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

Deep Generative Models for Enhancing Molecular Simulations

Project Description

Deep generative models have shown great promise in various fields, including LLMs (ChatGPT, Deepseek), image and video generation (Stable Diffusion), and scientific applications (AlphaFold and MatterGen).
Molecular simulations are a crucial tool for understanding biological and chemical processes. They can help us explore how drugs bind to proteins to treat diseases or determine the properties of material structures. However, first-principle simulations based on quantum dynamics are computationally expensive. Deep learning provides a promising approach to overcoming the long-standing challenge of balancing accuracy and efficiency in molecular simulations.
This project aims to integrate generative models (e.g., diffusion models and flow matching) with graph neural networks to efficiently generate molecular samples. These samples can be leveraged for machine learning potential training, particularly in multiscale modeling at both atomistic and coarse-grained levels. A key application of this research is studying the co-assembly process of peptide-based molecules.
This project is under **Prof. Dr. Julija Zavadlav** (Professur für Multiscale Modeling of Fluid Materials) and offers potential collaboration opportunities with external researchers.

Objectives

- Understand and develop state-of-the-art generative models and GNN pipelines.
- Generate equilibrium molecular samples, starting from simple systems and progressing to more complex molecules.
- Generate conditional molecular samples tailored to specific molecular systems.
- Apply the generated samples to enhance machine learning potentials across different scales.

Ideal candidates should have experience with a modern deep learning library, such as **PyTorch or JAX,** and be willing to learn at least one of the following topics during the project: molecular dynamics simulation or statistical physics.
It is highly recommended that applicants have completed the following courses:

- Machine Learning for Graphs and Sequential Data (IN2323)
- Advanced Machine Learning: Deep Generative Models (CIT4230003)

Application
If interested, email weilong.chen@tum.de with:

1. A brief introduction with background and motivation.
2. Your transcript of records.