Cooper Delaney Lorsung

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Education

Carnegie Mellon University — **Pittsburgh, Pennsylvania**
Doctor of Philosophy (PhD) in Mechanical Engineering — December 2024 (Expected)

Harvard University — **Cambridge, Massachusetts**
Master of Engineering in Computational Science and Engineering — May 2021

University of Illinois at Urbana-Champaign — **Urbana, Illinois**
Bachelor of Science with Honors in Engineering Physics — May 2019
Awards: Robert E. Hetrick Outstanding Undergraduate Research Award

PhD Research Experience

PhD Candidate - Carnegie Mellon University — July 2021 - Present
Advisor: Amir Barati Farimani
Thesis: *Pretraining and Transformers for Accelerating Solutions to Partial Differential Equations*

Explain Like I'm Five: Using LLMs to Improve PDE Surrogate Models with Text

- Developed multimodal framework for PDEs using popular Llama and SentenceTransformer LLMs
- Generated benchmark data sets by varying coefficients, boundary conditions, and initial conditions
- Showed up to 64.2% reduction in error on autoregressive rollout and 21% in next-step prediction

Physics Informed Contrastive Learning

- Developed a weighted contrastive learning approach that utilizes physics-informed loss function
- Designed novel magnitude-aware cosine similarity metric to measure similarity of PDE systems
- Improved fine-tuning performance for multiple neural operator models across different data sets

Physics informed token transformer for solving partial differential equations

- Constructed a novel text-based encoding of 2D Navier-Stokes, 1D Heat, Burgers, and KdV equations
- Designed multiview framework to train transformer and physics-based model embeddings
- Evaluated framework showing up to an order of magnitude reduction in error for 1D and 2D tasks

Mesh Deep Q Network: A Deep Reinforcement Learning Framework for Mesh Improvement in Computational Fluid Dynamics

- Developed Double DQN Framework to remove vertices in CFD mesh and preserve calculated drag value
- Implemented Graph Neural Network based Deep Q Network for vertex selection and action evaluation
- Deployed network that removed 5% of vertices in a 2D airfoil mesh with drag error within 0.1%

Additional Research Projects

Water Model Designed with Symbolic Regression

- Adapted existing many-particle Graph Neural Network model to learn forces in water simulations
- Developed force extraction procedure to allow for symbolic regression of GNN predictions
- Found current GNNs are unable to reliably distinguish between Coulomb and Lennard-Jones forces

High-Throughput Segregation Kinetics and Identification of Metastable Surface Alloys by DRL

- Parallelized CatGYM environment for surface segregation kinetics learning
- Adapted CatGYM to computing clusters using Ray in order to leverage pretrained energy calculators
- Ran binary and ternary Pd-Ni-Au alloys to determine surface segregation kinetics

AugLiChem: Data Augmentation Library of Chemical Structures for Machine Learning

- Deployed open-source package with automatic data downloading and data preprocessing
- Tuned data augmentation techniques for material and molecular data for Graph Neural Networks
- Improved Predictive accuracy up to 37% for popular GNN models and data sets

Skills

- Programming Languages: significant experience with Python, familiar with C++, CUDA
- Machine Learning Libraries: PyTorch, Scikit-Learn, Numpy, Scipy, Matplotlib, HuggingFace
- Parallel Computing: Slurm, developing with RLLib and Python Multiprocessing, familiar with OpenMPI
- Methods: Computational Fluid Dynamics, Molecular Dynamics, Density Functional Theory
- Tools: LAMMPS, VMD, OpenMM, FEniCS, GMsh
- Containerization: familiarity with Docker, Singularity

Additional Research Experience

Masters Research - Harvard University January 2020 - May 2021

Advisor: Weiwei Pan, Principal Investigator: Finale Doshi-Velez

Thesis: *Understanding Uncertainty in Bayesian Deep Learning*

Uncertainty-Aware (UNA) Bases for Bayesian Regression using Multi-Headed Auxiliary Networks

