

The Hong Kong University of Science and Technology

### **Department of Mathematics**

# **PhD THESIS EXAMINATION**

## **Overcoming Training Challenges in Neural Network based PDE** Solvers: Theory, Algorithms, and Applications

By

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#### <u>ABSTRACT</u>

Neural network-based methods have become a promising tool for solving partial differential equations (PDEs), especially in settings involving complex geometries, high dimensions, and integration with empirical data. Despite their flexibility, these models face training challenges such as slow convergence, and limited accuracy. This thesis systematically investigates the training dynamics and proposes algorithmic and theoretical advances to improve the efficiency of neural network based PDE solvers. First, we analyze the role of automatic differentiation (AD) and introduce a novel training metric, truncated entropy, to elucidate the superior performance of AD over finite difference (FD) methods from a training perspective. Next, by examining the spectral properties of associated kernel matrices, we quantify training difficulty via the concept of effective rank, and propose two initialization strategies — Partition of Unity (PoU) and Variance Scaling (VS) — that significantly improve convergence across frameworks such as PINNs, Deep Ritz, and DeepONet. Finally, we introduce Homotopy Dynamics, a framework designed to solve singularly perturbed problems by gradually deforming PDE parameters during training, with both theoretical convergence guarantees and strong empirical performance. Collectively, these contributions provide a principled foundation and practical tools for advancing the robustness, scalability, and applicability of neural network-based scientific computing.

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