

HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-025

Data-driven Discovery of the Morphology of Liquid Inclusions with Surface Energy

About AFRL:

Air Force Research Laboratory (AFRL) is a scientific research organization operated by the United States Air Force Materiel Command. AFRL is dedicated to leading the discovery, development, and integration of aerospace warfighting technologies, planning, and executing the Air Force science and technology program, and providing warfighting capabilities to United States air, space, and cyberspace forces.

The Air Force Research Laboratory Materials and Manufacturing Directorate uses a combination of novel and high-impact experiments, in-house high-fidelity HPC simulation software, and machine learning to characterize and predict the performance of current and emerging materials.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

Liquid inclusion morphology is controlled during resin infusion by tuning flow velocities, pressure gradients, and flow paths. For liquid metal composites, chemical and mixing processes control the distributions of inclusion sizes. The team will uncover processing-morphology relationships by leveraging a Monte Carlo based AFRL code which simulates the equilibrium morphology of liquid inclusions given their volume fractions, size distributions, surface tensions, temperature, and ambient pressure gradient. The intern will gain valuable experience in HEC and Monte Carlo methods while generating data. Our hypothesis is that a phase transition exists from evenly dispersed inclusions to large clusters. Dimensional reduction (e.g., UMAP) and deep learning (e.g., CNNs) will be used to classify morphologies, inspired by recent work which utilizes ML for understanding phases of matter (Carrasquilla and Melko, Nat. Phys., 2017).

To achieve the goals of the project, the intern will:

Week 1: The intern will spend the first week getting acclimated to AFRL, getting access to computational resources, and will have the opportunity to review the research goals, the fundamentals of Monte Carlo, liquid inclusions, and machine learning.

Weeks 1-3: The intern will collaborate with mentors to generate preliminary simulation data for different volume fractions, size distributions, surface tensions, temperatures, and ambient pressure gradients. Preliminary data will be statistically analyzed to design a broader parameter study. Classification methods will begin development in tandem.

Weeks 4-5: Because both the processing parameters and morphological features live in high dimensional space, a powerful dimensional reduction technique, UMAP, will be used to probe processing-morphology relationships.

Weeks 6-8: The intern will classify morphologies (and potentially phases) using convolution neural networks.

Weeks 9-10: The intern will complete final deliverables, participate in the annual AFRL poster session, final HIP presentation, and create documentation to ensure facile intellectual transfer and continuation of the research.

The intern will learn debugging, automated workflows, data management, data analysis, data visualization, and applied ML--all of which are broadly applicable to STEM fields. Monte Carlo methods are ubiquitous in modeling systems with randomness (e.g., weather forecasting, ground water, biology, financial markets, etc.). Beyond technical tasks, the intern learns about AFRL, network, attend talks and seminars (e.g., "MlrACLE Forum" on machine learning), and enhance communication skills.

ANTICIPATED START DATE:

May 2024 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

Preferred qualifications include:

- Degree obtained or sought in Data Science, Chemical Engineering, Physics, Chemistry, Computer Science, Mechanical Engineering
- Advanced undergraduate or graduate student
- Some knowledge of programming such as MATLAB, Python, C++, and/or Julia is preferred
- Knowledge of machine learning is a plus

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's
- Doctoral

DISCIPLINE NEEDED:

- Computer, Information, and Data Sciences
- Engineering
- Chemistry and Materials Sciences
- Physics
- Science and Engineering related