- Helped develop framework for uncertainty awareness in Neural Linear Models with auxiliary regressors
- Implemented robust and replicable experimental pipeline for benchmarks and downstream tasks
- Developed Radial Uncertainty Benchmark for evaluation of predictive uncertainty in data scarce regions

Additional Research Projects

Advisor: Sauro Succi

Solving the Fokker-Planck Equation for 1-D Protein Folding Potential

- Solved and analyzed the Fokker-Planck equation for a protein folding potential numerically
- Found eigenvalues and eigenvectors evolved randomly using horizontal visibility graph method

Undergraduate Research Assistant - UIUC May 2018 - August 2019

Advisor: Lucas Wagner

Benchmarking Diffusion Monte Carlo against VASP for Silicon-Oxygen Compounds

- Ran Density Functional Theory calculations to calculate trial wavefunction used in Quantum Monte Carlo
- Explored many sources of error including basis set, finite size effects, and k-point resolution

PyQMC: A python module that implements real-space quantum Monte Carlo techniques.

- Implemented reblocking for error estimation correlated time-series data
- Added force-bias monte carlo moves and electron-ion interaction in the Jastrow factor for PyQMC

Selected Publications

[1] Thakur, S., **Lorsung, C**, et. al. "Learned Uncertainty-Aware (LUNA) Bases for Bayesian Regression using Multi-Headed Auxiliary Networks." ICML Workshop on Uncertainty and Robustness in Deep Learning (2020)

[2] Magar, R., Wang, Y., **Lorsung, C.**, Liang, C., Ramasubramanian, H., Li, P., & Farimani, A. B. (2022). AugLiChem: data augmentation library of chemical structures for machine learning. Machine Learning: Science and Technology, 3(4), 045015. doi:10.1088/2632-2153/ac9c84

[3] **Lorsung, Cooper**, and Amir Barati Farimani. 'Mesh Deep Q Network: A Deep Reinforcement Learning Framework for Improving Meshes in Computational Fluid Dynamics'. *AIP Advances*, vol. 13, no. 1, Jan. 2023, p. 015026, https://doi.org10.1063/5.0138039.

[4] **Lorsung, C.**, Li, Z., Barati Farimani, A. "Physics informed token transformer for solving partial differential equations". 2024 Mach. Learn.: Sci. Technol. 5 015032

[5] Zhou, A., **Lorsung, C.**, Hemmasian, A., Barati Farimani, A. "Strategies for Pretraining Neural Operators". *Transactions on Machine Learning Research,* 2024, https://openreview.net/pdf?id=9vEVeX9oIv

[6] **Lorsung, C.**, Barati Farimani, A. "PICL: Physics Informed Contrastive Learning for Informed Contrastive Learning for Partial Differential Equations", in submission at *APL Machine Learning*

Projects

Carnegie Mellon University 10-714: Deep Learning Systems Fall 2023

Automatic Differentiation for Implicit Neural Networks

- Developed automatic differentiation package *Needle*
- Implemented backpropagation for standard mathematical operations with C++ and CUDA backends
- Trained implicit layers for numerical optimization of constraints

Harvard University AM205: Advanced Scientific Computing: Numerical Methods Fall 2019

Techniques for Missile Tracking, Projection, and Interception

- Designed missile interception algorithm using finite difference based projection of system variables
- Implemented enemy and response missile system that resulted in successful interception

Teaching Experience

Teaching Assistant - Carnegie Mellon University

- 24-888: Introduction to Deep Learning - online course design Fall 2023
- 24-788: Introduction to Deep Learning/24-789: Intermediate Deep Learning For Engineers Spring 2023

Teaching Fellow - Harvard University

- AM 207: Advanced Scientific Computing: Stochastic Methods for Data Analysis, Inference and Optimization Fall 2020
- CS109a/AC209a: Data Science 1: Introduction to Data Science Fall 2020