Matthew Adams
https://mattaadams.github.io/
Email : mattaadams1@gmail.com
Mobile : +1-865-951-9994

Experience

MN-AM Remote
Software Engineer *2023 - Present*

- **Worked asynchronously within a global development team across multiple time zones**, contributing to feature development, performing code reviews, and writing unit tests while coordinating through GitLab, Jira, and Microsoft Teams.
- Automated an expert-curated scientific **classification model** in Python and integrated it into the software backend, accelerating expert-driven research
- Identified and resolved bottlenecks in a predictive model by optimizing data pipeline workflows and file processing, achieving an **80% reduction in runtime**.

U.S. Environmental Protection Agency Durham, NC
Data Modeling Specialist (ORAU Subcontractor) *2021 - 2023*

- Improved a **Feature Engineering** method by transforming a chemical fingerprinting tool into a more universal format to allow for expanded applications in toxicology predictions of target chemical substances
- Performed in-depth pairwise comparison analysis across different chemical fingerprint sets using **Exploratory Data Analysis** to identify differences in information captured across chemical spaces.
- Developed **data pipelines** which extracted and aggregated data from MongoDB collections and transformed to loaded into multiple machine learning (ML) models
- Implemented a **Graph Neural Network** model in Python which led to a predictive capacity improvement of 20% in comparison with traditional ML models

Carnegie Mellon University Pittsburgh, PA
Graduate Research Assistant *2019 - 2020*

- Performed in-depth **statistical analysis** of composition effects on catalyst surface performance with computational calculations to reduce the required search space for screening by 70%
- Designed a flexible framework with PyTorch for **active learning with Deep Learning Neural-Network** potentials leading to a reduction of 60% in computational time while maintaining accurate results
- **Manipulated large dataframes** containing atomic structure information with MongoDB database in Python
- Collaborated in improvement of projects through implementation of **Continuous Integration**

Oak Ridge National Laboratory Oak Ridge, TN
Research Intern *Summer 2019*

- Implemented a unique workflow through combining density functional tight binding with metadynamics which **accelerated scanning** of the free energy profile of a system by a factor of 1000
- Implemented **neural-network assisted molecular dynamics simulations** to reduce the error below 10%.
- Ran Python Jupyter notebook experiments for **neural network hyper-parameter optimization**.

Education

Carnegie Mellon University Pittsburgh, PA
Master of Science in Chemical Engineering *2020*

University of Tennessee, Knoxville Knoxville, TN
Bachelor of Science in Chemical Engineering *2019*

Skills

- **Languages**: Python, JavaScript, SQL, CSS/HTML, Bash
- **Frameworks**: PyTorch, TensorFlow, Django, NodeJS, ReactJS
- **Technologies**: Docker, Kubernetes, REST APIs, MongoDB, Git, GitLab, VSCode, Linux (Ubuntu), Jira, Confluence

Projects

For additional projects and source code, visit https://mattaadams.github.io/

Q-Wall Game (Personal Project) | *Python (TensorFlow, Pygame)*

- Developed a **Deep Q-Learning** agent in TensorFlow capable of accurate navigation inside a Pygame environment

Sorting Algorithm Visualizer (Personal Project) | *JavaScript, ReactJS, HTML/CSS*

- Developed and deployed a website app through GitHub Pages which **visualizes popular sorting algorithms**

ReciPy Maker (Personal Project) | *Python (Django, Scikit-learn), Bootstrap, PostgreSQL, Docker, Heroku, AWS (S3)*

- Utilized Python scripts to scrape web data for data collection and transformation using BeautifulSOUP
- Created a Django Website App which allows for users to create and save their favorite recipes
- Implemented and deployed a Recipe Recommendation System with a **RESTful API** using Django Rest Framework

Publications

1. Grace Patlewicz, Antony J. Williams, Matthew Adams, Imran Shah, and Katie Paul-Friedman. A cheminformatics workflow to select representative tsca chemicals for new approach methodology (nam) screening. *Chemical Research in Toxicology*, 38(1):129–144, 2025. PMID: 39655894

2. Matthew Adams, Hannah Hidle, Daniel Chang, Ann M. Richard, Antony J. Williams, Imran Shah, and Grace Patlewicz. Development of a csrml version of the analog identification methodology (aim) fragments and their evaluation within the generalised read-across (genra) approach. *Computational Toxicology*, 25:100256, 2023

3. Ann M. Richard, Ryan Lougee, Matthew Adams, Hannah Hidle, Chihae Yang, James Rathman, Tomasz Magdziarz, Bruno Bienfait, Antony J. Williams, and Grace Patlewicz. A new csrml structure-based fingerprint method for profiling and categorizing per- and polyfluoroalkyl substances (pfas). *Chemical Research in Toxicology*, 36(3):508–534, 2023

4. Muhammed Shuaibi, Yuge Hu, Xiangyun Lei, Benjamin M. Comer, Matt Adams, Jacob Paras, Rui Qi Chen, Eric Musa, Joseph Musielewicz, Andrew A. Peterson, Andrew J. Medford, and Zachary Ulissi. Amptorch: A python package for scalable fingerprint-based neural network training on multi-element systems with integrated uncertainty quantification. *Journal of Open Source Software*, 8(87):5035, 2023