

Subject card

Subject name and code	Numerical methods with algorithms for physical sciences, PG_00129569						
Field of study	Chemistry						
Date of commencement of studies	October 2025		Academic year of realisation of subject		2026/2027		
Education level	Master's studies		Subject group		Optional subject group		
Mode of study	full-time studies		Mode of delivery		at the university		
Year of study	2		Language of instruction		Arabic		
Semester of study	4		ECTS credits		2.0		
Learning profile	academic		Assessment form		credit		
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Adam Sieradzan				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	30.0	0.0	0.0	30
	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	30		5.0		15.0	50
Subject objectives	Familiarizing the students with the numerical algorithms applied in chemistry. Preparing the students to write own numerical applications, including existing numerical libraries in the procesess.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry.	[SW2] presentation/project/paper/report
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student defines and solves problems related to the specifics of floating point arithmetic that arise when using available packages of quantum chemistry, molecular mechanics and dynamics, chemometrics, etc. The student solves computational problems that arise in chemistry and related subjects when using software libraries available at computer centers, or on the Internet. For this purpose, the student designs simple numerical applications using in-house or library procedures.	[SU1] oral statement/conversation/discussion [SU2] presentation/project/paper/report [SU6] demonstration of practical skills
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the ability of working in a team.	[SK1] oral statement/conversation/discussion [SK2] presentation/project/paper/report [SK8] observation of student's independent or team work
	[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the responsibility for his/her personal account on the workstation.	[SK1] oral statement/conversation/discussion [SK2] presentation/project/paper/report
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry.	[SW2] presentation/project/paper/report
	[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student describes floating point arithmetic's problems and explains the causes and implications of floating point round-offs. Defines the concept of the algorithm. Describes the basic numerical algorithms applied in solving equations and systems of linear and nonlinear equations, target function minimization and solving the initial and boundary problems for ordinary and partial differential equations, respectively. The student describes the numerical methods that can be applied so solve a given problem of computational chemistry or chemometry	[SW2] presentation/project/paper/report

Subject contents	Algorithm and its correctness. Errors in numerical calculations; Wilkinsons lemmas. Condition number of a problem. Overflow (INF), underflow, NaN. Interpolation: Lagrange and Newton schemes. Numerical differentiation. Numerical integration: the Newton-Coates and Gauss quadratures. Solution of linear equations systems: the Gauss, Gauss-Jordan, Cholesky, Householder, and QR algorithms. Solution of eigenvalue problem in quantum chemistry. Solution of nonlinear equations: the Newton, regula falsi, secant, Pegasus, and bisection algorithms. Solution of systems of nonlinear equations; calculation of equilibrium concentrations in multicomponent systems as an example. Local minimization of functions in single and several variables in relation to conformational analysis with molecular mechanics. Introduction to global optimization algorithms and their relation to the problem of finding the most stable structures of molecules and crystals. Least-squares algorithms in fitting models to experimental data: linear and nonlinear regression (the Newtona-Gauss, Newtona, i Levenberg-Marquardt methods): application in the determination of equilibrium constants. Statistical assessment of the goodness of fit and of the confidence levels of the determined parameters. Determination of parameters from noisy or insufficient data: the maximum entropy method. Algorithm for solving ordinary differential equations: application to chemical kinetics and molecular dynamics. Algorithms for solving partial differentia equations: applications to the electrochemical analysis (e.g., calculation of cyclic voltamperometry and polarography profiles) and to the calculation of electrostatic solvation energy of macromolecules. Fourier transformation and its application to the processing of IR and NMR spectra. Cluster analysis algorithms. Factor analysis algorithms and their application to the decomposition of UV spectra, QSAR, and conformational analysis.		
Prerequisites and co-requisites	Introduction to Python programming Basis of calculus and linear algebra, ability to use the LINUX operating system.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	task performance reports	51.0%	100.0%
Recommended reading	Basic literature	Siegmund Brandt, Data Analysis - Statistical and Computational Methods for Scientists and Engineers, Springer 2014 Extracurricular readings Qingkai Kong, Timmy Siau, Alexandre Bayen, Python Programming and Numerical Methods A Guide for Engineers and Scientists, Academic Press 2020	
	Supplementary literature	Python Programming for Arduino - Desai Pratik	
	eResources addresses		
Example issues/ example questions/ tasks being completed			
Work placement	Not applicable		

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