FAKULTETY kierunek MODELOWANIE MATEMATYCZNE I ANALIZA DANYCH st. II

INTRODUCTION TO COMPUTATIONAL MATHEMATICS IN QUANTUM MECHANICS
Educational Objectives (Cele kształcenia)
The course combines mathematical theory and hands-on computation. During the practical sessions students will implement numerical algorithms in Python and visualise quantum phenomena. After completing the course students will understand how computational mathematics can be used to explore quantum mechanics, how numerical algorithms for partial differential equations are constructed, and how simulations can reveal the behaviour of mathematical models arising in physics.
Requirements (Wymagania)
Basic knowledge of calculus, linear algebra and ordinary differential equations. Elementary familiarity with Python programming is recommended. The course Computational Mathematics of Evolutionary Equations is not required but recommended, as it provides useful background on basic numerical methods and computational techniques.
Program content **(Treści programowe)**
Quantum mechanics describes some of the most fascinating phenomena in nature: particles behaving like waves, quantum tunnelling, and the dynamics of microscopic systems. These phenomena are governed by the Schrödinger equation, a fundamental equation whose solutions typically cannot be written explicitly. In this course we will learn how mathematics and computation allow us to simulate and visualise quantum systems. We gradually move from physical intuition to mathematical models and computational algorithms, focusing on one central equation: the linear Schrödinger equation (SE). We begin with a short introduction to classical mechanics and Hamiltonian systems, which provide the conceptual bridge between classical and quantum descriptions of physical systems. Next, we introduce the basic principles of quantum mechanics, including wave functions, the probability interpretation, operators representing physical observables, and simple systems such as the harmonic oscillator. The emphasis will be on understanding how physical quantities are represented mathematically. The core of the course focuses on the SE. We first study the free SE, using Fourier transform techniques to understand the structure of its solutions. We then consider the time-dependent SE with potentials, discuss time-dependent and conservative systems, and explore fundamental conservation laws such as mass and energy conservation. In the computational part of the course we introduce numerical methods used to simulate quantum dynamics. Students will learn splitting and composition methods for time integration and explore issues of numerical stability and structure-preserving

algorithms. Gaussian wave packets will provide an example of mesh-free approximation methods. For spatial discretisation we introduce several powerful approximation techniques, including Galerkin methods, collocation methods, and the Chebyshev method.
List of literature (Wykaz literatury)
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.