AYUSH JAIN

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EDUCATION

Georgia Institute of Technology; Atlanta, Georgia G.P.A.– 3.76
Ph.D. Computational Science & Engineering *Expected Graduation: Dec 2025*
M.S. Computational Science & Engineering *Graduation: May 2024*

Georgia Institute of Technology; Atlanta, Georgia G.P.A.– 3.74
B.S. Materials Science & Engineering *Graduation: May 2021*

EXPERIENCE

Carbon3D May 2023 – Nov 2023
ML Research Intern *Redwood City, CA*

- Built Carbon's first AI for Simulation engine, using geometric data from 100+ finite element simulations with 1M+ elements each, utilized PyTorch, Deep Graph Library, and C++; highlighted in an NVIDIA Technical Blog
- Published LatticeGraphNet, a Graph Neural Operator to predict the compressive responses of latticed elastomeric meta-materials; *Engineering With Computers, 2024*
- Implemented streamlined transformation of low dimensional geometric lattices in Carbon's DesignEngine, in C++

Ramprasad Group Aug 2021 – Present
Graduate Research Assistant, Polymer Manufacturing Informatics *Atlanta, GA*

- Building an autonomous robotic experimentation platform for materials discovery by integrating GROMACS, PyTorch, PostgreSQL, Flask, and custom Bayesian optimization software
- Developed PolyGen, a latent diffusion model that generates periodic, DFT-accurate 3D polymer structures from repeat unit chemistries, capturing conformational flexibility and connectivity. Preprint.
- Implemented a closed-loop active learning module that uses multi-objective noisy Bayesian optimization to aid the scientific discovery of novel 3D printing materials; *ACS Applied Materials & Interfaces, March 2024*
- Pioneered a novel Physics-Enforced NN that increased physical intuition of materials properties by >7x, using PyTorch; *Presented at NeurIPS AI4Mat Workshop 2024, Nature npj Computational Materials, Feb 2025*

Zitara Technologies (Startup) June 2021 – Aug 2021
Employee #12 – Data Science and Software Engineering Intern *San Francisco, CA*

- Created a validation pipeline to pinpoint production ML model errors in battery health prediction throughout a product's lifecycle, using Pandas, Numpy, and Scikitlearn
- Built lab automation and alert tools that tracked battery experiment progress and detected anomalies by integrating Google Sheets API, Slack API, AWS S3, experiment sensor data, and Jenkins for CI/CD

Hewlett Packard May 2020 – Dec 2020
Machine Learning Intern *Corvallis, OR (REMOTE)*

- Benchmarked a Generative Adversarial Network (GAN) to predict 3D printed part deformation, using Tensorflow
- Built data pipelines to process and load 500+ 3D finite element simulation results to GAN inputs

GE Aviation June 2019 – Aug 2019
Data Science Intern *Newark, DE*

- Implemented a time-series anomaly detection model on nano-layer deposition processes with an 85% success rate, using R with integrated real-time SQL queries
- Reduced process failure by 75% by correcting a parameter based on data from 100+ manufacturing cycles

PROJECTS

Sci-LLM *Present*

- Bridging natural language and Bayesian optimization to accelerate small-batch scientific research.

NLP for Social Impact of MonkeyPox Dec 2022

- Identified hostile sentiment of MPox conversations on Reddit using BERT and Linear Discriminant Analysis
- Designed classification metrics and conducted a taxonomy of 19K+ conversations, collected using PushShift API

ADDITIONAL SKILLS

Technical: High Performance Computing Clusters, Molecular Dynamics, Computer Vision, NLP, AWS S3, CI/CD

Software: Python, C/C++, MPI, Java, SQL, R, MATLAB, Javascript (D3), Hadoop, Spark