University of Gdańsk

Subject card

Subject name and code	Introduction to Computational Mathematics in Quantum Mechanics, PG_00209693						
Field of study	Mathematics						
Date of commencement of studies	October 2026		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	1		Language of instruction		English		
Semester of study	2		ECTS credits		5.0		
Learning profile	academic		Assessment form		credit		
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		3.0	62.0		125
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 or related fields, the complex relationships between them and their development trends	Student knows and understands in depth the theory of Fourier analysis, operator theory, and numerical methods for partial differential equations, recognises the connections between these areas, and understands their development in the context of computational mathematics and quantum mechanics.	[SW4] test/exam - oral or written
[MATMU2_U05] is able to apply new or adapt existing methods and tools from a selected field of mathematics and information and communication technologies in related fields	Student applies numerical methods (splitting methods, spectral methods, Galerkin methods) and programming tools (Python) to simulate quantum systems and solve problems in related areas of mathematics and physics.	[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	see table below

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