Ellis R. Crabtree

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Education

Johns Hopkins University — Baltimore, MD
Doctor of Philosophy (Ph.D.) in Chemical and Biomolecular Engineering — *Aug. 2019 – June 2024*

Johns Hopkins University — Baltimore, MD
Master of Science (M.S.) in Applied Mathematics and Statistics — *Aug. 2022 – June 2024*

The University of Alabama — Tuscaloosa, AL
Bachelor of Science in Chemical Engineering — *Aug. 2014 – May 2019*

Experience

NASA Postdoctoral Fellow — June 2024 – Present
NASA Marshall Space Flight Center — *Huntsville, AL*

- Supporting the biological and physical sciences division as well as the materials and processes division, primarily focusing on computational modeling
- Developed machine learning generative models to generate alloy compositions consistent with prescribed microscopic properties as well as predict other properties of the generated compositions
- Developed finite element analysis code to simulate aluminum alloys undergoing welding and used the produced thermal data to model precipitation

PhD Candidate — Aug. 2019 – June 2024
Johns Hopkins University — *Baltimore, MD*

- Utilized generative models (including, but not limited to GANs, Diffusion Models, LLMs, VAEs, etc.) and dimensionality reduction methods for expediting the sampling of dynamical systems
- Participated in many collaborative research projects pertaining to the computational analysis of dynamical systems, particularly of systems involving small molecules and chemical reactors
- Acted as system administrator for local HPC server, managing packages, job queueing system, and other aspects to facilitate projects that required high amounts of compute

Visiting Data Scientist — June 2022 – June 2023
Sandia National Labs — *Livermore, CA*

- Developed deep learning architectures and numerical methods for reduced-order modeling and uncertainty quantification of systems of interest to the DOE
- Researched the use of dimensionality reduction methods to produce reduced-order surrogate models for microstructure evolution in alloys and composite materials

Projects

GAN and Diffusion Model Assisted Sampling | *Python, Pytorch, OpenMM, Git* — June 2020 – Present

- Developed a framework to use ML generative models in tandem with physics-based simulations
- Developed an additional framework to directly run physics-based simulations biased by latent space variables
- Variations of latent diffusion models are in development (in collaboration with JHU and NASA)
- Project resulted in various publications in high impact journals and Arxiv (3 publications to date)

Molecular Analysis of Ionic Polyimides | *FORTRAN, GROMACS, Git* — Jan. 2015 – May 2020

- Developed code to analyze the free surface area and pore size distribution of large molecules
- Developed a framework to simulate ionically charged polymer chains in ionic liquid solvent
- Committed 5,000+ lines to existing codebases via Git
- Project resulted in 3 publications in high impact computational chemistry journals

Technical Skills

Programming Languages: Python, C/C++, Java, JavaScript, Go, SQL (Postgres), HTML/CSS, FORTRAN
Software Packages: GROMACS, LAMMPS, Rosetta, Thermo-Calc, OpenMM
Frameworks/Platforms: Flux (a High Performance Computing Framework), CUDA, React, Node.js
Developer Tools: Git, Docker, Google Cloud Platform, Vim, VS Code, Visual Studio
Libraries: Pytorch, Tensorflow, Jax, scikit-learn, pandas, NumPy, Matplotlib