University of Gdańsk

Subject card

Subject name and code	Introduction to Computational Mathematics in Quantum Mechanics, PG_00208796						
Field of study	Mathematics						
Date of commencement of studies	October 2025		Academic year of realisation of subject		2026/2027		
Education level	Master’s studies		Subject group		Obligatory subject group in the field of study Optional subject group		
Mode of study	full-time studies		Mode of delivery		at the university		
Year of study	2		Language of instruction		English Lectures are delivered in English by a Polish-speaking instructor, laboratory sessions are delivered also in English, but by a German-speaking instructor.		
Semester of study	4		ECTS credits		6.0		
Learning profile	academic		Assessment form		exam		
Conducting unit							
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Karolina Kropielnicka				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	30.0	0.0	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		10.0	80.0		150
Subject objectives	The aim of the course is to introduce students to the mathematical and computational methods used to simulate quantum mechanical systems. Students will learn how to model physical phenomena governed by the Schrödinger equation, implement numerical algorithms in Python, and visualise quantum dynamics. The course bridges classical and quantum descriptions of physical systems, combining rigorous mathematical theory with hands-on computation.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[MATMU2_W01] knows and understands in-depth the theory of selected areas of mathematics	Student knows and understands the theory of selected mathematical areas: functional analysis, Fourier analysis, and numerical methods for PDEs.	[SW4] test/exam - oral or written
	[MATMU2_U07] is able to define his/her interests and develop them; in particular, is able to establish contact with specialists in his/her field, e.g. understand their lectures intended for young mathematicians	Student communicates their interests in computational mathematics and quantum mechanics, and is able to discuss them with specialists.	[SU4] test/exam - oral or written
	[MATMU2_U03] can understand mathematical texts of various types from selected fields of mathematics	Student reads and understands mathematical texts of varying character related to quantum mechanics and numerical analysis.	[SU4] test/exam - oral or written
	[MATMU2_K04] is ready to understand and appreciate the importance of intellectual honesty in one's own and other people's actions; ethical conduct	Student appreciates the intellectual value of mathematical rigour in the construction of reliable numerical algorithms.	[SK4] test/exam - oral or written
	[MATMU2_K05] is ready to independently search for information in literature, also in foreign languages	Student independently searches for information in scientific literature, including English-language sources.	[SK4] test/exam - oral or written
	[MATMU2_U05] can perform proofs in a selected field and, if necessary, also use tools from other areas of mathematics	Student carries out proofs and derives numerical schemes in the field of quantum mechanics, using tools from other areas of mathematics as needed.	[SU4] test/exam - oral or written
	[MATMU2_W03] knows and understands in-depth a selected field of theoretical or applied mathematics and is able to understand the formulations of issues in this field that are still at the research stage and knows the connections of issues in this field with other areas of mathematics	Student knows and understands an area of applied mathematics (numerical quantum dynamics) in depth, and recognises connections with other fields.	[SW4] test/exam - oral or written
	[MATMU2_U06] is able to apply methods and examples from a selected field of mathematics in related fields	Student applies methods from computational mathematics to problems in quantum mechanics and related fields.	[SU4] test/exam - oral or written
	[MATMU2_K06] is ready to formulate opinions on basic mathematical issues	Student is prepared to form opinions on fundamental questions of computational mathematics and its role in the physical sciences.	[SK4] test/exam - oral or written
	[MATMU2_K01] is willing to acknowledge the limitations of his or her own knowledge and is willing to pursue further education	Student recognises the boundaries of their knowledge of quantum mechanics and numerical methods, and identifies areas requiring further study.	[SK4] test/exam - oral or written
	[MATMU2_U01] can construct mathematical reasoning: prove theorems and refute hypotheses through construction and selection of counterexamples	Student constructs mathematical reasoning: derives properties of solutions to the Schrödinger equation and provides counterexamples where appropriate.	[SU4] test/exam - oral or written
	[MATMU2_K02] is ready to precisely formulate questions to deepen his/her understanding of a given topic or find missing elements of reasoning	Student formulates precise questions about quantum mechanical models and numerical algorithms to identify gaps in their understanding.	[SK4] test/exam - oral or written
	[MATMU2_W02] knows and understands well the role and importance of the construction of mathematical reasoning	Student knows and understands the role of mathematical reasoning underlying splitting methods, Galerkin methods, and spectral discretisation.	[SW4] test/exam - oral or written
	[MATMU2_U04] is able, at an advanced level and including modern mathematics, to apply and present, orally and in writing, methods of at least one selected branch of mathematics	Student applies contemporary mathematics — Fourier transforms, operator theory, numerical integration — at an advanced level, both orally and in writing.	[SU4] test/exam - oral or written

Subject contents	COURSE CONTENT **1.** Introduction to classical mechanics and Hamiltonian systems. **2.** Principles of quantum mechanics: wave functions, probability interpretation, observables, harmonic oscillator. **3.** The free linear Schrödinger equation; Fourier transform techniques. **4.** Time-dependent Schrödinger equation with potentials; conservation laws (mass, energy). **5.** Splitting and composition methods for time integration; numerical stability; structure-preserving algorithms. **6.** Gaussian wave packets as mesh-free approximation methods. **7.** Spatial discretisation: Galerkin methods, collocation methods, Chebyshev method. **8.** Implementation of numerical algorithms in Python; visualisation of quantum phenomena.
Prerequisites and co-requisites	Basic knowledge of calculus, linear algebra, and ordinary differential equations.
Assessment methods and criteria	Subject passing criteria: written exam; Passing threshold: 51.0%; Percentage of the final grade: 100.0%
Recommended reading	Basic literature: 1. C. Lubich, *From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis*, European Mathematical Society, 2008. 2. B. C. Hall, *Quantum Theory for Mathematicians*, Springer, 2013. Supplementary literature: 1. W. Scherer, *Mathematics of Quantum Computing: An Introduction*, Springer, 2019. eResources addresses:
Example issues/ example questions/ tasks being completed	**1. PL:** Wyprowadź prawo zachowania masy dla liniowego równania Schrödingera. **EN:** Derive the conservation of mass for the linear Schrödinger equation. **2.** Implement a Strang splitting scheme for the time-dependent Schrödinger equation in Python. **3.** Apply the Chebyshev spectral method for spatial discretisation of the Schrödinger equation. **4.** Simulate and visualise the dynamics of a Gaussian wave packet in a harmonic potential. **5.** Analyse the numerical stability of a given time integration scheme.
Work placement	Not applicable

Subject passing criteria	Passing threshold	Percentage of the final grade
written exam	51.0%	100.0%

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