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
Hours	**28**
Courses	14
TP	14
Number of positions	**25**

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/