

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
<b>Hours</b>	<b>4 weekly</b>
Lecture	2 weekly
Exercises	2 weekly
<b>Number of positions</b>	

**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>