Cooper Delaney Lorsung

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Education

Carnegie Mellon University **August 2021 - Present**

Doctor of Philosophy (PhD) in Mechanical Engineering

Harvard University **August 2019 - May 2021**

Master of Engineering in Computational Science and Engineering

Thesis: *Understanding Uncertainty in Bayesian Deep Learning* advised by Weiwei Pan

University of Illinois at Urbana-Champaign **August 2015 - May 2019**

Bachelor of Science with Honors in Engineering Physics

Awards: Robert E. Hetrick Outstanding Undergraduate Research Award

Research Experience

Carnegie Mellon University, PhD Candidate **July 2021 - Present**

PI: Amir Barati Farimani

Multiview Neural Operator Learning

- Designed a novel text-based encoding of 2D Navier-Stokes, 1D Heat, Burgers, and KdV equations
- Used popular Neural Operator models like Fourier Neural Operators for physics-based data driven learning
- Designed multiview framework to pretrain transformer and physics-based model embeddings

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

- Developed Double DQN Framework to iteratively remove vertices in CFD mesh while preserving calculated drag value
- Used Graph Neural Network based DQN for vertex selection and action evaluation
- Successfully removed 5% of vertices in a 2D airfoil mesh with computed drag error within 0.1%

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
- Successfully recovered Argon Lennard-Jones parameters
- 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 Deep Reinforcement Learning

- 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

- Tuned data augmentation techniques for chemical and molecular data for use with Graph Neural Networks (GNN)
- Benchmarked popular GNN models across various datasets, showing improved predictive accuracy
- Developed open-source package with automatic data downloading and preprocessing

Harvard University, Graduate Researcher **January 2020 - May 2021**

Advisor: Weiwei Pan, PI: Finale Doshi-Velez

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

- Helped develop framework for uncertainty awareness in Neural Linear Models
- Encodes uncertainty using auxiliary regressors and Gaussian Process reference functions
- Designed and implemented experimental pipeline for standard benchmarks and downstream tasks, leading to more robust and replicable results
- Developed Radial Uncertainty Benchmark for evaluation of predictive uncertainty in data scarce regions

Solving the Fokker-Planck Equation for 1-D Protein Folding Potential, PI: Sauro Succi

- Numerically solved and analyzed the Fokker-Planck equation for a protein folding potential
- Decomposed the potential with spectral methods using Chebyshev basis
- Analyzed potential's eigenvalue and eigenvector evolution using the horizontal visibility graph method

University of Illinois at Urbana-Champaign, Undergraduate Researcher **May 2018 – August 2019**
PI: 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
- Implemented force-bias monte carlo moves and electron-ion interaction in the Jastrow factor for PyQMC

Work Experience

Carnegie Mellon University, Teaching Assistant **January 2023 - Present**

- 24-788: Introduction to Deep Learning/24-789: Intermediate Deep Learning For Engineers Mini Courses
- Designed homework and recitation for training Neural Networks, Diffusion models, and handling data
- Hosted office hours and graded homeworks

Harvard University, Teaching Fellow **August 2020 - December 2020**

- AM 207: Advanced Scientific Computing: Stochastic Methods for Data Analysis, Inference and Optimization
- Held office hours and advised final projects on deep bayesian models
- CS109a/AC209a: Data Science 1: Introduction to Data Science
- Held office hours, graded, and advised final projects on lifetime mortality estimation

Technologies

- Python: significant experience with standard machine learning libraries such as PyTorch, Scikit-Learn, Numpy, Scipy, Matplotlib
- Parallel Computing: using Slurm and Torque, developing with RLLib, and python multiprocessing
- Methods: Computational Fluid Dynamics, Molecular Dynamics, Density Functional Theory
- Containerization: experience with Docker and Singularity

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] Wheeler, William A., et al. "Pyqmc An All-Python Real-Space Quantum Monte Carlo Module in pyscf." *The Journal of Chemical Physics*, vol. 158, no. 11, 2023, p. 114801, https://doi.org/10.1063/5.0139024.

In Submission

[1] Cao, Z., Wang, Y., **Lorsung, C.**, Barati Farimani, A. "Neural Network Predicts Ion Concentration Profiles under Nanoconfinement" in submission at *The Journal for Chemical Physics*

[2] **Lorsung, C.**, Li, Z., Barati Farimani, A. "Physics Informed Token Transformer" in submission at *The Journal for Computational Physics*

Open Source Contributions:

AugLiChem: modularized data augmentations and adapted AugLy framework to our use case, implemented automatic data downloading, cleaning, and processing for ease of use in model training,

Mesh Deep Q Network: designed airfoil mesh environment, parallelized DQN training using RLLib's Ray, designed robust data pipeline from airfoil, to simulation, to DQN training, adapted docker image to singularity

PyQMC: Implemented reblocking for error estimation correlated time-series data and force-bias monte carlo moves and electron-ion interaction in the Jastrow factor for PyQMC during the early stages of development