Riddhiman Raut

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Ph.D. candidate in Mechanical Engineering and Computational Science with expertise in scientific machine learning, graph neural networks, and high-performance computing. Experienced in developing efficient, scalable surrogate models for complex physics simulations. Seeking applied scientist and research roles at the intersection of AI, HPC, and computational modeling.

EDUCATION

The Pennsylvania State University, PA, USA Dec 2025
Ph.D. Mechanical Engineering, Minor Computational Science *GPA: 3.85*

EXPERIENCE

Pasteur Labs New York City, NY
Simulation Intelligence Intern May 2025 - August 2025

- Improved rollout stability in autoregressive surrogates by 40% for reliable long-horizon predictions
- Cut training time by 45% and compute needs by 87% using pushforward and temporal bundling
- Deployed novel, production-ready GNNs for steady-state modeling, expanding company's surrogate portfolio.
- Spearheading a review paper and position paper to publish scientific findings.

Tools used
Programming: Python (JAX, PyTorch, TensorFlow, DGL); **Machine Learning:** Large Language Models, Transformers, Graph Neural Networks, Neural Operators, Physics-informed Neural Networks; **High Performance Computing:** GPU acceleration **(**CUDA), Kernel Programming, Slurm, Distributed Data Parallel; **DevOps:** Azure ML, GitHub CI/CD

PROJECTS

Scalable Graph Neural Networks for Additive Manufacturing October 2023 - July 2024

- Built graph convolutional networks for scan-path optimization in laser powder bed fusion
- Demonstrated scalability and generalizability for 2x, 3x, and 4x domains using transfer learning
- Publication: "Scalable and transferable graph neural networks for predicting temperature evolution in laser powder bed fusion", ArXiv

Multiscale Graph Neural Networks for Turbulence Modeling August 2024 - May 2025

- Developed GNN architecture for modeling steady-state turbulent flow around turbine pin-fins, showing 10x improvement over GCNs, GraphSAGE, and MeshGraphNets
- Publication: "Multiscale graph neural network for turbulent flow prediction around complex pin-fin structures" [in review, *Physics of Fluids*]

Feature-interpretable Graph Neural Networks December 2024 - May 2025

- Built feature-specific interpretability module for multiscale message-passing graph neural networks
- Publication: "FIGNN: Feature-Specific Interpretability for Graph Neural Network Surrogate Models", [in review, *CMAME*]

Tools used
Programming: Python (PyTorch, PyG, DGL); **Machine Learning:** Transformers, Graph Neural Networks, Neural Operators, Physics-informed Neural Networks; **High Performance Computing:** CUDA, Slurm, Distributed Data Parallel; **Software:** ANSYS, OpenFOAM, Autodesk Netfabb, COMSOL

LEADERSHIP, COURSEWORK, & ADDITIONAL SKILLS

Leadership

- Mentoring Schreyer Honors student in research on Geometric Neural Operators and Diffusion Models.
- Delivered graduate-level lectures on machine learning.

Skills
Programming: C++ (OpenMP, MPI, CUDA), Julia, ROS; **High Performance Computing:** GPU Kernel Programming