HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-26-005

Atomistic, Coarse-Grained, and Machine Learning-Guided Modeling for Energetic Materials Under Extreme Conditions

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.

The Detonation Science and Modeling Branch within DEVCOM ARL performs a variety of experimental and computational research on energetic materials.

RESEARCH LOCATION: Aberdeen Proving Ground, MD

PROJECT DESCRIPTION:

Large-scale computational studies involving HPC platforms aimed at understanding the response of energetic materials to extreme conditions such as those observed under shock. HPC modeling using atomistic and particle-based coarse-grained models developed at the ARL will be used to access nano- and micro- scales which are mostly beyond the reach of the experimental techniques. The analysis of the results of the simulations will involve application of modern Machine Learning (ML) tools such as ImageJ, OpenCV, and PyTorch to unravel important physics behind the response of energetic materials to external extreme temperatures and pressures.

Under the guidance of mentors, the intern will gain knowledge and experience in:

1.) Preparing atomistic and coarse-grained simulation setups mirroring the experimentally observed structures of two energetic molecular materials: TATB and RDX.
2.) Getting familiar with bottom-up coarse-grained models for TATB and RDX developed at the ARL.
3.) Running on HPC platforms molecular simulation packages (such as LAMMPS) to model the energetic materials under shock impact at atomistic and coarse-grained levels.
4.) Analyzing output from the HPC simulations using the variety of ML tools, such as open-source ImageJ, OpenCV, and PyTorch for pattern recognition, with the aim to infer the physical processes at a range of scales leading the experimentally observed behavior of the energetic materials under the shock. This activity will involve extensive scripting using Python, MATLAB, R, Tcl lg. and shell script.
5.) Visualization of the results of HPC simulations.
6.) Presenting results in an open-lit publication (ARL report or journal paper), at world-class events such as Biennial Conf of the APS Topical Group on Compression of Condensed Matter or transitioned to DoW partners and publishing in limited distribution reports.

Activities for HIP interns will include:

- Daily mentoring in-person at APG
- Accessing HPC resources
- Developing setups for simulation of energetic materials on HPC platforms
- Familiarizing with the theory of coarse-graining, shock physics, and molecular dynamics simulation and relevant ML techniques
- Running simulation jobs on the HPC platforms
- Processing outputs using ML and other tools
- Extracting the relevant physics from the simulations using with ML-style tools
- Coding scripts to process output and compute relevant physical properties of the simulated systems
- Use of visualization software
- Interns will be able to have a tour of DEVCOM ARL's facilities at the Aberdeen Proving Ground, including manufacturing labs, test ranges, and analytical labs

Results of the research may be published in the open literature, presented at world-class events such as Biennial Conference of the APS Topical Group on Compression of Condensed Matter, or transitioned to DoW partners and published in limited distribution reports. Regardless of research outcomes, each intern should significantly improve their knowledge of molecular simulation techniques, HPC platforms, ML for material science in conjunction with shock physics. The project allows the opportunity to interact with a wide range of experimentalists and theoreticians at the ARL.

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:

Candidates should have prior knowledge of large scale molecular simulation and machine learning, with basic knowledge of shock physics. Basic knowledge of molecular dynamics simulation techniques using atomistic and coarse grain models is preferred.

Knowledge of chemistry or energetic materials is also favorable. Python, Mat Lab, Tcl, and shell scripting programming skills and some familiarity with concepts of machine learning is highly preferable.

The ideal candidate is a graduate student but will consider highly motivated undergraduates and recent PhD graduates.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's
- Doctoral

DISCIPLINE NEEDED:

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