PHYS-403 **Computer simulation of physical systems I**

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Cursus	Sem.	Type
Computational science and Engineering	MA1, MA3	Opt.
Computational science and engineering minor	H	Opt.
Ing.-phys	MA1, MA3	Opt.
Mechanical engineering	MA1, MA3	Opt.
Physicien	MA1, MA3	Opt.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	Oral
Workload	120h
Weeks	14
Hours	**4 weekly**
Courses	2 weekly
Exercises	2 weekly
Number of positions	

Summary

The two main topics covered by this course are classical molecular dynamics and the Monte Carlo method.

Content

The main focus of this course is the conceptual understanding of the potential and limitations of various simulation algorithms in the context of classical molecular dynamics and the Monte Carlo method. The Lennard-Jones liquid is extensively used for both methodologies as a case study for practical application. The codes for running the simulations are license-free and are provided. The emphasis of this course is on extracting physically relevant information from the simulations. Since the codes are provided, programming abilities may be helpful but do not correspond to the targets of this course. The main themes touched upon in the course are given below:

Ordinary differential equations: methods for numerical integration: multistep algorithms and implicit algorithms.

Classical molecular dynamics: Verlet algorithm, predictor-corrector algorithms, determination of macroscopic parameters, Nosé-Hoover thermostat, constraints, Ewald summations, 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.

Learning Prerequisites

Recommended courses

Statistical physics

Important concepts to start the course

Basic concepts from statistical physics

Learning Outcomes

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

- Model a physical problem by a computer simulation
- Interpret experimental properties using a computer program
- Carry out computer simulations

- Synthesize results in the form of a scientific report
- Choose an appropriate simulation method among those seen in the course
- Describe the simulation algorithms seen in the course
- Carry out computer simulations based on molecular dynamics and the Monte Carlo method
- Interpret experimental properties using computer simulations based on molecular dynamics and the Monte Carlo method
- Apply the methodologies seen in the course
- Explain the simulation algorithms seen in the course and associated issues.
- Assess / Evaluate errors associated with physical properties extracted from the simulations

Assessment methods

Report + oral exam = 1 grade

Resources

Virtual desktop infrastructure (VDI)

Yes

Ressources en bibliothèque

- Computational physics : an introduction / F.J. Vesely
- Computational physics / J. M. Thijssen
- Computational physics / S. E. Koonin

Websites

- http://moodle.epfl.ch/course/view.php?id=3711

Moodle Link

- https://go.epfl.ch/PHYS-403