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

Large Scale Molecular Dynamics with GNNs and LAMMPS

Multiscale phenomena appear in various fields from life sciences to engineering, due to an interplay of disparate spatial and temporal scales. In the Multiscale Modeling of Fluid Materials group, we aim to understand these phenomena by employing accurate micro and mesoscopic molecular models on large scales.

Graph Neural Network (GNN) are promising models in the field of Molecular Dynamics. To enable scaling accurate GNN-based simulations to millions of atoms, this IDP aims to interface promising GNN architectures written in JAX with the established simulation framework LAMMPS. To perform resource-intensive computations, we will provide you access to our chair's GPU cluster.

Your IDP will consist of the following tasks:

- Familiarize yourself with Molecular Dynamics
- Design a JAX interface to run state-of-the-art GNN models in LAMMPS
- Benchmark the interface in large-scale computations

If you are interested in this IDP, please reach out to paul.fuchs@tum.de with a short introduction and your transcript of records.