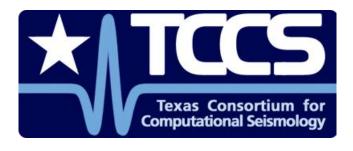
Frontiers in Computational Mathematics

A conference in honor of Björn Engquist's 80th birthday

April 10-12, 2025

The University of Texas at Austin

Sponsors









INSTITUTE FOR COMPUTATIONAL ENGINEERING & SCIENCES

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Background

Professor Björn Engquist is a prominent mathematician renowned for his contributions to applied and computational mathematics. He received his Ph.D. in numerical analysis from Uppsala University, Sweden, in 1975 and has held significant academic positions including professorships at the University of California, Los Angeles (UCLA), and Princeton University, where he served as the Michael Henry Stater University Professor of Mathematics and Applied and Computational Mathematics.

Currently, Engquist is a faculty member at the University of Texas at Austin, holding the Computational and Applied Mathematics Chair I and directing the Center for Numerical Analysis at the Oden Institute for Computational Engineering and Sciences. His research focuses on the development,



analysis, and application of numerical methods for differential equations in multiscale problems, fluid mechanics, and wave propagation.

Engquist has been honored with numerous accolades, including membership in the Royal Swedish Academy of Sciences, the Royal Swedish Academy of Engineering Sciences, and the Norwegian Academy of Science and Letters. He is also a Fellow of the Society for Industrial and Applied Mathematics (SIAM). He has received prestigious awards such as the SIAM Prize in Scientific Computing, the Henrici Prize, and the ICIAM Pioneer Prize.

Throughout his career, he has supervised over 40 Ph.D. students and actively promotes interdisciplinary collaboration in mathematics and its applications. Engquist's impact on the field resonates through his innovative research and dedication to education.

Schedule at a Glance

Talks held in Avaya Auditorium (POB 2.302)



DAY 1: THURSDAY APRIL 10, 2025

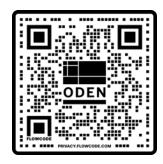
| 8:30am-9:30am | Registration and Refreshments |
|-----------------|---|
| 9:30am-9:45am | Opening Remarks |
| 9:45am-10:15am | Stan Osher, University of California, Los Angeles |
| 10:15am-10:45am | Olof Runborg, KTH Royal Institute of Technology |
| 10:45am-11:15am | Coffee Break |
| 11:15am-11:45am | Lexing Ying, Stanford University |
| 11:45am-12:15pm | Sergey Fomel, The University of Texas at Austin |
| 12:15pm-1:45pm | Lunch (POB 6.102) |
| 1:45pm-2:15pm | Eitan Tadmor, University of Maryland |
| 2:15pm-2:45pm | Chi-Wang Shu, Brown University |
| 2:45pm-3:15pm | Coffee Break |
| 3:15pm-3:45pm | Jian-Guo Liu, Duke University |
| 3:45pm-4:15pm | Hongkai Zhao, Duke University |
| 4:15pm-4:45pm | Christina Frederick, New Jersey Institute of Technology |
| 4:50pm-5:00pm | Group Photo |
| 5:30pm - 7:30pm | Reception, AT&T Center Courtyard |

DAY 2: FRIDAY APRIL 11, 2025

| 9:00am-9:30am | Weinan E, Peking University |
|-----------------|---|
| 9:30am-10:00am | Anna-Karin Tornberg, KTH Royal Institute of Technology |
| 10:00am-10:30am | Coffee Break |
| 10:30am-11:00am | Yi Sun, University of South Carolina |
| 11:00am-11:30am | Eric Chung, Chinese University of Hong Kong |
| 11:30am-1:00pm | Lunch (POB 6.102) |
| 1:00pm-1:30pm | Russ Caflish, Courant Institute, New York University |
| 1:30pm-2:00pm | Yoonsang Lee, Dartmouth University |
| 2:00pm-2:30pm | Yunan Yang, Cornell University |
| 2:30pm-3:00pm | Coffee Break |
| 3:00pm-4:00pm | Tony Chan, Thomas Y. Hou, David Kan, Richard Sharp, and Karen Willcox |

Schedule at a Glance

Talks held in Avaya Auditorium (POB 2.302)



