HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM RESEARCH PROJECT #: HPCMP-HIP-25-023

Evaluating the Parallel Performance and Fidelity of State-of-the-Art Solid Mechanics Computational Tools

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:

Modeling the initiation and evolution of complex crack networks remains an invaluable technique to understand how materials, components, and structures will fail. These fracture models enable virtual experiments that are used to optimize physical experiments, improve manufacturing processes, design materials and structures, and accelerate certification of new materials and vehicles. Though there are a variety of methods to model fracture, discrete damage models offer the advantage of accurately capturing the discontinuity in the displacement field. However, multiple scientific computational tools have been developed throughout the defense community to facilitate this type of simulation. There is interest in merging in-house AFRL tools with government-funded tools with wider adoption, and this project aims to compare the performance and capabilities of several tools to inform the decision-making process.

The overall objective of this project is to characterize and benchmark the performance of three government-developed computational tools capable of discretely modeling fracture: BSAM (a mature research code written in Fortran), SPAWC (a modular and scalable research code written in C++), and MOOSE (a well-established open-source C++ code developed by Idaho National Labs). Each code employs distinct numerical methods and fracture models. The project will involve creating an equivalent model in each code to facilitate direct performance comparison using 1) shared memory single-node systems, 2) CPUs across multiple nodes via MPI, 3) a single GPU, and 4) multiple GPUs across multiple nodes. In addition to measuring the computational efficiency of each code, another project outcome will be a summary of the fracture modeling features available in each tool.

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 simulations on an HPC system.

Week 2: Learn about containerization and how to compile the computational tools relevant to this project on DoD systems.

Week 3-4. Learn how to run, benchmark, and visualize results for MOOSE.

Week 5-6. Learn how to run, benchmark, and visualize results for BSAM.

Week 7-8. Learn how to run, benchmark, and visualize results for SPAWC.

Weeks 9-10. Author a report summarizing the research, document all code and results, give a research presentation to research team, and present at the HIP symposium.

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 a variety of computational tools and computing environments, and show how findings can impact a broader community of researchers in the lab. If desired, the intern can choose to pursue authoring a DoD technical report.

ANTICIPATED START DATE:

May 2025 – 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 mechanical engineering, material science, aerospace engineering, or computer science/engineering program.
- Be proficient in at least one well-known programming language (Python, C++, etc.).
- Have experience documenting code and research efforts.
- Be at least minimally familiar with benchmarking programs.

Qualifications that are not required but would be helpful include:

- Familiarity with common Linux commands and shell scripting.
- Familiarity with Gitlab CI/CD pipelines.
- Familiarity with containers technology.
- Familiarity with job scheduling and typical workflows in HPC environments
- Familiarity with running scientific computational tools.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's
- Doctoral

DISCIPLINE NEEDED:

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