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 / S. E. Koonin  
• Computational physics / J. M. Thijssen

Websites

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