DAY 3: SATURDAY APRIL 12, 2025

| 9:00am-9:30am | Thomas Hou, California Institute of Technology |
|-----------------|---|
| 9:30am-10:00am | Robert Moser, The University of Texas at Austin |
| 10:00am-10:30am | Coffee Break |
| 10:30am-11:00am | Xiaochuan Tian, University of California, San Diego |
| 11:00am-11:30am | Kui Ren, Columbia University |
| 11:30am-1:00pm | Lunch (Avaya Atrium) |
| 1:00pm-1:30pm | Haomin Zhou, Georgia Institute of Technology |
| 1:30pm-2:00pm | Sean Carney, Union College |
| 2:00pm-2:30pm | Richard Tsai, The University of Texas at Austin |
| 2:30pm | Coffee Break |

Office Space

Office space is available for use in POB 2.126 and POB 2.130.

Title and Abstract

Russ Caflisch: Optimization for the Boltzmann Equation

The kinetics of rarefied gases and plasmas are described by the Boltzmann equation and numerically approximated by the Direct Simulation Monte Carlo (DSMC) method. We present an optimization method for DSMC, derived from an augmented Lagrangian. After a forward (in time) solution of DSMC, adjoint variables are found by a backwards solver. They are equal to velocity derivatives of an objective function, which can then be optimized. This is joint work with Yunan Yang (Cornell) and Denis Silantyev (U Colorado, Colorado Springs).

Sean Carney: Uncertainty in Uncertainty and Rockafellian Relaxation

A critical aspect of PDE constrained optimization is to account for uncertainty in the underlying physical models, for example in model coefficients, boundary conditions, and initial data. Uncertainty in physical systems is modeled with random variables, however, in practice there may be some nontrivial ambiguity in the underlying probability distribution from which they are sampled. As stochastic optimal control problems are known to be ill-conditioned to perturbations in the sampling distribution, we describe an analytic framework that is better conditioned to such "meta-uncertainties" and conclude with numerical examples.

Eric Chung: Robust Multiscale Methods for a Class of High-Contrast Heterogeneous Sign-Changing Problems

The mathematical formulation of sign-changing problems involves a linear second-order partial differential equation in the divergence form, where the coefficient can assume positive and negative values in different subdomains. These problems find their physical background in negative-index metamaterials, either as inclusions embedded into common materials as the matrix or vice versa. In this paper, we propose a numerical method based on the constraint energy minimizing generalized multiscale finite element method (CEM-GMsFEM) specifically designed for sign-changing problems. The construction of auxiliary spaces in the original CEM-GMsFEM is tailored to accommodate the sign-changing setting. The numerical results demonstrate the effectiveness of the proposed method in handling sophisticated coefficient profiles and the robustness of coefficient contrast ratios. Under several technical assumptions and by applying the T-coercivity theory, we establish the inf-sup stability and provide an a priori error estimate for the proposed method. The research is partially supported by the Hong Kong RGC General Research Fund Projects 14305222 and 14305423.

Qiang Du: Integral Models with Nonlocal Operators: Applications and Recent Developments

Recent applications and theoretical developments of models of integral equations using nonlocal operators have shown promise as effective alternatives to local models, especially in the presence of singularities and anomalies. These models also serve as continuum limits for large-scale discrete models used in data learning and network analysis. We present these models on bounded spatial domains and discuss related modeling, analysis, and computational issues.

Weinan E: Understanding the Principles Behind Deep Learning

Deep learning has been a big success. It has been rather mysterious and at times appears to be some kind of "black magic". We will take a look at deep learning from the usual viewpoint of numerical analysis, namely approximation theory, stability, etc, try to put some rationale behind deep learning.

Christina Frederick: Uncovering One-Way Flow Mechanisms in Looped Network Models

We demonstrate flow rectification and valveless pumping in macroscale fluidic networks with loops, inspired by the directed airflow in bird lungs. When subjected to oscillatory forcing at high Reynolds numbers, multiloop networks exhibit persistent circulation, with experiments and simulations showing that stronger DC flows emerge at higher forcing frequencies and amplitudes. Flow visualizations reveal that vortex shedding at junctions acts as a passive valving mechanism, suggesting new strategies for controlling inertial flows through network topology. This is joint work with Quynh M. Nguyen, Anand U. Oza, Stephen Childress, and Leif Ristroph.

