



Subject card

Subject name and code	Computational physics, PG_00060225						
Field of study	Fizyka obliczeniowa						
Date of commencement of studies	October 2023		Academic year of realisation of subject		2025/2026		
Education level	first-cycle studies		Subject group		Optional subject group Subject group related to scientific research in the field of study		
Mode of study	Full-time studies		Mode of delivery		at the university		
Year of study	3		Language of instruction		Polish		
Semester of study	5		ECTS credits		5.0		
Learning profile	general academic profile		Assessment form		exam		
Conducting unit	Institute of Physics and Applied Computer Science -> Faculty of Applied Physics and Mathematics -> Wydział Politechniki Gdańskiej						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Marta Łabuda				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	30.0	0.0	0.0	60
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	Number of study hours	60		5.0		60.0	125
Subject objectives	The aim of the course is to familiarize students with advanced computational and simulation methods used in selected fields of physics (particularly electrodynamics, quantum physics, and modern physics). The course also covers programming techniques for these methods and discusses typical problems associated with their implementation.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K6_U04] Can plan and conduct experiments, critically analyze their results, draw conclusions and form opinions. Has laboratory work experience.	Student is able to plan and carry out a computer simulation of a physical phenomenon, select appropriate numerical methods, and evaluate the accuracy and stability of the obtained results. Student is able to critically analyze the results of numerical calculations and simulations, compare them with experimental or theoretical data, draw conclusions, and present them in the form of a report or graphical visualization.	[SU2] Ocena umiejętności analizy informacji [SU3] Ocena umiejętności wykorzystania wiedzy uzyskanej w ramach przedmiotu
	[K6_W02] Has systematized knowledge of the basics of physics, including mechanics, thermodynamics, electricity and magnetism, optics, atomic and particle physics, solid-state physics, nuclear and elementary particle physics.	The student knows the basic numerical methods used to solve physical equations describing phenomena from various fields of physics (including mechanics, thermodynamics, electrodynamics, and quantum physics). The student understands how computational methods enable quantitative analysis and simulation of physical phenomena across different scales — from classical systems to microscopic processes in atomic and solid-state physics.	[SW1] Ocena wiedzy faktograficznej
	[K6_W01] Understands the importance of physics and its applications in connection to civilization.	Student understands the role of computational methods in the development of modern physics and technology, as well as their impact on civilizational progress (e.g. energy, medicine, information technologies, climate). Student is aware that the ability to apply computational methods constitutes an essential component of a modern physicist's competencies in the context of scientific, industrial, and sustainable civilizational development.	[SW1] Ocena wiedzy faktograficznej
	[K6_U02] Can analyze and solve simple scientific and technical problems, based on possessed knowledge, using analytical, numerical, simulation and experimental methods.	The student is able to analyze a problem and find its solution.	[SU4] Ocena umiejętności korzystania z metod i narzędzi
	[K6_K05] Can present own work results, transfer information in a commonly understandable manner, communicate and self-evaluate, as well as constructively evaluate the effects of other persons' work.	The students are able to present the results of their work.	[SK3] Ocena umiejętności organizacji pracy

