

HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-021

Computational Investigation of the Structure, Dynamics, and Design of Ice-Nucleating Proteins

About AFRL:

The biomaterials group under the materials research directorate at the Air Force Research Lab (AFRL) participates in the High-Performance Computing Internship Program (HIP) offered by the Department of Defense High Performance Computing Modernization Program (DoD-HPCMP). The biomaterials group has been mentoring students from the science and engineering fields since 2008 (under JEOM and HIP) and seeks students for internship opportunities where they receive training in state-of-the-art high-performance computing on projects relevant to the DoD mission and/or their future careers.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

Ice-nucleating proteins (INPs) are a family of proteins that promote the nucleation of ice at higher temperatures. As average global temperatures rise, the permafrost upon which Arctic DoD installations are built begins to melt. Therefore, a solution for keeping the permafrost frozen at higher ambient temperatures has become increasingly necessary. One such solution can be found in INPs. As part of a strong collaboration with our experimental colleagues, the modeling team at AFRL/RXEB will mentor a HIP intern to research in the computational investigation of INPs as a means of stabilizing DoD installations in "cold regions."

The scientific problems addressed by this project are two-fold: 1) investigate the mechanism of action of ice nucleating proteins (INPs), particularly their effect on the point of liquid-liquid phase separation (LLPS) and 2) identify candidate INPs for further experimental investigation. Solving these problems will require a variety of computational techniques, including, but not limited to de novo protein structural modeling, molecular dynamics simulations, and bioinformatics (including static and dynamic network analysis of protein-protein and residue-residue interaction networks).

Each summer, scores of interns are present in the Materials and Manufacturing Directorate (AFRL/RX) laboratories. While day-to-day activities of an HPC intern depend strongly on the nature of the project initiated, typical activities from previous years are listed below:

1.) Training:

The student will attend training workshops provided by AFRL/AFIT and surrounding institutions, such as resume and publication writing workshops, and will be encouraged to develop presentation skills via poster or oral presentations.

2.) Professional Networking and Data Dissemination:

Examples of previous and expected routes of data dissemination and networking:

- Student will participate in local meetings, presenting findings at computational group meetings, research team meetings, and branch-wide research meetings. Also, AFRL/RX holds a student poster session at the end of each summer.
- Student is encouraged to disseminate findings in poster sessions and oral presentations at regional and national conferences. Previously, students in this group have presented findings at regional conferences of the ACS Regional meeting, the National Graduate Polymer Research Conference, the ASM International regional meeting, the ACS National Meeting and Exposition and APS Meetings.
- It is expected the student will participate in tours of local HPC facilities to gain an understanding of the operational support of the HPC systems they use.
- Students are encouraged to use local courses to expand their knowledge of the science behind the simulations as well as the breadth and depth of available HPC applications.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

The ideal candidate will be a student in a science or engineering field with limited background in data handling and program operation typical to HPC. This internship will help the student improve their capability to formulate pertinent scientific questions and use HPC to answer them.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's
- Doctoral

DISCIPLINE NEEDED:

- Chemistry and Materials Science
- Computer, Information, and Data Sciences
- Engineering
- Life Health and Medical Sciences
- Mathematics and Statistics
- Physics
- Science and Engineering related