

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 2026 | Academic year of realisation of subject | | | 2027/2028 | | |
| 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 | | | English | | |
| 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 processes. | | | | | | |

| Learning outcomes | Course outcome | Subject outcome | Method of verification |
|-------------------|---|--|--|
| | [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 |
| | [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_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_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_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_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 |

| Subject contents | <p>Algorithm and its correctness. Errors in numerical calculations; Wilkinsons lemmas. Condition number of a problem. Overflow (INF), underflow, NaN.</p> <p>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 Newton-Gauss, Newton, 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 differential 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.</p> | | | | | | | | |
|--|---|--|-------------------|-------------------------------|--------------------------|-------|--------|--|--|
| 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 | <table border="1"> <thead> <tr> <th data-bbox="456 797 790 824">Subject passing criteria</th> <th data-bbox="802 797 1136 824">Passing threshold</th> <th data-bbox="1141 797 1474 824">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="456 831 790 857">task performance reports</td> <td data-bbox="802 831 1136 857">51.0%</td> <td data-bbox="1141 831 1474 857">100.0%</td> </tr> </tbody> </table> | Subject passing criteria | Passing threshold | Percentage of the final grade | task performance reports | 51.0% | 100.0% | | |
| Subject passing criteria | Passing threshold | Percentage of the final grade | | | | | | | |
| task performance reports | 51.0% | 100.0% | | | | | | | |
| Recommended reading | Basic literature | Siegmond 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 | | | | | | | | |

Document generated electronically. Does not require a seal or signature.