Shehtab Zaman

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Education

Binghamton University, State University of New York

Ph.D in Computer Science	Expected 2023
Master of Science in Computer Science - 3.9/4.0	December 2020
Bachelor of Science in Mathematical Physics with a Minor in Computer Science - 3.9/4.0	January 2019

Technical Skills

Programming Languages	Python, C++, JavaScript, Java, SQL, Mathematica
Proficient	Unix, Git, CUDA, MySQL, MongoDB, PyTorch, LaTeX, Angular, Numpy, NVSHMEM

Professional Experience

CS Department - Binghamton University – *Graduate Research Assistant*   **December 2019 - Present**

- Led a team of undergraduate and graduate students to study and optimize 3D generative modelling in collaboration with Total Energies
- Co-authored, designed, and maintained open-source library for highly optimized 3D grid generation
- Designed and implemented a novel deep learning workflow based on matrix product states to solve quantum Ising models
- Developed deep generative machine learning models for inverse materials design of novel metal-organic frameworks (MOF) using 3D GANs and VAEs
- Created deep neural network models such as 3D-CNN and GCNN for high throughput property characterization of MOFs

Lawrence Livermore National Laboratory – *Computing Scholar*   **May 2022 - August 2022**

- Parallelized graph neural network via partition parallelism to support billion scale graphs on the Livermore Big Artificial Neural Network (LBANN) toolking
- Implented first of it's kind shared memory GPU kernels for Gather-Scatter operations using NVidia's NVSHMEM library
- Performed kernel profiling and tooling on multi-GPU distributed CUDA kernels

Lawrence Livermore National Laboratory – *Computing Scholar*   **May 2021 - August 2021**

- Implemented generic edge-conditioned graph neural network on LBANN
- Implemented distributed tensor parallel edge convolution kernels for generic graph neural networks utilizing NCCL-based GPU-GPU communications
- Achieved and 12x strong scaling on 16 and 93x weak scaling 100 GPUs on molecular graph energy prediction

Lawrence Livermore National Laboratory – *Data Science Institute - Research Scholar*   **May 2020 - August 2020**

- Investigated scalable geometric and 3D deep learning with the LBANN toolkit on GPU accelerated HPC systems
- Implemented distributed, GPU accelerated Graph Convolutional Neural Networks in Python and C++
- Designed custom data ingestion pipelines for Numpy,and HDF5 files for high performance computing workloads on HPC systems

CS Department - Binghamton University – *Automata Theory Teaching Assistant*   **January 2019 - December 2019**

- Prepared materials for and lectured during weekly 1.5 hour discussion class on models of computation
- Led weekly tutorial sessions with students in small groups to assist students with learning objectives, and assignments

Information Technology Services - Binghamton University – *Computing infrastructure Intern*   **May 2019 - August 2019**

- Documented cluster usage workflows with SLURM, Singularity, and LMOD for research faculty to best utilize the 166 node cluster
- Explored usability and implementation of containerization with Docker and Singularity, and a science gateway on top of the high performance cluster

Publications & Posters

ParticleGrid: Enabling Deep Learning using 3D Representation of Materials　　**October 2022**
Ethan Ferguson*, Shehtab Zaman*, Cecile Pereira, Denis Akhiyarov, Mauricio Araya-Polo, Kenneth Chiu
IEEE 18th International Conference on eScience (eScience) 2022

Parallelizing Graph Neural Networks via Matrix Compaction for Edge-Conditioned Networks　　**May 2022**
Shehtab Zaman, Tim Moon, Tom Benson, Sam Adé Jacobs, Kenneth Chiu, Brian Van Essen
22nd IEEE International Symposium on Cluster, Cloud and Internet Computing (CCGrid) 2022

MoleculeFlow: A Deep Generative Workflow for 3D Molecular Generation　　**December 2021**
Ethan Ferguson*, Shehtab Zaman*, Mauricio Araya-Polo, Denis Akhiyarov, Kenneth Chiu, Cécile Pereira
ELLIS Machine Learning for Molecule Discovery Workshop

Graph Neural Network for Metal Organic Framework Potential Energy Approximation　　**December 2020**
Shehtab Zaman, Christopher Owen, Kenneth Chiu, Michael Lawler
ML for Molecules Workshop at NeurIPS 2020

Real-Space Visualization of Quantum Phase Transition by Network Topology　　**July 2019**
Shehtab Zaman, Wei Cheng Lee
Physical Review E Vol. 100 Issue 1

Towards Run Time Estimation of the Gaussian Chemistry Code for SEAGrid Science Gateway　　**July 2019**
Angel Beltre, Shehtab Zaman, Kenneth Chiu, Sudhakar Pamidighantam, Xingye Qiao, Madhusudhan Govindaraju
Practice & Experience in Advanced Research Computing Conference

Presentations

ParticleGrid: A Library for 3D Molecular Representation for Deep Learning　　**March 2022**
Shehtab Zaman, Ethan Ferguson, Kenneth Chiu, Mauricio Araya, Denis Akhiyarov, Cecille Pereira
APS March Meeting 2022

Graph Neural Network for Metal Organic Framework Potential Energy Approximation: Energy Landscape Database and Rigidity　　**March 2021**
Christopher Owen, Shehtab Zaman
APS March Meeting 2021

Towards Inverse Design of Metal-Organic Frameworks to Maximize Hydrogen Storage using Deep Learning　　**March 2021**
Kevin Phillips, Shehtab Zaman, Kenneth Chiu, Michael Lawler
APS March Meeting 2021

Predicting Geometric Properties of Metal-Organic Frameworks by Fusing 3D and Graph Convolutional Neural Networks　　**March 2021**
Jacob Barkovitch, Musen Zhou, Shehtab Zaman, Ken Chiu, Michael Lawler, Jianzhong Wu
APS March Meeting 2021

Honors & Awards

Teaching Assistant of the Year – *Computer Science Department*　　**January 2020**
- Awarded for excellence as the Computing and Automata Theory teaching assistant

Robert J Penfield Award – *Undergraduate Award for Junior Physics Student*　　**April 2018**
- Awarded due to outstanding academic promise in physics

Hack Cooper Finalist and Best Video Hack Winner – *Immerse*　　**October 2016**
- Created a touch-free gesture controlled media player that feature an infrared sensor