UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Computational Materials Science

2526-1-FSM02Q022

Aims

The main goal of the Course is to provide to the students some key theoretical/computational tools for approaching at the atomic scale thermodynamics and kinetics of materials.

Knowledge and understanding
At the end of the course the student knows:

- the main concepts of thermodynamics and kinetics at the basis of computational material science
- the main computational techniques for modeling atom dynamics and the difference between classical and quantum approaches
- the key algorithms in use for implementing Molecular Dynamics and Monte-Carlo approaches

Applying knowledge and understanding
At the end of the course the student is able to:

- implement basic codes for simulating atomic scale dynamics
- perform numerical/statistical analysis on data and extract quantities of physical relevance
- adapt/modify simulation codes and select suitable parameters to tackle different materials or physical conditions
- recognise the use and importance of computer analysis and simulations in materials science

Making judgements
At the end of the course the student is able

- choose the best computational approach to perform simulations depending on the kind of the specific problem, scale and quantities to be evaluated
- identify possible flaws and limits of simulations by inspecting key quantities and adequate statistics

Communication skills

At the end of the course, the student will be able to describe and to explain orally, with the appropriate language, the topics of the class. Moreover, the student will learn how to summarize simulation results into effective plots, pictures and/or videos and to report them through a slide presentation (see assessment modality).

Learning skills
The student will be able to apply the acquired knowledge to understand and eventually implement autonomously more advanced techniques inherent to the methods discussed in the class or other affine computational approaches by referring to textbooks or scientific literature. Moreover, the course will give the students the necessary background to understand the documentation and user manuals of existing simulation softwares of Molecular Dynamics and Monte-Carlo simulations enabling a more conscious and transparent use of such tools.

Contents

Summary of basic concepts in classical statistical mechanics, adiabatic approximation, classical approximation for the motion of nuclei, ab initio and classical molecular dynamics, scientific coding with Matlab, implementation of a molecular dynamics code, application of the molecular dynamics code, kinetic and configurational Monte Carlo including implementation

Detailed program

Summary of basic concepts in classical statistical mechanics: canonical and microcanonical ensembles. Time averages and microcanonical averages: the ergodic theorem. Thermodynamic limit and equivalence of ensembles.

Adiabatic approximation: nuclear and electronics time scales and their separation. Electronic hamiltonian. Classical treatment of the nuclear motion: nuclear hamiltionian and interatomic potential. Ab initio vs classical molecular dynamics: semiempirical potentials and their limitations.

Pair and manybody potentials. Crystal-packing fraction and connection with the choice of the potential. The Lennard-Jones potential. Introduction of a cutoff radius and dependence of physical quantities on it.

Introduction to scientific coding, with examples in Matlab. Coding of a function computing the energy of a crystal using Lennard-Jones interatomic potentials. Function for computing neighbors' lists.

*** Molecular Dynamics**
Algorithms for integrating the equations of motion: configurational and velocity Verlet. Initial velocities; timestep optimization. Computing forces in a molecular dynamics code: theory and implementation. Writing of a complete Molecular Dynamics code based on Lennard-Jones potentials. Advanced topics: (a) temperature control in Molecular Dynamics using thermostats and/or velocity rescaling (b) thermal cycles/simulated annealing (c) linear-scaling Molecular Dynamics codes.

Exercise on Molecular Dynamics to be discussed at the exam (part 1 of 3).

*** Kinetic Monte Carlo**
The time scale problem; transition state theory; distribution of first-escape times. Concept of Markov chains, Master equation and the detailed-balance condition. Formulation of the Kinetic Monte Carlo method.

The Bortz-Kalos-Lebowitz algorithm and implementation of a Kinetic Monte Carlo code describing crystal growth processes.

Exercise on Kinetic Monte Carlo to be discussed at the exam (part 2 of 3).

*** Metropolis Monte Carlo**
Importance sampling and evaluation of equilibrium properties of a system by configurational Metropolis Monte Carlo. Implementation of a Metropolis Monte Carlo code.

Exercise on Monte Carlo Metropolis to be discussed at the exam (part 3 of 3).

Prerequisites

Basic classical (Boltzmann distribution, isolated systems, systems at constant temperature) and quantum mechanics (wave/particle duality, Schrodinger equation, Pauli esclusion principle), as from a Bachelor in Materials Science/Physics or analogous.
Knowledge of scientific coding can help but it is not mandatory as dedicated lectures will be given.

Teaching form

The full course consists of 30 lessons of 2 hours each, all taking place in presence in a computer laboratory. With the exception of a limited set of initial lectures, each concept is immediately exemplified and elaborated with the help of computer simulations. At half course a first problem is assigned: students are required to solve it by using their first complete (molecular dynamics) code. A second set of lectures about Monte Carlo methods follows with computer applications based on both Kinetic Monte Carlo and Metropolis Monte Carlo approaches. Students are then requested to solve an assigned problem on both methods by implementing under teacher guidance the respective codes during the laboratory activities.

Lessons are distinguished in:

- 8 two-hours lessons in delivered modality
- 18 two-hours practice lessons including a part in delivered modality during which the teacher illustrates concepts on which the students will be asked to work in interactive modality
- 4 two-hours practice lessons in interactive mode

The Course is given in English, but students can also ask questions in Italian.

Textbook and teaching resource

All lectures given by the teacher in presence are accompanied by slides which can be downloaded from the e-learning platform. While lectures are not taken from a specific text, most topics can be found in "Understanding Molecular Simulation: From Algorithms to Applications" by Smit and Frenkel.

Semester

First semester (End of September-January)

Assessment method

The exam is **oral only**. More specifically, the exam starts from the evaluation of the simulation results of the three parts of the exercises assigned during the Course and implemented by the students during the activities in the computer laboratory. To that goal, students are requested to prepare a **presentation of their results by slides** and to expose orally such content in a **time no longer than 15 minutes**, i.e. indicating only the key steps without details or explanations not requested. The teachers evaluate the clarity of the slides and the selection of topics and ask questions on the contents. Then a few open questions are asked on the general program of the Course, leading to the final mark.

There are no ongoing tests planned.

Office hours

Every day but by appointment to be agreed via email at least two days in advance.

Sustainable Development Goals

QUALITY EDUCATION