# HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-25-024

## Exploring Recent Nonlinear Solution Methods for Solving Challenging Highly Nonlinear Equations Emerging from Cohesive Fracture

**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 the certification of new materials and vehicles. However, cohesive fracture models often lead to computationally challenging nonlinear equations, as the residual is highly sensitive to small changes in the displacement field near a crack tip. Current tools leverage variations of traditional Newton methods, but a rich set of nonlinear solution methods have been developed across various disciplines. This project aims to evaluate the effectiveness of several of these alternative methods when applied to large-scale cohesive fracture simulations.

The overall objective of this project is to characterize and benchmark the performance of various nonlinear solution methods available within the popular C++ large-scale math package PETSc. An in-house computational tool capable of discrete fracture modeling, SPAWC, will serve as the testing framework. SPAWC is a modular and scalable research code written in C++ that already interfaces with Intel's MKL and PETSc. Performance will be evaluated for each method based on several key metrics: the number of iterations required for convergence, convergence behavior, computational cost per iteration, and scalability across multiple CPUs and GPUs.

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: Survey nonlinear methods available in PETSc and propose test plan.

Week 3: Setup a small scale cohesive fracture model in SPAWC.

Weeks 4-5: Explore the performance of various nonlinear solvers for the small scale problem.

Week 6: Setup a large scale cohesive fracture model in SPAWC that leverages distributed computing.

Weeks 7-8: Explore the performance of various nonlinear solvers for the large scale problem for varying number of CPUs/GPUs.

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 an applied mathematics, computer science/engineering, or STEM related program with an emphasis on numerical methods.
- Be proficient in both Python and C++.
- Have experience documenting code and research efforts.
- Have a strong numerical methods background.

Qualifications that are not required but would be helpful include:

- Familiarity with common Linux commands and shell scripting.
- Familiarity with PETSc.
- Familiarity with nonlinear solution methods for non-convex functions.
- Familiarity with job scheduling and typical workflows in HPC environments.

**ACADEMIC LEVEL:**

Degree received within the last 60 months or currently pursuing:

- Master’s
- Doctoral

**DISCIPLINE NEEDED:**

- Mathematics & Statistics
- Computer, Information, and Data Sciences
- Engineering
- Science and Engineering related