Multi-scale Modeling of Energetic Materials: Informing the Mesoscale in a Bottom-up Fashion

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 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 will develop, implement, and test enhancements to the current generation software, and then to transition these into the LAMMPS software and/or the hierarchical multiscale modeling framework.

The proposed project will investigate bottom-up, hierarchical multiscale approaches that scale-bridge atomistic, molecular dynamics (MD) and microscale, coarse grain (CG) descriptions of energetic material (EM) to inform a mesoscale and macroscale models implemented within continuum codes. The multiscale framework will provide a fundamental understanding of the effects of microstructure on meso-scale phenomena crucial to the shock initiation of heterogeneous EMs.

The microstructural heterogeneities that dictate the response of EM composites to various stimuli require multiscale modeling. In recent years, our group has developed computational capabilities (i.e., Dissipative Particle Dynamics, DPD) necessary to represent salient physical and chemical features of material microstructure. From recent HPCMP Frontier and HIP projects, the DPD models and methods have been integrated into the LAMMPS software package and transitioned into continuum level approaches through the scale-bridging Hierarchical Multiscale Simulation (HMS) software developed at ARL and the SCIMITAR3D software.

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The overarching goals of the proposed project are the following. First, to compare head-to-head the physical modeling, mathematical and numerical fundamentals of SCIMITAR3D and DPD; to establish that continuum models in SCIMITAR3D can be employed to bridge DPD and macro-scale codes such as ALE-3D. Second, to evaluate the use of SCIMITARD within the predictive multi-scale framework of HMS in an efficient implementation, taking advantage of the fundamental physics models from DPD and real microstructure volume elements that can be simulated by SCIMITAR3D.

Through guidance from the mentors, the intern will be expected to complete several simulations, analyze the data generated, and present their research 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 software and/or hierarchical multiscale framework.

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 research 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 2025 – 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