FSI3250 Advanced Simulation Methods in Statistical Physics 7.5 credits

Avancerade simuleringsmetoder i statistisk fysik

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment

Course syllabus for FSI3250 valid from Spring 2009

Grading scale

Education cycle

Third cycle

Specific prerequisites

Familiarity with computers and basic programming ability.
Basic statistical physics.
Elementary probability theory.
Basic course in computer simulations recommended, but not compulsory.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After completed course, the PhD student should:

- have a deep theoretical understanding of several Monte Carlo and molecular dynamics methods.
- have hands-on experience from implementing and using these techniques.
- be able carry out simulations in different ensembles.
- be able to carry out advanced data analysis using, e.g., reweighting.
- know when to apply the different methods.
- be able to develop new simulation methods.

Course contents

- Basics of molecular dynamics
- Basics of Monte Carlo simulations
- Markov chain theory • Detailed balance, Metropolis method, Heat bath method, etc • Convergence • Dynamical point of view, simulating rare events using N-fold way
- Data analysis: • Estimating errors. Autocorrelation times. • Histogram reweighting
- Simulations in different ensembles: • MC in NPT, Grand canonical, (Micro canonical) ensembles • MD in Canonical, NPT ensembles, etc
- Simulations in extended ensembles: • Parallel tempering (aka Replica exchange MC) • Multicanonical, Simulated tempering, ... • Wang-Landau method
- Free energy calculations • Integration method (temperature, density, or other parameters) • Umbrella sampling • Particle insertion
- Cluster updates and worm algorithms • Swendsen-Wang, Wolff
- Quantum Monte Carlo: • Path integral MC: Mapping to classical problem • Stochastic series expansion (SSE) • Worm algorithm

Disposition

Computer simulations are invaluable in modern science. Molecular dynamics aims to integrate the equations of motion of a physical system, thus mimicking the real dynamics of natural phenomena. In this way we can learn many things about complex phenomena that are difficult or even impossible to obtain in other ways.

Monte Carlo simulations, on the other hand, take a short cut and directly generate samples from the probability distribution that governs the statistical properties of a system. The Monte Carlo method is not one method, but rather a framework of great generality, that can be applied to many different fields, not only statistical physics, but also statistics, finance, bioinformatics, engineering, etc.

Using the computer as a virtual lab, one can avoid many complications of real experiments, and instead carry out computer experiments. Besides reducing costs, this can, in many cases, allow for much more precise control over the external parameters, and eliminate measurement uncertainties (instead there will be statistical errors). So this is very useful both when exploring the consequences of an underlying complicated theory, and when one wants to compare theories with effective idealized models.

This course will give you a theoretical understanding of advanced simulation methods, as well as provide hands on experience using state-of-the-art methods. We go through the theoretical basis of molecular dynamics and Monte Carlo algorithms, and discuss various ways to speed up simulations, using cluster update methods, parallel tempering, etc. We discuss how to use the sampled data in more efficient ways, and methods for the calculation of free energies, something which is not straightforward. While the application area for the course is statistical physics, the methods discussed here apply to many other problems too.

Course literature

There is no specific course textbook. The course literature consists of lecture notes and several research articles as well as several textbooks can be used.

Examination

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Other requirements for final grade

To fulfill the course requirements you should complete the computer labs/projects and give a short presentation (15-20 min) of a special topic of your choice.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.