Professorship of Multiscale Modeling of Fluid Materials
TUM School of Engineering and Design
Technical University of Munich

Large Scale Molecular Dynamics with GNNs and LAMMPS

Most scientific phenomena across various fields, from life sciences to engineering, are multiscale due to an interplay of disparate spatial and temporal scales. In the Multiscale Modeling of Fluid Materials group, we are focusing on tackling such problems with multiscale modeling and simulations, where we merge micro and meso/macroscopic models. Graph Neural Network (GNN) potential models are promising candidates for bridging between models at different scales. However, the absence of support for GNN potentials in classical Molecular Dynamics frameworks hinders the application to large-scale simulations.

This thesis aims to interface promising GNN architectures written in JAX with the established simulation framework LAMMPS, scaling accurate simulations to millions of atoms. To perform resource-intensive computations, we will provide access to our chair's GPU cluster.

If you are interested in the project or have further questions, please write a short mail to paul.fuchs@tum.de. Please include a short presentation of yourself and your transcript of records.

The thesis will include the following tasks:

- Familiarize yourself with Molecular Dynamics Simulation
- Research GNN architectures and train a model
- Integrate the GNN into LAMMPS using your interface
- Validate the integration by running simulations

Requirements:

- Machine-Learning practice
- Good expertise in programming with C++
- Knowledge of JAX and XLA is advantageous
- Highly motivated