Simulation methods in statistical physics

Lecturer
Bortolo Matteo MOGNETTI (Coordinator)

Course mnemonic
PHYS-F481

ECTS credits
5 credits

Language(s) of instruction
English

Course period
Second term

Campus
Plaine

Course content

The Monte Carlo Method
- random number generators
- sampling stochastic variables

Dynamic Monte-Carlo simulations
- Markov chains
- Ergodicity and (super) detailed balance
- Generative models
- Data analysis

Critical phenomena
- Finite-size scaling
- Self-avoiding walks

Ensembles
- simulations in the microcanonical ensemble
- simulations in the canonical ensemble
- simulations in the isobaric-isothermal ensemble
- simulations in the grand-canonical ensemble
- the Gibbs ensemble
- biased sampling
- free energy and density of states calculations

Molecular Dynamics
- symplectic integrators
- Nosé–Hoover thermostat

Objectives (and/or specific learning outcomes)

Understanding of the principal simulation techniques (Monte Carlo and Molecular Dynamics) used in Statistichal Mechanics.

Ability to design and implement algorithms to sample probability distributions.

Teaching method and learning activities

classroom teaching

theoretical and exercice (including programming) classes

Contribution to the teaching profile

1.4 1.3 and 1.2

References, bibliography and recommended reading

[[span]]

D. E. Knuth, *The art of computer programming* (chapter 3), Addison Wesley

A. Sokal, *Monte Carlo Methods in Statistical Mechanics: Foundations and New Algorithms.* In: DeWitt-Morette C., Cartier P., Folacci A. (eds) Functional Integration.

D. Frenkel and B. Smit *Understanding Molecular Simulation: From Algorithms to Applications,* Elsevier

D. P. Landau and K. Binder A guide to Monte Carlo simulations in statistical physics, Cambridge university press

Other information

Place(s) of teaching

Plaine

Contact(s)

Bortolo.Matteo.Mognetti@ulb.be

Evaluation method(s)

Other

Evaluation method(s) (additional information)

A Oral examination

B Study and presentation of a scientific article relevant for the course

Determination of the mark (including the weighting of partial marks)

A 70%

B 30%

Main language(s) of evaluation

French and English

Programmes

Programmes proposing this course at the faculty of Sciences

MA-PHYS | Master in Physics | finalité Research/unit 1 and finalité Teaching/unit 1