HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-013

Generating Synthetic Ceramic-Matrix Composite Microstructures Through Generative AI/ML

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 composites performance team at 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:

Ceramic-matrix composites (CMCs) exhibit complex microstructural features, such as non-uniform fiber coatings, residual phases, microcracks, and voids. Characterizing the effect of each microstructural feature on the resulting performance is key to enabling high-temperature materials for space and hypersonic applications. High-fidelity physics-based simulations and human expertise can connect the microstructural features to properties at a higher scale, but the simulations are predicated on having an accurate geometric model of a realistic microstructure. This project aims to select and train a generative machine learning model based on existing microscale X-Ray CT data that AFRL has collected to be able to create realistic CMC microstructural features based on given fiber positions.

The overall goal pertaining to material engineering for the project is to develop a machine learning model that can generate synthetic CMC microstructures with realistic, complex features, which is currently intractable without machine learning. The scope of this project specifically focuses on generating realistic patterns of residual Si in SiC/SiC CMCs based on the fiber positions, but importantly, the methodology can be applied to a range of microstructural features and materials. To train such a model, the project will leverage terabytes of X-Ray CT images of actual SiC/SiC microstructures, which has been segmented and labeled through other projects in AFRL.

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

Week 1: Complete in-processing, obtain access to a DoD HPC system, and learn how schedule jobs involving GPUs

Weeks 2-3: Learn about generative adversarial networks (GANs) suitable for image data through tutorials and simple problems within a popular ML framework, such as PyTorch

Weeks 4-5: Construct and train several types of GANs based on a small set of 2D slices from labeled X-Ray CT data, comparing the performance of the considered models

Week 6: Extend at least one of the methods to be able generate residual Si features for a small 3D region of a microstructure

Weeks 7-8: Develop a method to use the generative AI/ML model, which operates on a small domain, to generate large microstructures through an overlapping domain approach

Weeks 9-10: Author a report summarizing the work, document all code, and give a research presentation to research team and another to the broader AFRL RX community

In addition to the activities related to the project directly, the intern will have the opportunity to attend seminars focused on computing, machine learning, and material science; attend technical meetings across a variety of disciplines; participate in tours in the computing and material labs; and network with experts across disciplines. These activities will give the intern the opportunity to lead a research project typical to those in government labs, develop an understanding of CMC microstructures, and show how data science and machine learning can be leveraged in scientific and engineering disciplines. If desired, the intern can choose to pursue publishing the work given its novelty.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

The ideal candidate should:

- Be enrolled in a computer science, material science, data science, or engineering program
- Have a working-level understanding of Python
- Have taken an introduction to machine learning

Qualifications that are not required but would be helpful include:

- Familiarity with GANS
- Familiarity with job scheduling and typical workflows in HPC environments
- Familiarity with CMC microstructures

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Master's
- Doctoral

DISCIPLINE NEEDED:

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