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

Accelerated Molecular Dynamics for Rare Event Sampling

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 focus on tackling such problems with multiscale modeling and simulations.

State-of-the-art approaches to speed up Molecular Dynamics simulations require detailed knowledge about the slow processes of a system. Neural Networks (NNs) are powerful models to extract knowledge from high-fidelity data. Therefore, the thesis aims to leverage NN models to discover slow modes in Molecular Dynamics simulations.

The thesis will include the following tasks:

- Researching state-of-the-art approaches from the literature
- Implementing approaches into our chairs' framework
- Validating implementation on benchmark systems

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

Requirements:

- Good understanding of physics and statistics
- Machine learning practice
- Python programming proficiency
- Highly motivated