

# 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 Statistical Mechanics.

Ability to design and implement algorithms to sample probability distributions.

## Teaching method and learning activities

classroom teaching

theoretical and exercise (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

