

Deep Learning for Molecular Dynamics Simulations (AI for Science)

AlphaFold, which recently won the Nobel Prize, successfully solved a long-standing problem in computational biology: predicting a protein's three-dimensional structure from its amino acid sequence. However, obtaining static protein structures is only part of the story. Researchers are also interested in understanding **how protein structures change over time** (dynamical properties) and properties are typically studied using molecular dynamics (MD) simulations.

Traditional first-principles simulations based on quantum dynamics are highly accurate but computationally expensive, limiting their scalability. Deep learning provides a promising alternative by balancing accuracy and computational efficiency. It enables the integration of scientific domain knowledge (e.g., physical laws) with advanced neural network architectures such as Graph Neural Networks (GNNs) and Transformers.

This thesis aims to integrate state-of-the-art neural networks to efficiently perform molecular dynamics simulations. The project is under Professurship of Multiscale Modeling of Fluid Materials and offers potential collaboration opportunities with external research partners.

Objectives

- Understand and develop state-of-the-art **GNNs** and **Transformers**.
- Gain familiarity with **geometric deep learning** (GDL) and understand how geometric priors affect computational efficiency.
- Design and benchmark Transformer-based neural network potentials.
- Apply advanced techniques such as **LoRA (Low-Rank Adaptation)**, **RoPE (Rotary Positional Embedding)**, and **MoE (Mixture of Experts)**.

We are looking for technically strong Master's students with a keen interest in AI/ML methods and their scientific applications.

Preferred skills and interests

- Familiarity with probability theory and statistics.
- Interest in dynamical systems, physics, chemistry, or applied mathematics.
- Strong time management and a proactive mindset.

You will gain:

- Hands-on coding and experimentation with state-of-the-art AI methods for physics-inspired problems.
- Learn how to collaborate with others in an international research environment.
- Opportunities to contribute to high-quality scientific publications.

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

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

