

MSE-639

**Statistical methods in atomistic computer simulations**

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.
Materials Science and Engineering		Opt.

Language of teaching	English
Credits	2
Session	
Exam	Project report
Workload	60h
<b>Hours</b>	<b>28</b>
Courses	14
TP	14
<b>Number of positions</b>	<b>25</b>

**Frequency**

Every 2 years

**Remark**

Postponed until further notice

**Summary**

The course gives an overview of atomistic simulation methods, combining theoretical lectures and hands-on sessions. It covers the basics (molecular dynamics and monte carlo sampling) and also more advanced topics (accelerated sampling of rare events, and non-linear dimensionality reduction)

**Content**

Sampling the constant-temperature ensemble in atomistic simulations

- Canonical averages and importance sampling
- Monte Carlo, detailed balance and the Metropolis algorithm
- Molecular dynamics, integrators, energy conservation
- Autocorrelation functions, correlation time and statistical efficiency

Thermostatting molecular dynamics

- Breaking energy conservation and getting into the canonical ensemble
- Global and local thermostats, deterministic and stochastic thermostats
- Langevin dynamics. Stochastic differential equations and sampling efficiency
- Colored-noise generalized Langevin dynamics

Rare events. Getting dynamics from ensemble averages

- Rare events and time-scale separation
- Transition-state theory on the potential energy surface
- Collective coordinates. Free energy and TST on the free-energy surface
- Beyond TST. Bennett-Chandler method, committor analysis

Re-weighted sampling and adaptive biasing

- Re-weighting a trajectory to get averages in a different ensemble
- Statistics of re-weighting. Sampling efficiency of weighted averages
- Umbrella sampling and adaptive (Wang-Landau) biasing
- Metadynamics. Basics, examples and caveats

Linear and non-linear dimensionality reduction

- Dimensionality reduction -- coarse-graining the description of structurally complex systems
- Linear projection: principal component analysis; classical multidimensional scaling
- Non-linear dissimilarity reduction: ISOMAP, locally-linear embedding
- Sketch map: using proximity matching to describe atomistic problems

**Keywords**

Introductory knowledge of statistical mechanics and probability, basic programming skills preferably in FORTRAN. Some

familiarity with working in a Linux environment is preferable

### **Learning Prerequisites**

#### **Recommended courses**

Introductory knowledge of statistical mechanics and probability, basic programming skills, preferably in FORTRAN or Python

### **Assessment methods**

Project report

### **Resources**

#### **Websites**

- <http://cosmo.epfl.ch/>