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

Pasquarello Alfredo

Cursus	Sem.	Type
Computational science and Engineering	MA1, MA3	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

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

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

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