Introduction to computer simulations - course description

General information

Course name	Introduction to computer simulations
Course ID	13.2-WF-FizP-ItCS-S17
Faculty	Faculty of Physics and Astronomy
Field of study	Physics
Education profile	academic
Level of studies	First-cycle Erasmus programme
Beginning semester	winter term 2017/2018

Course information

Semester	6
ECTS credits to win	4
Course type	obligatory
Teaching language	english
Author of syllabus	

Classes forms

The class form	Hours per semester (full-time)	Hours per week (full-time)	Hours per semester (part-time)	Hours per week (part-time)	Form of assignment
Laboratory	45	3	-	-	Credit with grade

Aim of the course

The aim of the course is to gain basic knowledge of computer simulations of selected methods for problems of deterministic and Monte Carlo-type issues. Students should acquire skills of implementation of this knowledge by designing an algorithm and a computer program and then interpreting the results of computer simulations. Specific examples will include e.g. problems of molecular dynamics of a single particle, molecular dynamics with constraints, modeling Brownian motion and other random events for different distributions of random variables.

Prerequisites

Programming skills in C / C + +, Python or Java and knowledge of numerical methods

Scope

- Representation of numbers, excess and underflow errors, truncation error (finite difference method), the stability of numerical algorithms.

- Algorithms for solving the equation of motion: Euler, Verlet, velocity Verlet, leap-frog predictor-corrector algorithm, the choice of the time step, the stability and accuracy of the algorithms, numerical solution of the harmonic oscillator 1D and 2D.

- Monte Carlo algorithms (random number generators, random variables with different probability distributions, Metropolis algorithm, stochastic equations).

- Cellular automata.

- Genetic algorithms.

Teaching methods

laboratory exercises, discussions, independent work with a specialized scientific literature in Polish and English, and work with the technical documentation, search for information on the Internet.

Learning outcomes and methods of theirs verification

Outcome description	Outcome symbols	Methods of verification	The class form
Students expand their ability to acquire knowledge in different ways using a variety of sources		• a discussion • a project • activity during the classes	• Laboratory
Students have an extended knowledge of classical physics of interacting systems with particular emphasis on the impact parameters potential impact on the stability and behavior of the studied systems		• a discussion • a project • activity during the classes	• Laboratory

Outcome description	Outcome symbols	Methods of verification	The class form
Students have has expertise in the following areas: numerical error analysis, numerical solution of differential equations, implementation, and application design to simulate the physical processes of the molecular dynamics of interacting particles, integration methods of Monte Carlo, Metropolis algorithm, the results of numerical analysis, random number generators		• a discussion • a project • activity during the classes	• Laboratory
They have skills in data analysis, they have knowledge which is acquired during the studies of scientific literature		• a discussion • a project • activity during the classes	• Laboratory
Students have expanding awareness of the need to update the technical knowledge on the available techniques and simulation results as well as awareness of the impact of research on the development of computer technology, including in particular nanotechnology.		• a discussion • a project • activity during the classes	• Laboratory

Assignment conditions

Laboratory: positive evaluation of the tests, the execution of the project. The final evaluation of the laboratory: evaluation of tests of 60%, the assessment of the project 40%.

Recommended reading

[1] J. C. Berendsen and W. F. Van Gunsteren, Practical Algorithms for Dynamic Simulations in Molecular dynamics simulations of statistical mechanical systems, Proceedings of the Enrico Fermi Summer School, p.43-45, Soc. Italinana de Fisica, Bologna 1985. 154

[2] Stephen Wolfram, Statistical mechanics of cellular automata, Rev. Mod. Phys. 55, 601-644 (1983).

[3] Tao Pang, An Introduction to Computational Physics, Cambridge University Press (2006).

Further reading

[1] William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, Numerical recipes, The art of scientific computing, third edition 2007.

Notes

Modified by dr hab. Maria Przybylska, prof. UZ (last modification: 27-10-2017 20:38)