Subject contents	Course content – lecture Modeling of nanoscale systems in a computational context. Modeling of the dielectric function Drude and Lorentz models. Finite-difference (FDTD) and finite-element (FEM) methods for solving Maxwells equations. Transformation from the time domain to the frequency domain using the discrete Fourier transform (DFT). Fundamentals of quantum mechanics in a computational context. Born-Oppenheimer approximation. Self-consistent field (SCF) methods and configuration interaction (CI). Other quantum chemistry methods (density functional theory DFT, coupled cluster CC, and others). Analysis of selected computer codes performing quantum-mechanical calculations (e.g., GRASP, ORCA, and others). Presentation of problems related to programming these computational methods and practical approaches to solving them (issues related to the high computational complexity of problems, convergence issues in self-consistent field methods, problems arising from inaccurate numerical representation of real numbers in computer memory, communication issues between different modules of software packages, etc.). Elements of modern physics. Investigation of symmetry breaking (C, P, T) in physics as a method for testing the Standard Model. Methods for calculating and measuring electric dipole moments of atoms and molecules.		
	Course content – laboratory Heat propagation simulations on a plate made of a selected material, e.g., using COMSOL/FreeFEM. Graphical visualization of results. (4 hours) Simulations of visible light propagation through arrays of gold/silver nanoparticles using OmniSim, MiePlot, MEEP, or other software packages. (4 hours) Use of the GRASP package for quantum-mechanical calculations of atomic structures: energy levels, oscillator strengths, and transition probabilities for selected multi-electron atoms. (4 hours) Calculations of electric dipole moments (EDM) of selected atoms and molecules as examples of symmetry breaking. Using GRASP, COWF packages, and custom programming. (4 hours) Calculations of the structure of selected molecules and their spectroscopic parameters, including IR/UV spectra. (4 hours) Determination of potential energy curves (surfaces). (4 hours) Fundamentals of molecular dynamics: solving equations of motion, modeling simple chemical reactions. (4 hours) High-precision calculations using the Multiple Precision Integers and Rationals (MPIR) library. (2 hours)		
Prerequisites and co-requisites	Basics of numerical methods.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Lab	50.0%	60.0%
	Exam	50.0%	40.0%

Recommended reading	Basic literature	J. F. Dobrowolski, Fizyka obliczeniowa. Podstawy i zastosowania, Wydawnictwo Naukowe PWN, Warszawa 2018 M. Kowalski, Symulacje komputerowe w fizyce i chemii kwantowej, Wydawnictwo Naukowe PWN, 2016 R. Zienkiewicz, Metody elementów skończonych w mechanice i fizyce, Wydawnictwo Naukowo-Techniczne, Warszawa 2015 A. Grabowski, Podstawy dynamiki molekularnej i modelowania komputerowego, Wydawnictwo Naukowe PWN, 2017 J. R. Reitz, F. J. Milford, Podstawy elektrodynamiki (tłumaczenie polskie), WNT, Warszawa 2014 A. Herman, Atomy i kwanty. Wprowadzenie do współczesnej spektroskopii atomowej, PWN 2006 M. Mansuripur, Field, Force, Energy and Momentum in Classical Electrodynamics (wydanie poprawione), Bentham Science Publishers, 2017 P. Jönsson, G. Gaigalas, C.F. Fischer, J. Bieroń, I.P. Grant, T. Brage, J. Ekman, M. Godefroid, J. Grumer, J. Li, W. Li, GRASP Manual for Users. Atoms, 11(4), 68 (2023). https://doi.org/10.3390/atoms11040068
	Supplementary literature	M. Wróblewski, Metody numeryczne w fizyce, Wydawnictwo Naukowe PWN, 2015 T. K. Kołodziejwski, Fizyka współczesna w zadaniach obliczeniowych, Wydawnictwo Naukowe PWN, 2016 B. Khriplovich, S.K. Lamoreaux, CP Violation Without Strangeness, Springer Berlin, Heidelberg 1997 P. Jönsson, M. Godefroid, G. Gaigalas, J. Ekman, J. Grumer, W. Li, J. Li, T. Brage, I.P. Grant, J. Bieroń, C.F. Fischer, An Introduction to Relativistic Theory as Implemented in GRASP, Atoms, 11(1), 7 (2023). https://doi.org/10.3390/atoms11010007
	eResources addresses	
Example issues/ example questions/ tasks being completed	Simulations of heat propagation and electromagnetic wave propagation How can finite-difference (FDTD) and finite-element (FEM) methods be used to model heat conduction in materials or light propagation through nanostructures? Quantum-mechanical calculations of atomic and molecular structures How do calculations of electric dipole moments of atoms and molecules allow the study of symmetry breaking (C, P, T) in modern physics? How can molecular dynamics simulations be implemented, equations of motion for particles solved, and simple chemical reactions modeled in a computational context?	
Practical activities within the subject	Not applicable	