

MSE-639

Statistical methods in atomistic computer simulations

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| Cursus | Sem. | Type |
|-----------------------------------|------|------|
| Materials Science and Engineering | | Obl. |

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|----------------------------|----------------|
| Language of teaching | English |
| Credits | 2 |
| Session | |
| Exam | Project report |
| Workload | 60h |
| Hours | 28 |
| Courses | 14 |
| TP | 14 |
| Number of positions | 25 |

Frequency

Every 2 years

Remark

Next time: 2018-19

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>