The Hong Kong University of Science and Technology

Department of Mathematics

PhD THESIS EXAMINATION

PDE-Driven Methods for Scientific Discovery: Dislocation Simulation, Protein Design, and Neural PDE Solvers

By

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ABSTRACT

Partial differential equations (PDEs) serve as the cornerstone of mathematical modeling across scientific disciplines, from predicting material defects to simulating biomolecular interactions. This thesis demonstrates how embedding physical principles into computational algorithms can unlock new scientific capabilities, including material science, drug discovery and Neural PDE solvers. In the first part, we present a continuum formulation for dislocation climb velocity based on densities of dislocations. The obtained continuum formulation is an accurate approximation of the Green's function based discrete dislocation dynamics method. The continuum dislocation climb formulation has the advantage of accounting for both the long-range effects of vacancy diffusion and that of the Peach-Koehler climb force, and the two long-range effects are canceled into a short-range effect (integral with fast-decaying kernel) and in some special cases, a completely local effect. This obtained continuum dislocation climb velocity can be applied in any available continuum dislocation dynamics frameworks. In the second part, we propose Poisson Flow based AntiBody Generator (PF-ABGen), a novel antibody structure and sequence designer. We adopt the protein structure representation with torsion and bond angles, which allows us to represent the conformations more elegantly, and take advantage of the efficient sampling procedure of the Poisson Flow Generative Model. Our computational experiments demonstrate that PF-ABGen can generate natural and realistic antibodies in an efficient and reliable way. Notably, PF-ABGen can also be applied to antibody design with variable lengths. In the third part, we present a robust neural operator framework that enhances stability through adversarial training while preserving accuracy. We formulate operator learning as a min-max optimization problem, where the model is trained to achieve consistent performance under both normal and adversarial conditions. We demonstrate that our method not only achieves good performance on standard inputs, but also maintains high fidelity under adversarial perturbed inputs.

Date : **11 July 2025, Friday**

Time : **10:00 am**

Venue : **Room 4472 (Lifts 25-26)**

***Thesis Examination Committee*:**

Chairman	:	**Prof. Shuhuai YAO, MAE/HKUST**
Thesis Supervisor	:	**Prof. Yang XIANG, MATH/HKUST**
Member	:	**Prof. Zhichao PENG, MATH/HKUST**
Member	:	**Prof. Shing Yu LEUNG, MATH/HKUST**
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(Open to all faculty and students)

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