General Information

Course name	Computational Physics II	ECTS Credits	4
		Semester	W

Aims

To teach students to use computer as a tool of modeling of physical reality focusing on design of simulation projects to help to solve physical problems.

Content

1. Basic and advanced methods of Monte Carlo simulations of lattice spin systems. Types of local perturbation algorithms (Metropolis, Heat-bath, Glauber) and their performance.
2. Critical slowing-down of the relaxation process – nonlocal cluster methods of Monte Carlo simulation. Swendsen-Wang, Wolff and other advanced algorithms.
3. Statistical analysis of Monte Carlo data. Initial non-equilibrium period and transition to the equilibrium state.
4. Calculation of mean values and statistical errors in the equilibrium state. The adverse impact of temporal autocorrelation on their estimation.
5. Statistical errors, autocorrelation times and their numerical estimation. Binning and Jackknife analyses.
6. Histogram data processing. Reweighting by the simple histogram and multi-histogram methods.
7. Universality and finite-size scaling analysis. Universality classes and calculation of critical exponents.
8. Determination of the type of phase transition by finite-size scaling. The phase transitions of the first and second order. Binder cumulant.
9. Monte Carlo simulations of stochastic processes. A one-dimensional discrete random walk. Transition to a continuous random walk. Diffusion equation.
10. Basic quantum Monte Carlo simulations. Determination of the ground state of a quantum system based on the concept of random walks.
11. Random processes in the financial analysis. Geometric Brownian motion. Monte Carlo simulations of stock prices. Black-Scholes analysis.
12. Basic methods of molecular dynamics. Lennard-Jones potential. Verlet and velocity-Verlet discretization.
13. The implementation of the method of molecular dynamics. Periodic boundary conditions and other relevant conditions in the simulation of the finite system.

Assessment Methods and Criteria

Prerequisites: Numerical Methods; Statistical Mechanics. Continuous evaluation is based on students' activity in the classroom and work on assignments. The course ends with final oral examination.

Grading Scale (in %):
A: 91% - 100%
B: 81% - 90%
C: 71% - 80%
D: 61% - 70%
E: 51% - 60%
F: 0% - 50%

Grading System:
The University recognises the following six degrees for the evaluation of the study results:
a) A – excellent (excellent results) (numerical value 1)
b) B – very good (above average results) (1.5)
c) C – good (average results) (2)
d) D – satisfactory (acceptable results) (2.5)
e) E – sufficient (results meet the minimum criteria) (3)
f) FX –failed (requires further work) (4)

Bibliography

1. D.P. Landau, K. Binder: A Guide to Monte Carlo Simulations in Statistical Physics, Cambridge University Press, 2000.
2. B.A. Berg: Introduction to Markov Chain Monte Carlo Simulations and Their Statistical Analysis, http://www.worldscibooks.com/etextbook/5904/5904_intro.pdf
3. W. Janke: Lectures on Ising model, http://www.physik.uni-leipzig.de/~janke/Ising_Lectures_Lviv.html