COURSE DESCRIPTION CARD - SYLLABUS

Course name
Computer simulations [S1FT2>SK]

Course

Field of study
Technical Physics

Year/Semester
3/6

Area of study (specialization)
–

Profile of study
general academic

Level of study
first-cycle

Course offered in
Polish

Form of study
full-time

Requirements
compulsory

Number of hours

Lecture
15

Laboratory classes
0

Other (e.g. online)
0

Tutorials
0

Projects/seminars
0

Number of credit points

1,00

Coordinators

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Lecturers

Prerequisites

General knowledge of physics, mathematics and the basics of programming at the level achieved after five semestrs of study in the field of technical physics. The ability to solve simple physical problems based on the acquired knowledge, the ability to obtain information from indicated sources. Understanding the necessity of self-training.

Course objective

To acquaint students with computational techniques used to simulate physical phenomena with the use of C ++, Java or Python programming languages.

Course-related learning outcomes

Knowledge:
The student knows the mathematical apparatus necessary to describe the basic laws of physics and solve tasks related to the issues of technical physics, has an ordered and theoretically founded general knowledge of the structure and functions of nano- and microworld objects, knows the current state of advancement and is familiar with the latest development trends in the field of computer simulation of physical processes

Skills:
The student is able to:
1. apply the appropriate mathematical apparatus and perform computer simulations of basic physical phenomena and technical processes with the use of standard software

Social competences:
The student acquires competences allowing for:
1. independent and creative work on the given task
2. understanding the needs and possibilities of continuous training

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Learning outcome (symbol) Method of assessment Assessment criteria
W01, W10-W13, K01, K03, K08|open question/test|3: 51%-70%, 4: 71%-90%, 5: od 90%

Programme content

1. Elements of statistical physics.
2. Fundamentals of dynamics of nonlinear systems.
3. Molecular dynamics simulation methods:
a) motion equation integration algorithms,
b) periodic boundary conditions,
c) equilibrium and non-equilibrium molecular dynamics,
d) selected stochastic methods (Monte Carlo algorithm, Brown dynamics, Langevin dynamics),
4. Fundamentals of programming and creating computer simulations in Java and / or Python.
5. Fundamentals of data analysis and visualization using C++ and / or Java and / or Python.

Course topics

none

Teaching methods

Conversational lecture: multimedia presentation, simulation demonstrations, examples given on the blackboard, solving research problems.

Bibliography

Basic:
1. Materials from lectures (in Polish)
2. Podstawy fizyki statystycznej, Kerson Huang,Wydawnictwo Naukowe PWN, Warszawa 2006.
3. Understanding Molecular Simulation. From Algorithms to Applications, D. Frenkel, B. Smit, Academic Press.
4. Computer Similation of Liquids, M. P. Allen, D. J. Tildesley, Oxford University Press 2017

Additional:
1. Molecular Modeling Techniques in Material Sciences, J.-R. Hill, L. Subramanian, A. Maiti, Taylor&Francis 2005.
2. Molecular Modeling and Simulation. An Interdisciplinary Guide, T. Schlick, 2nd edition, Springer 2010.
3. The nature of Code, Daniel Shiffman 2012.

Breakdown of average student's workload

	Hours	ECTS
Total workload	25	1,00
Classes requiring direct contact with the teacher	17	0,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	8	0,50