HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HPCMP-HIP-24-026

From Molecular Dynamics to Electro-fluid Mechanics: Simulation of Electrowetting for the Next Generation of Space and Aerospace Composites Processing

About AFRL:

Air Force Research Laboratory (AFRL) is a scientific research organization operated by the United States Air Force Materiel Command. AFRL is dedicated to leading the discovery, development, and integration of aerospace warfighting technologies, planning, and executing the Air Force science and technology program, and providing warfighting capabilities to United States air, space, and cyberspace forces.

The Air Force Research Laboratory Materials and Manufacturing Directorate uses a combination of novel and high-impact experiments, in-house high-fidelity HPC simulation software, and machine learning to characterize and predict the performance of current and emerging materials.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

The team will advance electrowetting-enhanced infusion processes by molecular dynamics (MD) modeling (using LAMMPS) of resin responses in ambient electric fields, including polarization, rheological behavior, and surface tension. The insights gained from MD will inform the material responses utilized in electrohydrodynamic (EHD) simulations for resin infusion into fiber reinforcements. Key inquiries include: 1) determining optimal voltage properties (e.g., magnitude, AC vs. DC, frequency) for infusion quality and mitigating voids, 2) exploring the resin chemistry's influence on electrowetting effects, and 3) assessing the potential of utilizing the fringing electric field of a partially filled capacitor to drive flow into intricate geometrical features.

To achieve the goals of the project, the intern (s) will:

Intern 1:

Weeks 1-2: Establish and test an EHD model for benchmark flows–emphasis on electrically-driven Couette flow.

Weeks 3-6: Introduce carbon fibers with charge density. Infusion simulations into a fiber bundle, considering electrowetting and different pressures; compare void content.

Weeks 7-9: Extend the EHD model to mirror electrowetting experiments. MD data (by Intern 2) guide resin's response to electric fields, informing polarization, surface tension, and rheology. Parameter study to determine optimal voltage for infusion quality, alongside planning of final deliverables.

Intern 2:

Weeks 1-4: Identify intermolecular potentials for resins like RTM-6, simulating resin at equilibrium. LAMMPS non-equilibrium MD (NEMD) simulations confirm temperature/viscosity relationship against specifications.

Weeks 5-7: Expand the MD model with an electric field, calculating surface tension using the Irving and Kirkwood pressure tensor. Predicted polarization is compared with dielectric measurements.

Weeks 8-9: Entail computational experiments, analyzing electric field-polarization relationships, and assessing resin rheology's sensitivity to applied field.

Interns 1 & 2:

Weeks 10-11: Final deliverables are completed. Participation in the AFRL poster session, the HIP presentation, and documentation ensure knowledge transfer and research continuity.

CFD and MD are broadly applicable in engineering and science. The former serves automotive, aerospace, and marine industries; the latter is essential across computational materials science. Beyond technical tasks, interns learn about AFRL, network, attend talks and seminars (e.g., "MIrACLE Forum" on machine learning), and enhance communication skills.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

Preferred qualifications include:

- Degree obtained or sought in Mechanical Engineering, Chemical Engineering, Physics, or Chemistry
- Advanced undergraduate or graduate student, or post-doctoral
- Knowledge of either 1) computational fluid dynamics or 2) molecular dynamics
- Knowledge and coursework in electromagnetism is a plus (but not required)
- Some knowledge of programming such as MATLAB, Python, C++, and/or Julia is preferred

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor’s
- Master’s
- Doctoral

DISCIPLINE NEEDED:

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