Sergey Fomel: Partial Differential Equations in Seismic Data Analysis

I review some of the PDEs used in seismic reflection data analysis and the numerical methods for solving them.

Thomas Hou: Nearly Self-Similar Blowup of Generalized Axisymmetric Navier-Stokes Equations

We numerically investigate the nearly self-similar blowup of the generalized axisymmetric Navier-Stokes equations. First, we rigorously derive the axisymmetric Navier-Stokes equations with swirl in any integer dimensions, marking the first such derivation for dimensions greater than three. Building on this, we generalize the equations to arbitrary positive real-valued dimensions, preserving many known properties of the 3D axisymmetric Navier-Stokes equations. To address scaling instability, we dynamically vary the space dimension to balance advection scaling along the r and z directions. A major contribution of this work is the development of a novel two-scale dynamic rescaling formulation, leveraging the dimension as an additional degree of freedom. This approach enables us to demonstrate a one-scale self-similar blowup with solution-dependent viscosity. Notably, the self-similar profile satisfies the axisymmetric Navier-Stokes equations with constant viscosity. We observe that the effective dimension is approximately 3.188 and appears to converge toward 3 as background viscosity diminishes. Furthermore, we introduce a rescaled Navier-Stokes model derived by dynamically rescaling the axial velocity in 3D. Our numerical study shows that this rescaled Navier-Stokes model with two constant viscosity coefficients exhibits a nearly self-similar blowup with maximum vorticity growth on the order of O(1030).

Yoonsang Lee: Ensemble Bayesian Update: Analysis, Extension, and Application to Data Assimilation and Inverse Problems

Ensemble-based Bayesian updates play a crucial role in estimating system states with uncertainty by assimilating observational data. Applications such as numerical weather prediction, UAV localization, and epidemiology are well-known examples of the effectiveness of ensemble-based Bayesian methods. The use of ensembles in Bayesian updates addresses the challenge of estimating the system's prior distribution, which is often complicated by nonlinear dynamics and computationally intensive prediction models, frequently resulting in non-Gaussian distributions. While nonparametric particle filters are versatile in handling nonGaussian systems, ensemble filters that assume Gaussian priors have demonstrated greater robustness in high-dimensional settings. This talk will explore the stabilizing effect of the Gaussian assumption in ensemble filters and propose extensions to enhance their accuracy and convergence speed, particularly in the context of solving inverse problems.

Jian-Guo Liu: Least-Action Incompressible Flows and the Adhesion Model

Variational relaxation of the least-action principle for free-boundary incompressible flow yields pressureless Euler flow following Wasserstein geodesics. Action-minimizing incompressible flows are locally rigid, determined by convex and locally affine velocity potentials for initially convex bodies. An alternative characterization of these flows involves absence of mass concentration in Monge-Ampere measures associated with certain Hamilton-Jacobi equations. There is a close relation to the adhesion model in cosmology, a multi-D model which reduces to sticky particle flow in 1D.

Robert Moser: The Intersection of Turbulence Theory and Numerical Analysis in the Simulation of Turbulent Flows

Stanley Osher: Recent Results on Mean Field Games, Optimal Transport, and In-Context Learning

The subjects in my title have been advancing rapidly. I'll try to give a coherent overview.

Kui Ren: A Policy Iteration Method for Inverse Mean Field Problems

We propose a policy iteration method to solve an inverse problem for a mean-field game model, specifically to reconstruct the obstacle function in the game from the partial observation data of value functions, which represent the optimal costs for agents. The proposed approach decouples this complex inverse problem, which is an optimization problem constrained by a coupled nonlinear forward and backward PDE system in the MFG, into several iterations of solving linear PDEs and linear inverse problems. This method can also be viewed as a fixed-point iteration that simultaneously solves the MFG system and inversion. We further prove its linear rate of convergence. Numerical examples are provided to demonstrate the effectiveness of the proposed method. This is a joint work with Nathan Soedjak and Shanyin Tong.

