EPFL

MSE-305   **Introduction to atomic-scale modeling**

Ceriotti Michele

Cursus	Sem.	Type
Materials Science and Engineering	BA6	Obl.

Language of teaching	English
Credits	2
Session	Summer
Semester	Spring
Exam	During the semester
Workload	60h
Weeks	14
Hours	**2 weekly**
Courses	2 weekly
Number of positions	

Summary

This course provides an introduction to the modeling of matter at the atomic scale, using interactive jupyter notebooks to see several of the core concepts of materials science in action.

Content

Simulation and modeling has become an integral part of the process of designing and optimizing materials for the most diverse applications. Truly predictive simulations, that can estimate the properties of materials before they have ever been synthesized, require atomistic resolution. This course provides an introduction to some of the techniques that underlie atomic-scale simulations of materials. With a strong hands-on component, based on interactive Jupyter notebooks, we will revisit, and see in a new light, several basic concepts on the nanometer-scale description of matter, and see a number of different modelling techniques in action, from molecular dynamics to atomic-scale machine learning.

Keywords

materials modeling
atomic-scale simulations
programming
python
numerical methods

Learning Prerequisites

Required courses

Information, computation, communication

Recommended courses

Materials structure
Numerical analysis

Important concepts to start the course

Basic python, some familiarity with jupyter notebooks
No need for QM or statistical mechanics
Some finite-elements and continuum modeling and numerical methods
Basic understanding of materials science: crystallography, defects, mechanical properties, thermodynamics, phase transitions

Learning Outcomes

By the end of the course, the student must be able to:

- Examine the code underlying a Jupyter notebook
- Sketch short code snippets to model materials properties
- Interpret the result of simulations in the light of core concepts in materials science

Teaching methods

The course is based on a set of interactive Jupyter notebooks, which guide the student in a step-by-step fashion into computing the numerical outcomes of a microscopic model of matter. The notebooks require a minimal amount of programming knowledge, and are executed in class by the students, under the guidance of the teacher.

Expected student activities

Students should go through the notebooks, experimenting with the effect of different parameters on the results of the models, writing short snippets of code, and reading the accompanying text that describes the underlying theory. They should then revise the content at home, and answer a couple of open questions that are then assessed as the course progresses.

Assessment methods

The students are assessed during the course, based on the answers they give to short open-ended questions that require commenting on the core concepts presented in each notebook.