



Computer Simulation of Physical Systems I

PHYS-403

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Course 01/1

Presentation of the course

- Program
- Organisation
- Report
- General conditions from EPFL
- Evaluation
- Marking
- Motivation for following the exercise sessions

Program

Ordinary differential equations

methods for numerical integration: multistep algorithms and implicit algorithms.

Classical molecular dynamics I

Verlet algorithm, predictor-corrector algorithms, determination of macroscopic parameters, Nosé-Hoover thermostat, application to Lennard-Jones liquids.

Random variables

definitions and properties, generators and distribution functions, central-limit theorem.

Random walks

binomial and Gaussian distributions, particle diffusion, Brownian motion.

Monte Carlo integration

direct sampling, importance sampling, Metropolis algorithm, errors in correlated sampling, Monte-Carlo simulations of Lennard-Jones liquids and of two-dimensional spin systems.

Classical molecular dynamics II

Ewald summations, constraints.

Organisation

Courses

All courses will be given in presence in the class room CM012. Recordings of the material presented in 2021 are provided online.

Exercises

All exercise sessions will take place in the class room CO023. The time slot of the first exercise session on Tuesday 10th September 2024 at 15:15-17:00 (week 1) will be used to continue the course lectures, and will take place in room CM012. The first exercise session will start on Tuesday 17th September 2024 at 15:15 in room CO023 (week 2). There are no recordings of the exercise sessions.

Moodle page

This page contains all the material for the course including the recorded presentations, the corresponding PowerPoints, the documentation, the codes used in the exercise sessions, etc.: <https://moodle.epfl.ch/course/view.php?id=3711>

Report

Requirements

Detailed requirements for the report are provided in a sheet on Moodle page (Week 01).

Contents

The report covers topics that are addressed in the following exercise sessions:

Task II (Molecular dynamics of Lennard-Jones liquid)

Task III (NVT molecular dynamics with Nosé-Hoover thermostat)

Task VI (Monte Carlo simulation of Lennard-Jones liquid)

Supporting results are obtained during the exercise sessions. Codes for the execution of the tasks are provided.

Format

1 cover page + max 7 A4 pages including references, font size 12, line separation 1.25, font Helvetica, text should not approach borders by less than 2 cm.

Deadline for uploading reports on Moodle page

Wednesday 18 December 2024 at 13:00. A **paper version** of the report has to be handed in by the same time.

General conditions from EPFL

Individual report

At the Masters level, regulations of EPFL enforce that the work should be individual.

Language of the course

The report and the exam are in the language of the course, i.e. English.
Any desired change should comply with the regulations of EPFL.

Evaluation

Report

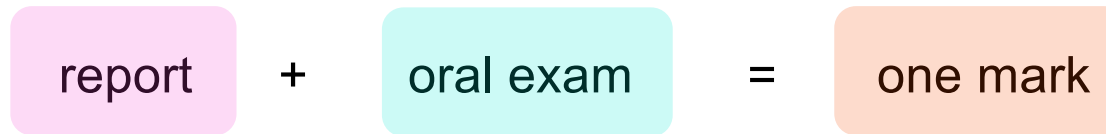
The report is evaluated on quality of the numerical results and of the presentation, overall discussion and interpretation.

Oral examination

All the material treated in the course is material that can be examined at the oral exam. Questions will be asked with the student in front of the black board. There will be no preparation time. The typical examination time is about 30 min with three topics being covered, but these are not strict conditions.

Marking

Final mark



The report is mandatory to access the exam

Weighing

The report could count at most up to 25% of the final mark.

For instance, with an excellent report,

- A partial mark of ≈ 3.5 at the oral exam could give a final mark of 4
- A partial mark of ≈ 5 at the oral exam could give a final mark of 5.25

Motivation for following the exercise sessions

- The same topics described in the course are illustrated through practical codes (Language: PYTHON 3, free, no license).
- All codes are provided and the implementation is thus available.
- In the case of some important codes for analysis, it is proposed to program these codes by yourself for those that prefer this learning approach.
- A deep understanding of the codes allows one to better understand the theoretical aspects discussed in the course, in view of the oral exam.
- The exercise sessions are necessary to prepare the report.
- However, the final exam is an oral examination (no coding).

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