Differentiable molecular dynamics simulations of non-equilibrium biomolecular systems

Engel Research Group at the University of Calgary

Preferred Start: Fall 2026
Application Deadline: January 25
Supervisor: Dr. Megan C. Engel, Assistant Professor, Biological Sciences Department, University of Calgary (megan.engel@ucalgary.ca)
Salary: $70,000 CAD per annum
Term: 2 years

Description

The Engel Research Group is recruiting an outstanding postdoctoral candidate to nominate for the prestigious Canada Impact+ Research Training Awards, to pursue interdisciplinary research at the intersection of biology, chemistry, physics, and machine learning. The overarching foci of the group are (i) to elucidate how naturally evolved systems have taken advantage of nonequilibrium physics to excel at their biological functions and (ii) to develop rational design principles for *de novo* nucleic acid and protein nanotechnology. To achieve these ends, the Engel Group harnesses advances in the hardware and software that undergird modern machine learning – particularly, automatic differentiation – to develop improved biomolecular models; perform innovative optimizations over molecular dynamics simulations of DNA, RNA, and proteins; and interface non-equilibrium physics theories with biological systems.

Available projects include:

- Investigating the optimality of the ATP synthase molecular motor through multi-scale differentiable molecular dynamics simulations;
- Elucidating control mechanisms for the epithelial-mesenchymal transition in cancer cells through differentiable molecular dynamics simulations and gene network modelling;
- Inverse design of external control protocols and active particle interactions to control spatiotemporal patterning in active matter systems;
- Contributing to the development of in-house software for improving biomolecular modelling according to the machine learning paradigm;
- Developing coarse-grained models of peptide nucleic acids (PNAs) in collaboration with experimentalists, using in-house software;
- Refining non-equilibrium alchemical techniques for computational drug discovery.

The specific project will be refined from the above options according to the candidate's interests and background. **Work in the Engel lab is fully computational/theoretical** with opportunities for close collaboration with experimental groups. The Engel group has dedicated, priority access to substantial HPC hardware including seven H100 GPU units. A document outlining what you can expect while working in the Engel lab can be found here.

The University of Calgary is committed to an equitable, diverse, and inclusive workforce. We welcome interest from all qualified persons. We encourage women; First Nations, Métis and Inuit persons;

members of visible minority groups; persons with disabilities; persons of any sexual orientation or gender identity and expression; and all those who may contribute to the further diversification of ideas and the University to apply.

Requirements

Essential

- A PhD degree or equivalent in biophysics, computational physics, applied mathematics, or similar from a recognized institution
- C1-level English proficiency (CEFR framework)
- Interest in computational biophysics
- Programming experience (Python preferred)
- **Applicant must not be currently based at a Canadian institution.**

Additional Details

Location: University of Calgary, Calgary, Alberta, Canada

Benefits: A generous health and dental benefits plan is provided to postdoctoral associates at no cost to the employee.

More information about postdoctoral work in the at the University of Calgary can be found here.

Application

Please email the following to megan.engel@ucalgary.ca:

- Transcripts (unofficial is fine) for both undergraduate and graduate degrees
- CV/resume
- Names and contact information for 2-3 references
- Brief (100-200 words) statement outlining why you are interested in researching in the Engel lab