error $O(\epsilon)$ in the operator norm as $\epsilon \to 0$, with high probability. Our assumptions on the regularity of the coefficients of the hyperbolic PDE are relatively weak given that hyperbolic PDEs do not have the "instantaneous smoothing effect" of elliptic and parabolic PDEs, and our recovery rate improves as the regularity of the coefficients increases.

The robust-preconditioner for Stokes-Darcy coupling problems with the mixed Darcy equation Xue Wang, Tufts University

We construct mesh-independent and parameter-robust monolithic solvers for the coupling Stokes-Darcy problem with mixed Darcy equation. In particular, our preconditioners does not contain any fraction operators by using the standard norm, so it is easy to implement in the code. In numerical experiments, we consider the conforming and nonconforming finite element methods for space discretization to verify the parameter-robustness of the proposed solvers.

Improving Greedy Algorithms for Rational Approximation

Zhongqin Xue, Tufts University

When developing robust preconditioners for multiphysics problems, fractional functions of the Laplace operator often arise and need to be inverted. Rational approximation in the uniform norm can be used to convert inverting those fractional operators into inverting a series of shifted Laplace operators. A desired property is that the poles of the approximation be negative so that the shifted Laplace operators remain symmetric positive definite, making them better conditioned. In [Li et al., arXiv:2305.18038], an orthogonal greedy algorithm (OGA) was proposed. Although the approach produces negative poles, the OGA provides rational approximation in the L2 norm. In this work, we address this issue by studying two greedy algorithms for finding rational approximations to such operators, allowing for efficient solution methods for these applications. The first algorithm improves OGA by adding one minimization step in the uniform norm to the procedure. The second approach employs the weak Chebyshev greedy algorithm (WCGA) in the uniform norm, which converges monotonely. We present analysis and numerical results demonstrating that both proposed algorithms ensure the poles are negative while providing rational approximation in the uniform norm. Furthermore, our approach can be extended to other approximation problems by expanding the dictionary used in the algorithm, demonstrating potential flexibility and applicability.

Control of Plasma Instability in Vlasov-Poisson System

Yukun Yue, University of Wisconsin, Madison

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