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Automated, Interpretable, and Scalable Scientific Machine Learning

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Although Artificial Intelligence (AI) has transformed vision and language modeling, Scientific Machine Learning (SciML) complements data-driven AI via a knowledge-driven approach, enhancing our understanding of the physical world. My work focuses on: 1) automating scientific reasoning with language models, 2) improving geometric interpretation, 3) developing foundation models for multiphysics.

Part 1: Automated PDE Control and Analysis with LLMs. Automating PDE control and analysis is crucial for dynamic systems like aerospace and fluid dynamics, where current methods are inefficient and lack scalability. My work focuses on automating, accelerating, and verifying PDE control using large language models (LLMs) to scale for real-world applications. We aim to synthesize boundary control inputs to optimize PDE systems in multiphysics applications like heat and wave propatation . LLMs translate control problems from natural to formal language, decompose tasks, and accelerate control across various PDE types (e.g., Heat, Navier-Stokes). Additionally, we automate well-posedness proofs for linear PDEs using semigroup theory and interact with tools like Lean to ensure correctness across diverse problem sets.

Part 2: Interpretable 3D Geometry Generation for Scientific Computing. 3D geometry generation can revolutionize scientific computing by enabling accurate modeling of complex dynamics, making it more interpretable. I focus on two core questions: ***(Q1)*** developing scalable, high-fidelity 3D methods that integrate heterogeneous views; ***(Q2)*** balancing computational efficiency with real-time accuracy. We bridge the gap between visual quality and simulation needs by integrating 3D reconstruction with fluid simulations, reducing uncertainty without ground-truth data. Our goal is to enhance data efficiency and generalizability using pretrained scientific models, focusing on sample generation and improved 3D reconstruction .

Part 3: Scalable Foundation Models for PDE Operator Learning. SciML faces two key challenges: the *need for extensive pretraining data* and *poor performance on unseen distributions*. To enhance data efficiency, I propose unsupervised pretraining for PDE operator learning using unlabeled PDE data and introduce a scalable in-context learning method that improves OOD performance without extra training costs . Our approach outperforms vision-pretrained models and handles challenging OOD cases, especially in high-frequency or chaotic dynamics. We further introduce Super-OOD-Bench , a comprehensive benchmark covering diverse physical systems, integrating domain-specific physics knowledge to boost OOD generalization.

Future Directions. I pursue broader scopes and impacts: 1) Automated control of distributed multiphysics systems with interactions across local agents; 2) More practical and realistic 3D geometries (water dams, clouds, airfoils); 3) Next-generation AI-enhanced fluid simulations that integrate data-driven and numerical methods. I will leverage my previous works on designing network architectures (highlighted as **"Featured Advance in Artificial Intelligence" in the US NSF newsletter (2022)**, winner of the **INNS and iSchools Doctoral Dissertation Awards (2024)**).

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