HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-029

Adaptation of the AppPottsRS SPPARKS Class for Efficient Grain Growth Simulations

About DEVCOM ARL:

The DEVCOM Army Research Laboratory (ARL) is designed to significantly increase the involvement of creative and highly trained scientists and engineers from academia and industry in scientific and technical areas of interest and relevance to the Army. Scientists and engineers at ARL help shape and execute the Army's program for meeting the challenge of developing technologies that will support Army forces in meeting future operational needs by pursuing scientific research and technological developments in diverse research fields.

RESEARCH LOCATION: Aberdeen Proving Ground, MD

PROJECT DESCRIPTION:

The program seeks a summer intern to conduct research on the algorithmic improvement of the AppPottsRS SPPARKS class [1,2], which will be used to simulate microstructural evolution with more accurate physics. The intern will develop algorithms to properly manage the interaction between a wide range of grain boundaries, as relevant to real microstructures. This will require basic understand of MPI programming, as well as usage of C++ maps, pairs and/or vectors. Furthermore, the intern will perform post-processing of the simulated microstructures in order to curate the data and extract useful microstructural information. These simulations will be conducted on Mustang and/or Narwhal, as appropriate.

One of the disadvantages of the current model is the poor management of the vast population of grain boundary combinations, especially when instantiating from a random distribution. Under the guidance of a mentor, the intern will develop an efficient implementation of a grain boundary tracker.

[1] Hernandez, E; AppPottsRS: A Read-Shockley Class for SPPARKS, ARL-TN-0913 (2018)

[2] Crossing the Mesoscale No-Man's Land via Parallel Kinetic Monte Carlo, SAND2009-6226 (2009)

The Army Research Laboratory has an active intern program that includes tours of several individual laboratories at locations in Aberdeen Proving Ground and Adelphi, MD. Throughout the summer, there are planned functions/socials at the team, branch, and division level to interact. Furthermore, there are frequent program, team, and branch meetings to help introduce interns to the culture at ARL.

Throughout the summer, the intern will receive hands-on training on using the DSRC systems, running simulations, and analyzing simulation data. Linux workstations will be used to train the intern on accessing the DSRC resources and transferring data to/from the clusters. The intern will be provided extensive training on creating and running the parallelized Potts-Monte Carlo models using SPPARKS. Additionally, the intern will be trained on using post-processing tools for studying the simulation results (e.g., paraview). Other local workshops and internal training opportunities will also be made available to the intern as needed.

There are multiple opportunities to network with other interns, postdoctoral associates, and ARL S&Es. The mentor will facilitate individual meetings between the intern and specific staff members whose research portfolio or professional experience best align with the student's intended professional path. Additionally, the intern will have the opportunity to interact with human resources and learn more about careers in the government defense laboratories.

The intern will be expected to compile the SPPARKS framework, and properly manage code development via the DSRCs GitLab instance. The intern will be expected to maintain regular communication with the mentors, including virtual and/or in-person meetings.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

Graduate students with interest in materials modeling.

Preferred skills:

- C/C++
- Basic/moderate understanding of parallel computing
- Understanding of microstructural evolution
- Knowledge on numerical methods (e.g., finite differences)

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Master's
- Doctoral

DISCIPLINE NEEDED:

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