

Module/Course Syllabus
Program: COMPUTER SCIENCE
 Full-time master degree program

Course:	Monographic lecture
Type of the course:	Directional
Course code:	I2S1.09
Year:	I
Semester:	1
Form of the degree program:	full-time
Form of classes and number of hours per semester:	15
Lecture	15
Number of ECTS credits:	1
Form of assessment:	course completion assessment
Course language:	English

Course objective (CO)	
CO1	Familiarizing students with the basics of simulation methods.
CO2	Gaining knowledge about transferring a real problem to the world of computer simulations.

Prerequisites in terms of knowledge, skills and other competencies	
1	Knowledge of the basics of algorithms and numerical methods.
2	Basic knowledge of differential and integral calculus.
3	Programming in selected languages: C, C++, Java, Python, Fortran.

Learning outcomes (LO)	
	In terms of knowledge:
LO 1	Has knowledge of simulation methods.
LO 2	Has a structured knowledge of the basics of Molecular Dynamics.
	In terms of skills:
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	In terms of social competence:
LO 3	He is ready to critically assess his knowledge and appreciate the importance of expert knowledge.

Course content	
Form of classes - lectures (L)	
	Course content
L1	Introduction: computer simulations: molecular dynamics.
L2	Impacts in the simulation system: type, range, right choice.
L3	Methods of solving Newton's equations of motion.
L4	Optimization of simulation calculations scale.
L5	Numerical methods of temperature thermostating.
L6	Calculation of averages for different thermodynamic systems.
L7	Application of Molecular Dynamics to stress modelling.

Didactic methods	
1	Lecture with multimedia presentation.

Assessment methods and criteria		
Assessment method symbol	Assessment method description	Passing threshold
A1	Test with closed, multiple choice and open questions.	51%
A2	Lecture attendance and activity	51%

Required textbooks and other course materials	
1	Frenkel, D., Smit, B., Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2002
2	Allen, M. P., Tildesley, D.J., Computer simulation in chemical physics, Springer Science & Business Media, 2012.
Recommended textbooks and other course materials	
1	Matyka, M., Symulacje komputerowe w fizyce, Helion, 2002.

Student workload	
Form of activity	Average number of hours to complete the activity
Contact hours with the lecturer, including:	15
<i>participation in lectures</i>	15
Student's own work, including:	10
<i>preparation for the exam</i>	10
Total student workload	25
Total number of ECTS credits	1

Learning outcomes matrix					
Learning outcome	Reference to learning outcomes defined for the master's program	Course objectives	Course content	Didactic methods	Assessment methods
LO 1	I2A_W01+	CO1,	L1	1	A1
LO 2	I2A_W06++ I2A_W08+++ I2A_W10+	CO1, CO2	L1-L7	1	A1
LO 3	I2A_K01+ I2A_K02++	CO1, CO2	L1-L7	1	A1, A2

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