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Alexa (Stewart) Freeman

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Career Objectives

Recent Computational Science and Engineering graduate pursuing full-time research or data scientist roles in Machine Learning, Data Science, or Scientific Computing.

Education

Georgia Institute of Technology, M.S. in Computational Science and Engineering *Expected August 2025*

Massachusetts Institute of Technology, B.S. from the Department of Physics *June 2022*

Publications

Ahrens, J., Arienti, M., et al., (2024). The ECP ALPINE project: In Situ and Post Hoc Visualization Infrastructure and Analysis Capabilities for Exascale.

Stewart, A., Terece L. Turton, David Rogers, James P. Ahrens, Soumya Dutta, (2022). Visualizing MFIX-Exa Codes for Chemical Looping Combustion.

Stewart, A., Lo, L.T., Korobkin, O., Sagert, I., Loiseau, J., Lim, H., Kaltenborn, M., Mauney, C., & Miller, J.. (2021). Realistic Kilonova Up Close.

Awards & Leadership

The International Conference for High Performance Computing: Scientific Visualization & Data Analytics Showcase, Finalist (2022).

The International Conference for High Performance Computing: Scientific Visualization & Data Analytics Showcase, Finalist (2021).

Community Service Chair, Boston AO Downtown Ministry (2021-2022).

Musical Director, MIT Asymptones (2019-2021).

Skills

Machine Learning: PyTorch, CNNs, Support Vector Machines, TensorFlow, Ridge Regression, LASSO, Naive Bayes, Style Transfer, PINNs, NLP, LLM, Neural Networks, OpenMP, Slurm, HPC.

Data Science / **Visualization:** Python, C++, Linux OS, BASH, Julia, Algorithm Development, Conda, Spack, MATLAB, R, Ascent, Paraview, yt Project, Jupyter, Colab, Pandas, NumPy, Matplotlib, Github. **Communication:** Teaching, Research, Scientific Visualization, Presentation and Organizational Skills.

Student Projects

<u>Multifidelity Modeling of Lagrangian Hydrodynamics Simulation</u> For a course at the Georgia Institute of Technology (Fall 2023)

https://github.com/astew95/nsm sml

o Collaborated with team members to investigate a learned correction term inside a multilayer perceptron (MLP) architecture, a novel approach when compared with current Scientific ML research methods.

o Produced a technical presentation as part of the Scientific Machine Learning Course Symposium at the Georgia Institute of Technology.

Physics-Informed Gram Matrix for Style Transfer

For a course at the Georgia Institute of Technology (Spring 2024)

https://github.com/astew-95/physical-style-transfer/tree/main

- o Deployed Style Transfer algorithm on novel dataset to extract meaningful patterns from CFD simulation data.
- O Demonstrated proficiency in implementing and understanding Convolutional Neural Networks (CNNs) through extracting and analyzing intermediate features in the Network.
- Proposed a novel physical interpretation of the Gram Matrix within Scientific Machine Learning applications.

Machine Learning for Drug Discovery of Lipid Nanoparticles

Undergraduate Research at the MIT Anderson Laboratory (Spring 2020)

- o Applied machine learning algorithm to SMILES representation data to support the discovery of molecular candidates for the activation of luciferase for LNP (lipid nanoparticles).
- o Improved lab-developed PyTorch ML pipeline through evaluating model performance, implementing cross-validation, and enhancing code readability.

Selected Experience

Graduate Research in the John Wise Lab

September 2023 – December 2023

- Leveraged The yt Project, a Python-based science toolkit to process and analyze HDF5 simulation data of cosmological particle simulations.
- Managed and processed data at scale through distributed computing practices, utilizing Georgia Tech's distributed HPC clusters.
- Created visualizations of large-scale simulations and conducted data analysis.
- Demonstrated proficiency in Python-based scientific computing and data tools, supporting high-impact research.

<u>Teaching Assistant – Georgia Institute of Technology, Atlanta, GA</u>

August 2022 – May 2024

- Graduate Teaching Assistant for Undergraduate courses Mathematical Physics and Introductory Physics I.
- Responsible for Grading and Student Evaluation.

Summer Student/Student Developer – Los Alamos National Laboratory, Los Alamos, NM May 2021 – November 2022

- Integrated a many-core capable visualization framework with LANL-developed physics simulation code leveraging git, BASH programming, Spack, python, and C++ API.
- Systematically determined bugs and installation issues of Ascent on Virtual Machines, working closely with developers to understand user-end software outcomes.
- CCS-3 Summer Student Finalist at the Scientific Visualization Showcase for HPC (2021 / 2022)
- Produced visualization of Lagrangian fluid simulations of compact objects using ParaView from LANL developed code. Rendered a realistic image of kilonova ejecta as it would appear for a nearby observer (2021).

Undergraduate Research – MIT Anderson Lab, Cambridge, MA

January 2020 – August 2020

- Applied machine learning algorithm to chemical structure data to support the discovery of molecular candidates for the activation of luciferase for LNP (lipid nanoparticles).
- Conducted data cleaning, cross-validation with over 90% validation error, and performance evaluation to understand limitations in generalizability.
- Improved Lab-developed PyTorch pipeline using Lab-oriented Best-practice Software Principles.

<u>Undergraduate Research – MIT Media Laboratory</u>

January 2020 – June 2020

- Deployed classification models to predict demographic features (race/gender) from fellowship applicant data using PyTorch.
- Engineered a data pipeline from scratch using web-scraping methods to source, clean, preprocess, and standardize over 40,000 fellowship records, including handling incomplete and inconsistent entries.
- Presented results to inform institutional analysis of equity in prestigious fellowship programs.