

Worksheet 9

Problems

Partial Differential Equations

(H) Exercise 1: Von Neumann Stability Analysis

Consider the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, 1)$$

together with boundary conditions $u(t, 0) = u(t, 1) = 0$. We apply two different discretization schemes using explicit and implicit Euler time-stepping and the standard second-order approximation of the spatial derivative:

Explicit:

$$\frac{u_j^{(m+1)} - u_j^{(m)}}{\tau} = \frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{h^2} \quad (1)$$

Implicit:

$$\frac{u_j^{(m+1)} - u_j^{(m)}}{\tau} = \frac{u_{j-1}^{(m+1)} - 2u_j^{(m+1)} + u_{j+1}^{(m+1)}}{h^2} \quad (2)$$

where h and τ denote mesh-size and time step and $u_j^{(m)} := u(m\tau, jh)$.

According to the von Neumann stability analysis, we assume the error in the solution to be of the type

$$u_j^{(m)} = (a_k)^m \sin(\pi k(jh)).$$

- Derive an explicit formula for the coefficient a_k in case of the explicit time-stepping, see equation 1. You may use the equality $\sin(A + B) + \sin(A - B) = 2 \sin(A) \cos(B)$.
- Typically, the error is not given by a single frequency, but by a superposition of several frequencies k ,

$$u_j^{(m)} = \sum_k c_k (a_k)^m \sin(\pi k(jh)).$$

Why is it enough to only consider single frequencies? What is the maximum frequency that we need to consider?

- (c) The error in the solution decays if it holds $|a_k| < 1$ for all coefficients a_k . Which condition do we have to satisfy for the explicit time-stepping scheme in order to achieve this?
- (d) Carry out the analysis from (c) for the implicit time-stepping scheme. Which condition arises in this case?

(H) Exercise 2: Wave Equation

Consider the wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$$

on the interval $x \in (0, 1)$ with initial conditions

$$u(t = 0, x) = e^{-100(x-0.4)^2}, \quad \frac{\partial u(t = 0, x)}{\partial t} = 0$$

and boundary conditions

$$u(t, x = 0) = u(t, x = 1) = 0.$$

Write a python script to solve this problem using finite differences on an equidistant grid with $N + 1$ grid points. The mesh-size is denoted by $h := 1/N$ and the time step by τ .

- (a) Discretize the temporal and spatial derivatives and formulate an update rule

$$u((m + 1)\tau, ih) = f(u(m\tau, ih), u(m\tau, (i + 1)h), u(m\tau, (i - 1)h), u((m - 1)\tau, ih))$$

where $i \in \{1, \dots, N - 1\}$, $m \in \mathbb{N}$.

- (b) How can we include the initial condition?
- (c) A formula that incorporates this particular initial condition and also preserves the accuracy of the scheme is given by

$$u(\tau, ih) := u(0, ih) + \frac{\tau^2}{2h^2}(u(0, (i - 1)h) - 2u(0, ih) + u(0, (i + 1)h))$$

and setting $u(t = 0, ih)$ as described above. Implement both your and this approach for the initial conditions in a python script and solve the problem for $\tau \in \{0.01, 0.02\}$, $N = 90$. Plot the solution in every time step and compare the results according to your initial condition. You may consider the time interval $t \in [0, 1]$. What do you observe?

- (d) Find the time step restriction from the von Neumann stability analysis.

(I) Exercise 3: Bacteria Transport Equation

One-dimensional transport of some bacteria concentration $c(t, x)$ in some media can be described by the equation

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial x} (vc) - \lambda c, \quad (3)$$

where $D > 0$ denotes the diffusivity of the bacteria, v the flow velocity in x direction, and λ the death rate of the bacteria.

Assume that we want to solve the problem numerically for periodic boundary conditions and all parameters D, v, λ are constant.

- (a) Formulate a finite difference scheme for equation (3) using first-order finite differences of the form

$$\frac{\partial f(x)}{\partial x} = \frac{f(x+h) - f(x)}{h}, \quad (4)$$

for the first-order derivative and the central difference scheme for the second-order derivatives. Use an equidistant grid with mesh size h in the x direction. State the order of the local discretization errors for both finite difference schemes.

Apply the explicit Euler scheme for the time derivative with time step size τ .

- (b) From the von Neumann stability analysis, find the magnitude of the error a_k . Take the error in the solution of type $\epsilon_j^{(m)} = a_k^m e^{i\pi k j h}$. What condition does the error magnitude a_k have to satisfy such that the numerical scheme from the previous tasks is stable?

(H*) Exercise 4: Free Charges in Semiconductors

There are semiconductors that do not conduct electric current unless they are exposed to light. Free electrons appear in this material due to the photo-effect. They can again get trapped and localized.

- (a) A thin layer of semiconductor has momentarily been exposed to light. This created a homogeneous density n_0 of free electrons. Write down the ODE for the free electrons density $n(t)$ and solve it if free electrons get trapped again at a rate $\alpha n(t)$ (number of free electrons trapped in a unit volume per unit time interval). What is $n(t \rightarrow \infty)$?
- (b) To improve the model, potential holes are introduced. In our model, potential holes will only keep one electron at the same time. If M is the number of potential holes, $m(t) = n_0 - n(t)$ is the number of localized electrons, then $\alpha(1 - m(t)/M)n(t)$ is number of trapped electrons in the potential holes per unit time interval. And the number of electrons that get free again per unit time interval is $\beta m(t)$. The resulting ODE is

$$\frac{dn(t)}{dt} = \beta(n_0 - n(t)) - \alpha \left(1 - \frac{n_0 - n(t)}{M}\right) n(t). \quad (5)$$

For $n_0 = 1, M = 1, \alpha = 2, \beta = 1$ find a physical ($n \geq 0$) stationary solution for the free electron concentration n_s of this equation.

- (c) Determine whether the physical ($n \geq 0$) stationary solution from (b) is stable.
- (d) If the semiconductor layer is thick, the generated density of free electrons n is no longer homogeneous. More electrons are freed near the surface and less inside the layer. The simplest model for the evolution of $n(x, t)$ considers diffusion along the layer depth x and is described by the following equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} - \gamma n, \quad (6)$$

where the coefficients D and γ are positive.

Provide a numerical scheme for this PDE. For the time discretization use the explicit Euler scheme and for the spatial discretization a central difference second-order scheme. For an example of a discretization grid see Figure 1.

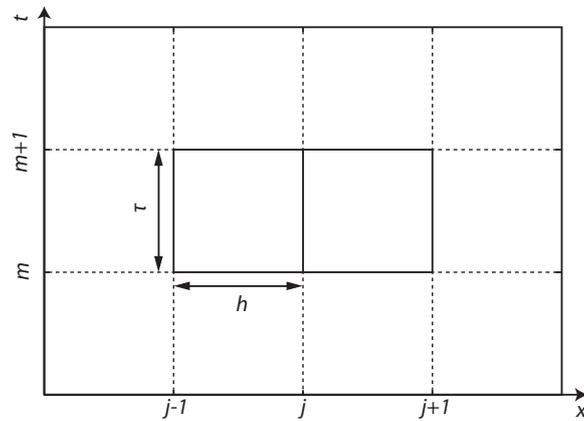


Figure 1: Discretization grid example.

- (e) Find the restriction for the time step size of the numerical scheme by using the von Neumann stability analysis.