

HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-035

Machine Learning for Energetic Materials

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. This particular opportunity has a focus on developing machine learning models for application to both explosives and propellants.

RESEARCH LOCATION: Aberdeen Proving Ground, MD

PROJECT DESCRIPTION:

DEVCOM ARL has previously published machine learning research on predicting a variety of physical and performance properties of explosives in the open literature. This HPC opportunity will build upon that research to consider propellant performance properties, polymer properties relevant to formulations, interpretable models, generative models, and fine-tuning of large-language models. Research problems will be tailored to the skills and interests of the intern. This project is designed to accommodate multiple intern applicants from different institutions who may have prior research. The broad lines of research are:

ML for propellant burning rate:

Recently a focus of the DARPA RIDE project, will extend upon that research using a limited distribution dataset created in part under the Enhanced Energetic Effects ARAP project. The team will combine academic data with DoD data for a more robust dataset and implement a new composition-based featurization for training with a DARPA RIDE method.

ML for pure material properties:

ARL has an existing in-house tool that predicts some safety and physical properties of explosives. The team will extend it by adding predictions of properties such as molecular strain, inflammability (for polymers), and interpretable models for detonation performance. Datasets will be on-hand and research will be in appropriate ML architectures.

A large-language model for energetics:

ARL currently have a corpus of several thousand PDFs related to energetics, and two base models (Llama 2 and NeoX) available for fine-tuning. The team will explore how well a fine-tuned LLM can stand in for an energetics SME chat.

Activities for HIP interns will include

- Daily mentoring in-person at APG
- Developing new representations of energetic materials for use with ML
- Coding new architectures in PyTorch/Tensorflow/scikit-learn
- Developing new methods for handling of small incomplete datasets and transfer learning.
- Tour of DEVCOM ARL's facilities at Aberdeen Proving Ground, including manufacturing labs, test ranges, and analytical labs
- Results of research may be published in the open literature, presented at world-class events such as the 2024 Gordon Research Conference on Energetic Materials, or transitioned to DoD partners and published in limited distribution reports.
- Interns will share cross-university knowledge.

Regardless of research outcomes, each intern should significantly improve their skills in programming and evaluation of ML models using python-based workflows. The mentor will share programming best practices and 'tips-and-tricks' for future job interviews, building upon a guide they first authored in 2018 (ARL-SR-0411, "A Primer on Machine Learning for Materials and Its Relevance to Army Challenges") which has been successfully used with other HIP interns.

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 have prior knowledge of python programming and some familiarity with concepts of machine learning. Knowledge of chemistry or energetic materials is also favorable. The ideal candidate is a graduate student who desire to pursue a career utilizing data science or machine learning. Highly motivated undergraduates and recent PhD graduates will also be considered.

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