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 that underlies the ability of ice nucleating proteins (INPros) to efficiently nucleate ice, and 2) identify and/or design candidate INPros 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, bioinformatics (including static and dynamic network analysis of protein-protein, residue-residue, water-water, and water-protein interaction networks), and machine learning using network data. As part of achieving its mission to support DoD interests, the AFRL BioRT modeling group has historically made significant use of DoD HPC resources.

For this project, significant computational hours on DoD supercomputers will be required to perform and analyze molecular dynamics simulations characterizing INPros that the group has modeled using de novo protein structure prediction tools (AlphaFold3). Hours will also be used to train machine learning models to predict properties related to ice nucleation efficiency.

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:

Training:

The intern 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.

- Participate in tours of local HPC facilities to gain an understanding of the operational support of the HPC systems they use.
- Interns 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.

Professional Networking and Data Dissemination:

- Intern 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.
- Intern is encouraged to disseminate findings in poster sessions and oral presentations at regional and national conferences. Previously, interns 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.

ANTICIPATED START DATE:

May 2025 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

The ideal candidate is a student in a science or engineering field with a background in data handling and program operation typical to HPC. This internship will help the student engage in the process of scientific inquiry through formulating pertinent scientific questions and using HPC resources to answer them.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's

DISCIPLINE NEEDED:

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