KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI
FUNDUSZ SPOŁECZNY

Course title	ECTS code
Numerical methods with algorithms for physical sciences	13.3.1318

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	Digital Chemistry
		specialization	wszystkie

Teaching staff

dr hab. Adam Sieradzan, profesor uczelni; prof. dr hab. Cezary Czaplewski, profesor uczelni

Forms of classes, the realization and number of hours

Forms of classes

Laboratory classes

The realization of activities

classroom instruction

Number of hours

Laboratory classes: 30 hours

ECTS credits

2
classes – 30 h
student's own work – 10 h
tutorial classes – 10 h
Total: 50 h – 2 ECTS

The academic cycle

2024/2025 summer semester

Type of course

an elective course

Language of instruction

English

Teaching methods

Case studies in computer laboratory

Form and method of assessment and basic criteria for eveluation or examination requirements

Final evaluation

Graded credit

Assessment methods

written reports for case studies including program codes, final assignment completion in the form of written report and/or oral presentation

The basic criteria for evaluation

according to "Rules and regulations for studies at the University of Gdansk"

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
Introduction to Python programming

B. Prerequisites
basis of calculus and linear algebra, ability to use the LINUX operating system

Aims of education

Familiarizing the students with the numerical algorithms applied in chemistry. Preparing the students to write own numerical applications, including using existing numerical libraries in the process.

Course contents

Algorithm and its correctness. Errors in numerical calculations; Wilkinson's 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.

Bibliography of literature

Bibliography of literature

Literature required to pass the course

Siegmund Brandt, Data Analysis - Statistical and Computational Methods for Scientists and Engineers, Springer 2014

Extracurricular readings

Qingkai Kong, Timmy Siauw, Alexandre Bayen, Python Programming and Numerical Methods
A Guide for Engineers and Scientists, Academic Press 2020

The learning outcomes (for the field of study and specialization)

K_W01: uses in-depth knowledge of spectroscopic methods of chemical compound analysis

K_W05: has extended knowledge in the field of the specialisation studied

K_W06: applies mathematics to the extent necessary to understand, describe and model chemical processes of extended complexity

K_U02: critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors

K_K01: knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so

K_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

Knowledge

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

Skills

The student defines and solves the problems connected with the specific features of floating-point arithmetic, which arise when using the available quantum chemistry, molecular mechanics and dynamics, chemometry, etc., packages. Solves the computational problems that arise in chemistry and related subjects while using the software libraries available in the computer centres or from the web. Designs, for this purpose, simple numerical applications that use own or library procedures.

Social competence

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. Develops the ability of working in a team

Contact

adam.sieradzan@ug.edu.pl