Differentiable Physics-Solvers in JAX for Uncertainty Quantification and Optimization

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:

The JAX Python library, largely developed by Google, provides building blocks for high-performance AI/ML models, such as JIT compilation, auto-differentiation, GPU acceleration and linear algebra. AFRL/RX in collaboration with other agencies and universities are exploring the framework to construct novel physics-based modeling tools that leverage AI/ML, auto differentiation, and heterogeneous computing. This summer project will use an existing code built on JAX to explore how differentiable solvers could be leveraged for uncertainty quantification and/or optimization problems.

This project will use the implementation of the finite element method (FEM) in the JAX Python library that was developed by AFRL RX and DoD HPCMP. The implementation provides a differentiable solver that allows the gradients of the solution with respect to any of the inputs to be efficiently computed. This provides the possibility to quickly compute the derivative of a solution with respect to the material properties, for example. The intern will use the aforementioned implementation to compute gradients for several problems of interest in material design and use the gradients to either guide uncertainty quantification or material design optimization. To achieve these aims, the project will require access and computational hours on DoD systems equipped with modern GPUs, such as Flyer. 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.

Weeks 2-3: Learn about FEM implementation in JAX.

Weeks 4-5. Implement functions to easily access gradients, construct several boundary value problems, and demonstrate ability to compute gradients.

Weeks 6-7. Explore the use of gradients to either optimize the material or estimate the uncertainty given uncertainty of the inputs.

Week 8. Perform benchmarking and analysis to characterize scaling on HPC.

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 learn how 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/June 2026 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

The ideal candidate will be a graduate student pursuing a degree in applied mathematics, computer science/engineering, or STEM related program with an emphasis on numerical methods.

Preferred skills:

- Be proficient in Python and familiar with 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 JAX
- Familiarity with job scheduling and typical workflows in HPC environments**.**

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor’s
- Master’s
- Doctoral

DISCIPLINE NEEDED:

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