HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-004

Multi-scale Modeling of Energetic Materials: Developing SCIMITAR3D as a Meso-scale Bridge

About DEVCOM ARL:

The DEVCOM Army Research Laboratory (ARL) is the Army's sole foundational research laboratory strategically placed under the Army Futures Command. ARL focuses on cutting-edge scientific discovery, technological innovation, and transition of knowledge products that offer incredible potential to improve the Army's chances of surviving and winning any future conflicts.

RESEARCH LOCATION: Aberdeen Proving Ground, MD

PROJECT DESCRIPTION:

The proposed project will investigate approaches and implementation routes through which the well-developed meso-scale continuum code SCIMITAR3D can be linked with the existing Hierarchical multiscale simulation (HMS) framework. The goal is to bridge meso-scale phenomena crucial to the shock initiation of heterogeneous energetic materials (HEs), bridging on the one hand to coarse-grain (CG) molecular descriptions, and on the other to homogenized macro-scale production codes such as ALE-3D.

The proposed project will support efforts in developing computational capabilities that can be used to acquire fundamental understanding of the effects of microstructure on the dynamic response of energetic materials. The intern's role in this project will be to develop, implement and test enhancements to the current generation software, and then to transition these into either the SCIMITAR3D or LAMMPS software.

Under the guidance of mentors, the intern will be expected to complete several simulations, analyze the data generated, and present in oral and written forms. The intern will be exposed to projects that will provide them with the opportunity to develop the computational skills that are necessary, including but not limited to, parallel programming, Python programming, and large data analysis. The intern will use HPC resources to setup and run large-scale, multi-core simulations using both LAMMPS and SCIMITAR3D. The properties generated by the simulations will be analyzed by the intern with various data-analysis tools (e.g., Python, shell scripts, Matlab), and visualized using standard software packages (e.g., Ovito, Materials Studio, Tecplot). A report of the project's findings will be completed at the end of the term, with the goal of publishing an open literature manuscript or an ARL technical report. Software enhancements developed by the intern will be transitioned into the LAMMPS and SCIMITAR3D software packages.

The intern will also have numerous opportunities to both advance their technical skills and expand their professional network. The intern will be provided with opportunities to present their work at weekly team meetings and at a laboratory-wide oral presentation competition among all summer interns (the annual ARL Summer Student Symposium), providing an excellent opportunity to network with the senior leadership and technical staff at ARL. In addition, lab tours of the Adelphi Laboratory Center and Aberdeen Proving Ground are organized to expose summer students to the research conducted at ARL, and the important technological challenges facing the Army.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

Candidates should be pursuing a degree in Physics, Chemistry, Materials, Chemical, or Mechanical engineering, Computer Science, or a related field. The successful candidates will have experience in computational modeling and simulation, Fortran, C++, and Python.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Master's
- Doctoral

DISCIPLINE NEEDED:

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