GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MATHEMATICAL METHODS IN CHEMISTRY, PG_00038882					
Field of study	Chemistry					
Date of commencement of studies	February 2023		Academic year of realisation of subject		2022/2023	
Education level	second-cycle studies		Subject group		Obligatory subject group in the field of study	
Mode of study	Full-time studies		Mode of delivery		at the university	
Year of study	1		Language of instruction		Polish	
Semester of study	1		ECTS credits		2.0	
Learning profile	general academic profile		Assessment form		exam	
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry					
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. inż. Jacek Czub			
	Teachers					
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	15.0	0.0	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	The aim of the course is to provide students with general knowledge and skills in advanced mathematical methods used in chemistry and related fields, with a special emphasis on linear algebra, vector analysis, Fourier series and transform, probability theory and numerical methods.					

Learning outcomes

Course outcome	Subject outcome	Method of verification
K7_W01	The student acquires in-depth knowledge of mathematical methods and tools for the study of quantum and theoretical chemistry, spectroscopy, crystallography, statistical thermodynamics, molecular biophysics and related fields on a quantitative level. The student learns the terminology and mathematical formalism used in linear algebra, vector analysis, Fourier analysis, theory of stochastic processes and numerical methods. The student learns to use the theoretical knowledge gained during the lecture to solve mathematically advanced problems of chemical importance by writing computer programs.	[SW1] Assessment of factual knowledge
K7_K01	The student understands the need for lifelong learning, and is able to inspire and organize the learning process of other people.	[SK5] Assessment of ability to solve problems that arise in practice
K7_U01	The student learns to confront the results of theoretical predictions with regard to the properties of chemical molecules with the literature and experimental data.	[SU1] Assessment of task fulfilment
K7_W02	The student learns the mathematical formalism of theoretical chemistry methods used to predict the properties of molecules, including the relationship between structure and reactivity.	[SW1] Assessment of factual knowledge

Subject contents

Lecture:

1. Linear algebra (operations on vectors and matrices, inner product axioms, systems of linear equations, multiple linear regression, four fundamental subspaces, orthogonal bases, orthogonal (unitary) matrices, eigenvalue problem, diagonalization, properties of symmetric (hermitian) matrices, similarity transformation, spectral decomposition of a matrix, positive-definite matrices, singular value decomposition, introduction to LCAO-MO method, Hueckel method, normal mode analysis, principal component analysis)
2. Vector analysis (parametric curves and surfaces, vectors tangent and normal to curves and surfaces, arc length, total differential and total derivative, chain rule, gradient and gradient operator, Lagrange multipliers, directional derivative, scalar and vector fields, integration -- change of variables, Jacobian, line and surface integrals, properties of a gradient field, curl of a vector field, flux of a vector field, Stokes theorem, Green theorems, divergence of a vector field, continuity equation, Gauss theorem, laplacian, diffusion equation, Poisson equation, Laplace equation, Poisson-Boltzmann equation, vector identities)
3. Fourier analysis (brief introduction to Sturm-Liouville theory, representing functions in orthogonal function bases, orthogonal polynomials, Fourier series and its convergence, Fourier basis, complex form of Fourier series, Fourier series of odd, even and piecewise continous functions, Parseval's identity, differentiating and integrating of Fourier series, Fourier transform, inverse Fourier transform, Dirac delta-function, application of Fourier transform in spectroscopy and crystallography, discrete Fourier transform, fast Fourier transform, convolution theorem and its applications, Nyquist-Shannon sampling theorem)
4. Stochastic processes theory (probability density, cumulative distribution function, stochastic processes and their properties, stationary stochastic processes, autocorrelation, white noise, Monte Carlo methods, Langevin equation and Brownian dynamics, introduction to Markov processes, Markov matrices and their spectral decomposition, Markov state models in chemical kinetics and in biology, Fokker-Planck and Smoluchowski equations)

Practicals:

1. Introduction to Octave programming (variables, control structures, routines, matrix and vector representation, operations on matrices and vectors)
2. Numerical approach to solving ordinary differential equations and to Markov modeling of (bio)chemical processes , simple models describing the kinetics of bistable reactions, dimerization thermodynamics, cooperativity at the molecular level.
3. Eigenvalue problem: principal component analysis & Hueckel method, quantum-chemical basis of aromaticity, effect of heteroatom on energy levels, fundamentals of electronic excitations
4. Eigenvalue problem: normal mode analysis in the context of IR spectroscopy, numerical prediction of IR spectra
5. Basics of vector analysis: numerical approach to optimization, minimization of multivariable function, optimization of the structure of atomic clusters
6. Selected topics in Fourier analysis: application of the fast Fourier transform to analysis of time series, in particular, discrete Fourier transform of free induction decay data from an NMR spectrometer; Fourier transform of images

Prerequisites and co-requisites	Basic background in calculus and linear algebra.
Assessment methods and criteria	<table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>Practicals</td><td>50.0%</td><td>70.0%</td></tr><tr><td>Lecture</td><td>50.0%</td><td>30.0%</td></tr></table>
Recommended reading	<table><tr><td>Basic literature</td><td>1. Donald A. McQuarrie "Mathematical Methods for Scientists and Engineers" 2. Erich Steiner "The Chemistry Maths Book" 3. Henry Margenau "The Mathematics of Physics and Chemistry" 4. Zbigniew Skoczylas, "Elementy analizy wektorowej: teoria, przykłady, zadania" (in polish only)</td></tr><tr><td>Supplementary literature</td><td>1. Gilbert Strang "LInear Algebra and Its Applications", 4th ed. 2. George B. Arfken, Hans J. Weber "Mathematics for Physicists", 7th ed.</td></tr><tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:</td></tr></table>
Example issues/ example questions/ tasks being completed	Examples of problems to be solved in the MATLAB/Octave environment: 1. *Create a routine z(v) that will take a vector of arguments, v = [x y], and return the value of an arbitrary function z = f(x,y), e.g.* $z = x^2 + 4y^2$*. Based on this routine, create another routine grad(v) that will take the vector of coordinates v = [x y] and return the normalized gradient, grad(v) = [gx gy]. Then, write a program which will do the followng: (1) read the starting point P, (2) calculate the gradient at point P, (3) move point P by a given step along the direction of negative gradient, (4) compute the resulting change in value of z = f(x,y), (5) repeat steps 2-4 until the value of the function ceases to decrease.* 2. *Use the toeplitz() function to create a tridiagonal matrix describing a hexatriene molecule according to the Hückel theory. Calculate the electronic energy of the conjugated π-system. Repeat the procedure with the matrix modified to represent benzene instead of hexatriene. Compare and comment on the results.*
Work placement	Not applicable