Innovative and Efficient Strategies for Stiff Differential Equations
Poster Session Abstracts
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A novel second-order accurate Strang splitting type exponential integrator for stiff systems

Saburi Rasheed, University of Louisiana at Lafayette

In this study, we construct a new second-order accurate exponential time differencing (ETD) scheme to solve two-dimensional semilinear parabolic problems with both nonsmooth and smooth initial and boundary data. The exponential integrator is also characterized by its L-stability, parallelizability, and computational efficiency. We utilize a non-Pad\' e type rational function, specifically, the real distinct pole (RDP), for approximating the matrix exponentials involved in the scheme. The novel Strang-splitting-type exponential integrator is employed to address various reaction-diffusion equations (RDEs) with homogeneous Dirichlet, Neumann, and periodic boundary conditions. Numerical examples validate that the proposed time-marching scheme is of second-order convergence rate and demonstrate superior accuracy and efficiency when compared with other competing second-order accurate ETD and implicit-explicit (IMEX) schemes.

SAV-based entropy-dissipative schemes for a class of kinetic equations

Shiheng Zhang, University of Washington

We introduce novel entropy-dissipative numerical schemes for a class of kinetic equations, leveraging the recently introduced scalar auxiliary variable (SAV) approach. Both first and second order schemes are constructed. Since the positivity of the solution is closely related to entropy, we also propose positivity-preserving versions of these schemes to ensure robustness, which include a scheme specially designed for the Boltzmann equation and a more general scheme using Lagrange multipliers.

Efficient Neural Network Methods For Numerical Partial Differential Equations

Cesar Herrera, Perdue University

ReLU neural networks (NNs) define a class of approximating functions capable of adaptively moving the mesh. In one dimension, this class is equivalent to free-knot linear splines (FKS), which can significantly improve approximation accuracy for non-smooth functions while drastically reducing the degrees of freedom. Unlike FKS, neural networks naturally extend to higher dimensions, making them a powerful tool for challenging problems with non-smooth or discontinuous solutions. A central difficulty is that determining the optimal adaptive mesh involves solving a high-dimensional, non-convex optimization problem. Our research aims to develop efficient neural network-based methods to address this challenge and use neural networks to tackle problems that are challenging for traditional mesh-based methods.

Stiffness in Deep Learning and How to Fix It

Fred Daum, Raytheon

Stiffness of the gradient flow is a crucial problem in deep learning. In particular, state-of-the-art methods (e.g., ADAM) adaptively adjust the learning rate to extremely small values (e.g., 0.0001 to 0.0000001). This is the same as using a tiny step size for numerical integration of the gradient flow to mitigate stiffness. The root cause is that the Hessian matrix of the loss function is very ill-conditioned, which is the same as the Jacobian of the gradient flow being ill-conditioned. In contrast, we do not use a gradient search, but rather we derive a completely new deep learning algorithm that minimizes the condition number of the Jacobian of the flow of particles. This allows us to increase the learning rate by many orders of magnitude relative to state-of-the-art deep learning methods. Typically our learning rate is on the order of 0.1 to 0.01. Hence, we can reduce the computer run time for training by many orders of magnitude.

Bounds-Constrained Finite Element Approximation of Time-Dependent Partial Differential Equations

John Stephens, Baylor University

Finite element methods provide accurate and efficient methods for the numerical solution of partial differential equations by means of restricting variational problems to finite-dimensional approximating spaces. However, they do not guarantee enforcement of bounds constraints inherent in the original problem. Previous work enforces these bounds constraints by replacing the variational equations with variational inequalities. We extend this approach to collocation-type Runge–Kutta methods for time-dependent problems, obtaining (formally) high order methods in both space and time. By using a novel reformulation of the collocation scheme, we can guarantee that the bounds constraints hold uniformly in time.