PHY-MV-BE-T04 – Computational physics with focus on time-dependent quantum mechanics

Lecture held winter term 2022/23 by Prof. Dr. Daria Gorelova, Universität Hamburg

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Contents

1 Explicit forward Euler method

Lecture 1–24.10.2022

Consider a first-order differential equation with boundary condition,

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = f(y(t), t) \text{ with } y(t_0) = y_0\,. \tag{1.1}$$

As f is a known function, we know the derivative at t_0:

$$\left.\frac{\mathrm{d}y(t)}{\mathrm{d}t}\right|_{t=t_0} = f(y(t_0), t_0) = f(y_0, t_0) \tag{1.2}$$

This is enough information to write down the tangent line of the solution at $t = t_0$:

$$y_{\text{tangent}}(t) = y_0 + f(y_0, t_0)(t - t_0) \tag{1.3}$$

We can now take some $t_1 > t_0$. Given t_1 is close enough to t_0,

Put some graphic here

2 Runge-Kutta and related methods

Lecture
2–07.11.2022

3 Crank-Nicholson Method

Lecture 3 – 14.11.2022

4 Numerov method

Lecture 4 – 21.11.2022

4.1 General Numerov method

Within the Numerov method, differential equations of the following type are treated:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = U(x) + V(x)y(x) \tag{4.1}$$

Exercise 4 – 21.11.2022

4.2 Anharmonic oscillator and shooting

In the exercise, the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{4.2}$$

with the potential

5 Fast-Fourier-Transform and Split Operator

Lecture 5 – 28.11.2022

6 Time-dependent Perturbation Theory and Numerical Integration

Lecture 6 – 05.12.2022

7 Monte-Carlo Methods and Ising Model

Lecture 7 –
12.12.2022

8 Lanczos Algorithm

Lecture 8 –
19.12.2022

9 Machine Learning

Lecture
9–16.01.2023