Olof Runborg: Solving Helmholtz Equation Using the Temporal Decomposition Method

Chi-Wang Shu: Stability of Time Discretizations for Semi-Discrete Schemes

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

Yi Sun: Kinetic Monte Carlo Simulations of Traffic Flows

We employ an efficient kinetic Monte Carlo (KMC) method to study traffic flow models on 1D and 2D lattices based on the exclusion principle and microscopic dynamics. This model implements stochastic rules for cars' movement based on the configuration of the traffic ahead of each car. In Part 1), we compare two different look-ahead rules: one is based on the distance from the car under consideration to the car in front of it, the other one depends on the car density ahead. In Part 2), we introduce a novel idea of multiple moves, which plays a key role in recovering the nonconcave flux in the macroscopic dynamics. In Part 3), we propose a look-ahead rule that depends on both the car density ahead and a generalized interaction function related to the distance between cars. For this case, we design an accelerated KMC method to reduce the computational complexity in the evaluation of the nonlocal transition rates. Our results show that the fluxes of the KMC simulations agree with the coarse-grained macroscopic averaged fluxes for the different look-ahead rules under various parameter settings. This talk includes the joint work with Cory Hauck, Changhui Tan and Ilya Timofeyev.

Eitan Tadmor: The Emergence of Entropy Solutions for Euler Alignment Equations

The hydrodynamic description for emergent behavior of interacting agents is governed by Euler alignment equations, driven by different protocols of pairwise communication kernels. We survey recent results in Euler alignment dynamics with emphasis on the multi-dimensional setting. A distinctive feature of alignment dynamics is the reversed direction of entropy. We discuss the role of a reversed entropy inequality in selecting mono-kinetic closure for emerging strong alignment solutions, we prove the existence of such solutions, and we characterize their related invariants which extend the 1-D notion of an "e" quantity.

Xiaochuan Tian: Sparse Solutions of Nonlinear PDEs via Radial Basis Function Networks

We propose a general framework for solving nonlinear PDEs using neural networks. To avoid overparameterization and eliminate redundant features, a regularization approach that encourages sparsity is explored within the framework of shallow radial basis function (RBF) networks. An adaptive training process iteratively adds neurons to maintain a compact network structure. Existence theory is established via the calculus of variations, and a representer theorem is derived for reproducing kernel Banach spaces (RKBS) associated with one-hidden-layer neural networks of possibly infinite width. An error estimate for the neural network approximation to the PDE is also derived. Training is performed using a second-order semismooth Newton method with gradient boosting. The approach is compared with the reproducing kernel Hilbert space (RKHS) framework and Gaussian process methods. This is a joint with Konstantin Pieper (Oak Ridge National Lab) and Zihan Shao (UC San Diego).

Anna-Karin Tornberg: Layer Potentials - Quadrature Error Estimates and Applications

When numerically solving PDEs reformulated as integral equations, so called layer potentials must be evaluated. The quadrature error associated with a regular quadrature rule for evaluation of such integrals increases rapidly when the evaluation point approaches the surface and the integrand becomes sharply peaked. Error estimates are needed to determine when the accuracy becomes insufficient, and then, a sufficiently accurate special quadrature method needs to be employed. In this talk, we discuss how to estimate quadrature errors, building up from simple integrals in one dimension to layer potentials over smooth surfaces in three dimensions. We also discuss a new special quadrature technique for axisymmetric surfaces with error control. The underlying technique is so-called interpolatory semi-analytical quadrature in conjunction with a singularity swap technique. Here, adaptive discretizations and parameters are set automatically given an error tolerance, utilizing further quadrature and interpolation error estimates derived for this purpose. Several different examples are shown, including examples with rigid particles in Stokes flow.

Richard Tsai: Deep Learning Approaches for Solving Differential Equations by Classical Convergent Numerical Schemes

I will present our approach using classical numerical methods in deep learning models to solve high-dimensional Hamilton-Jacobi equations and multiscale Hamiltonian systems. The approach uses a stochastic gradient descent-based optimization algorithm to minimize the least squares functionals defined by the numerical schemes. In the talk, I will discuss the advantages of using numerical schemes, including improved data and training efficiency, the ability to compute the viscosity solutions, and improved structure preservation compared to other popular approaches. I will also discuss some critical issues related to the critical points of the least squares functionals, the choice of activation functions, and network architecture.

