Machine learning for atomistic simulations, 3.0 credits

Maskininlärning för atomistiska simuleringar, 3.0 hp

Third-cycle education course

6FIFMB6

Department of Physics, Chemistry and Biology

Valid from: First half-year 2026

Approved by **Approved**

Registration number

Entry requirements

Entry requirement for studies on third-cycle education courses

- second-cycle degree,
- 240 credits in required courses, including at least 60 second-cycle credits, or
- acquisition of equivalent knowledge in some other manner

Specific information

The course targets all students directly involved in atomistic simulations, but also students from material science, data science, or even visualization, that are (perhaps through collaborations) interested in ML/AI applied to atomistic simulations. Requirement for this course are only basic math and python knowledge. Therefore, it will be a perfect introduction for students in order to start own projects or to better understand how to strengthen their collaborations.

Contents

The course will present in introduction to the foundations and applications of machine learning in atomic simulations, with a primary focus on machine learning interatomic potentials (MLIPs). It will cover the most commonly used descriptors, the underlaying mathematical formulations of the most relevant models and architectures, and introduce recently developed strategies for training data generation as well as model training. The course will finish with an overview of recent pre-trained foundation MLIPs, covering both "out-of-the-box" use and system specific transfer learning/fine-tuning schemes. We will particularly focus on the MACE architecture in two labs where students will learn how to generate data, efficiently select training data, train and apply machine learned interatomic potentials.

Educational methods

7 Lectures and 2 Labs.
The lectures will cover:
-Foundations and history of descriptors for atomistic systems
-Training data generation and databases; Foundation models
- Modern MLIP architectures and their relations: BP, GAP, ACE, MACE, Nequip, etc.
- Overview: pertained MLIPS, coordinate free models, generative models, workflows and limitations
Labs:
(1) Training data generation, selection, and potential training, error evaluation
(2) Molecular Dynamics and Mechanical Properties from MLIPS

Examination

Lab participation + report on lab

Grading

Two-grade scale

Course literature

A list of recommended literature will be provided by the course coordinator before the start of the course.

General information

The course is planned and carried out according to what is stated in this syllabus. Course evaluation, analysis and suggestions for improvement should be fed back to the Research and PhD studies Committee (FUN) by the course coordinator.
Teachers:
Lecturers: Florian Trybel & Johan Klarbring
Lab responsible: Abhijith S Parackal