The Hong Kong University of Science and Technology

Department of Mathematics

PhD THESIS EXAMINATION

Overcoming Computational Barriers through Neural Network PDE Solvers: Theory, Methodology and Application

By

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ABSTRACT

This thesis addresses three fundamental challenges in traditional numerical methods for solving partial differential equations (PDEs) through strategic integration with deep learning techniques. First, for nonlinear time-evolution PDEs, we introduce a neural hybrid solver that uses a convolutional neural network trained by a novel implicit-scheme-informed learning strategy to predict initial guesses for Newton's method. The proposed approach significantly reduces iteration counts and achieves acceleration while preserving the structure of solutions. Theoretical analysis of how initialization affects the iteration count is provided. Additionally, we analyze the generalization error of the proposed unsupervised learning strategy in both fully-discrete and semi-discrete settings. Second, to overcome the Kolmogorov barrier in multiscale kinetic transport equations, we develop reduced order models (ROMs) to predict solutions under the parametric setting. We first develop a piecewise linear ROM by introducing a novel goal-oriented adaptive time partitioning strategy with the aid of a coarsening strategy. Next, for problems where a local linear approximation is not sufficiently efficient, we further develop a hybrid ROM, which strategically applies autoencoder-based nonlinear ROMs only when necessary. Numerical experiments show that the proposed ROMs successfully predict full-order solutions at unseen parameter values with both efficiency and accuracy. Finally, we introduce a novel neural operator, the Split-Step Fourier Method Network (SSFMnet), designed for a wide range of nonlinear PDEs. Following the basic idea of spectral collocation, SSFMnet integrates Fourier integral kernels within each Split-Step layer, effectively overcoming the limitations of previous block-wise AutoFlow network architectures, which struggled with strong nonlinearities. Our varying resolution tests confirm that the proposed neural solver is aliasing-free, establishing it as a genuine neural operator.

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The student's thesis is now being displayed on the reception counter in the General Administration Office (Room 3461).