Yunan Yang: When Optimal Transportation Meets PDE-Based Inverse Problems

Optimal transportation (OT) has emerged as an important area in mathematical analysis and applied mathematics since Monge introduced it in 1781. Over the last century, its deep ties with differential geometry and kinetics theory have been uncovered, with Kantorovich's groundbreaking work in 1942 highlighting its effectiveness in addressing real-world challenges. In recent years, we have applied the concept of quadratic Wasserstein distance, derived from OT theory, to a range of inverse problems and complex, high dimensional kinetic PDE-constrained optimization problems, e.g., waveform inversion and dynamical system modeling. This approach overcomes traditional methods' limitations, such as the least-squares method, by addressing issues like nonconvexity and sensitivity to noise, and it introduces a novel geometric framework for gradients. Many of these works started at UT Austin in collaboration with Prof. Bjorn Engquist.

Lexing Ying: Eigenmatrix for Unstructured Sparse Recovery

We consider unstructured sparse recovery problems in a general form. Examples include rational approximation, spectral function estimation, Fourier inversion, Laplace inversion, and sparse deconvolution. The main challenges are the noise in the sample values and the unstructured nature of the sample locations. We propose eigenmatrix, a data-driven construction with desired approximate eigenvalues and eigenvectors. It offers a new general framework for these sparse recovery problems. If time permits, we will also discuss its applications in deconvolution problems from free probability and statistics.

Hongkai Zhao: A Simple and Efficient Best Response Strategy for Mean-Field Games

A mean-field game (MFG) seeks the Nash Equilibrium of a game involving a continuum of players, where the Nash Equilibrium corresponds to a fixed point of the best-response mapping. However, simple fixed-point iterations do not always guarantee convergence. Fictitious play is a very simple iterative algorithm that leverages a best-response mapping combined with a weighted average. In this talk, I will present a simple and unified convergence analysis with explicit convergence rate for the fictitious play algorithm in MFGs of general types, especially non-potential MFGs. Based on this analysis, we propose two strategies to accelerate fictitious play. The first uses a backtracking line search to optimize the weighting parameter, while the second employs a hierarchical grid strategy to enhance stability and computational efficiency. We demonstrate the effectiveness of these acceleration techniques and validate our convergence rate analysis with various numerical examples.

Haomin Zhou: Parameterized Wasserstein Geometric Flow

I will present a parameterization strategy that can be used to design algorithms simulating geometric flows on Wasserstein manifold, the probability density space equipped with optimal transport metric. The framework leverages the theory of optimal transport and the techniques like the push-forward operators and neural networks, leading to a system of ODEs for the parameters of neural networks. The resulting methods are mesh-less, basis-less, sample-based schemes that scale well to higher dimensional problems. The strategy works for Wasserstein gradient flows such as Fokker-Planck equation, and Wasserstein Hamiltonian flow like Schrodinger equation. Theoretical error bounds measured in Wasserstein metric is established. This presentation is based on joint work with Yijie Jin (Math, GT), Wuchen Li (South Carolina), Shu Liu (UCLA), Hao Wu (Wells Fargo), Xiaojing Ye (Georgia State), and Hongyuan Zha (CUHK-SZ).

Panel Discussion: AI and the Future of Computational Mathematics

Speakers:

Tony Chan - Former president of KAUST and HKUST Tom Hou - Charles Lee Powell Professor of Applied and Computational Mathematics, California Institute of Technology David Kan - Vice President of Sales, COMSOL Inc. Richard Sharp - Senior Principal Data Scientist, Cambridge Mobile Telematics

Karen Willcox - Director, Oden Institute for Computational Engineering and Sciences

Abstract

The rapid integration of artificial intelligence into computational mathematics is transforming the way we model complex systems, solve large-scale problems, and advance scientific discovery. From AI-driven numerical solvers to machine-learning-assisted theorem proving, the synergy between AI and computational methods is reshaping the field in profound ways.

This panel will explore the impact of AI on scientific computing, numerical analysis, and mathematical modeling, addressing both the opportunities and challenges it presents. Additionally, we will discuss the evolving skill set needed for careers in computational mathematics, whether in academia, industry, or national laboratories. What programming and analytical tools will be essential for the next generation of computational mathematicians? How can researchers effectively integrate AI-driven techniques into traditional workflows while maintaining mathematical rigor?

Join us for an insightful discussion with experts from across the field as we examine the future of computational mathematics in an AI-augmented world.

