Computer simulations - course description

General information

Course name	Computer simulations
Course ID	13.2-WF-FizD-CS- 17
Faculty	Faculty of Physics and Astronomy
Field of study	Physics
Education profile	academic
Level of studies	Second-cycle studies leading to MS degree
Beginning semester	winter term 2021/2022

Course information

Semester	2
ECTS credits to win	6
Available in specialities	Theoretical physics
Course type	obligatory
Teaching language	english
Author of syllabus	• prof. dr hab. Mirosław Dudek

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
Lecture	15	1	-	-	Exam
Laboratory	30	2	-	-	Credit with grade

Aim of the course

The aim of the course is to gain basic knowledge of computer simulation methods and the ability to choose the appropriate simulation model to the considered problem. Students should acquire skills in implementation of this knowledge by designing the proper algorithms and then interpreting the results of computer simulations.

Prerequisites

Ability to use some programming language.

Scope

- Representation of numbers, excess and underflow errors, truncation error (finite difference method), the stability of numerical algorithms.
- Algorithms for solving the equations of motion: Euler, Verlet, velocity Verlet, numerical solution of the harmonic oscillator.
- Monte Carlo algorithms (random number generators, random variables with different probability distributions, Metropolis algorithm, stochastic equations).
- Selected examples of applications (simulation of phase transitions, relaxation of the electric dipole)

Teaching methods

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

Learning outcomes and methods of theirs verification

Outcome description	Outcome symbols	Methods of verification	The class form
Students know numerical error analysis, numerical methods of solving differential equations, they can use molecular dynamics methods, methods of Monte Carlo.	• K2_W05	• a discussion • a test • an exam - oral, descriptive, test and other	• Lecture • Laboratory
They have skills in data analysis, they posses knowledge which is acquired during studies of the scientific literature.	• K2_U03 • K2_U05 • K2_U10	• a discussion • a test • an exam - oral, descriptive, test and other	• Lecture • Laboratory
Characteristic feature is the 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.	• K2_K01 • K2_K05	• a discussion • a test • an exam - oral, descriptive, test and other	• Lecture • Laboratory

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.	• K2_U10	• a discussion	• Laboratory
Students have an extended knowledge of classical physics of interacting systems.	• K2_W01	• an exam - oral, descriptive, test and other	• Laboratory
They have practical knowledge on modeling using pseudo-random number generator and deterministic methods.	• K2_W02	• a test • an exam - oral, descriptive, test and other	• Lecture • Laboratory

Assignment conditions

Lecture: positive evaluation of the test.

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%.

Before taking the exam the student must be credited with the exercises.

Final grade: arithmetic mean of the completion of the lecture and in excersises.

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.

[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 Marcin Kośmider (last modification: 09-05-2021 21:39)