Course Syllabus

Particle-based modeling: an introductory course to molecular dynamics simulations

Instructor: Kamran Karimi

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Class Hours: Thurs 9:30-11:00 am
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Class Room: TBA
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Course Description

Molecular dynamics (MD) has become a state-of-the-art computational tool to improve our understanding towards physics and chemistry of a broad range of solids and liquids by focusing on associated structure and dynamics at atomistic scales. This course aims at introducing the fundamentals of MD (underlying theories, models, and methodologies) and to uncover capabilities of atomistic modeling and its broad applicability in practical contexts. The topic should be of great relevance to graduate students in physics, materials science, and other engineering disciplines with great interest in developing numerical particle-based models of concern.

Prerequisites

- background in classical mechanics;
- prior knowledge of statistical mechanics and classical thermodynamics is a plus but the lectures should be self sufficient;
- basic knowledge of probabilities, ordinary differential equations, and integral calculus;
- experience with a scientific programming language (Fortran, C++) or a scripting language (Python, Matlab) is desirable but not required.

Course Objectives

- Developing skills in implementing basic molecular dynamics codes, running computer simulations, and postprocessing and analyzing their output;
- Ability to measure equilibrium and transport properties using both molecular dynamics simulations and Monte Carlo sampling techniques and understand underlying approximations and associated advantages and limitations.

Course Contents

1. Introduction (**2** weeks)
    - molecular modeling
    - computer simulations
    - intermolecular forces
2. Statistical mechanics (**2-3** weeks)
    - classical thermodynamics, thermal equilibrium
    - probability distributions and thermodynamic averaging
    - statistical ensembles and fluctuations
    - Hamiltonian and sampling
    - Virial theorem, equipartition of energy
3. Molecular dynamics (**5-6** weeks)
    - Newton's equations of motion for many-body systems
    - numerical integration, accuracy, and stability
    - classical potentials and force fields
    - periodic boundary conditions and neighbor lists
    - implementation of thermostats and barostats
4. Monte Carlo (**3** weeks)
    - sampling for different ensembles
    - thermodynamic properties: free energy, heat capacity estimation

Course Requirements

This course will include (between 7-9) homework assignments based on the materials covered in class. On top of that, there will be a term project involving computer programming and its successful application in a practical problem of interest with a written part and an oral presentation due at the end of the semester. The topics and relevant methodologies will be selected based upon a mutual agreement between the students (individually) and the instructor. No final exam!

Grading Policy

- Homework assignments **50%**;
- Written paper **35%**;
- Seminar-style presentation **15%**.

Textbooks

- Michael P Allen and Dominic J Tildesley.*Computer simulation of liquids*. Oxford university press, 2017;
- Frenkel, D., & Smit, B. (2001). *Understanding molecular simulation: from algorithms to applications* (Vol. 1). Elsevier.