Technische Universität München
Lehrstuhl für Informatik V
Univ.-Prof. Dr. M. Bader
M.Sc. S. Seckler, M.Sc. D. Jarema, M.Sc. A. Bakhtiari

WS 2016/17
Scientific Computing
16.01.2017/18.01.2017

Worksheet 10
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:

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

Implicit:

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

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

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

(a) Derive an explicit formula for the coefficient a_k in case of the explicit time-stepping, see equation 1. You may use the equality $\sin(A+B) + \sin(A-B) = 2\sin(A)\cos(B)$.

(b) Typically, the error is not given by a single frequency, but by a superposition of several frequencies k,

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

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

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

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

(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

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

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

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

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 $\epsilon_j^{(m)} = a_k^m e^{\imath\pi kjh}$. 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 $wn(t)$ (number of free electrons trapped in a unit volume per unit time interval). What is $n(t \to \infty)$?

(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

$$\frac{\mathrm{d}n(t)}{\mathrm{d}t} = \beta(n_0 - n(t)) - \alpha\left(1 - \frac{n_0 - n(t)}{M}\right)n(t). \tag{5}$$

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

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

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.

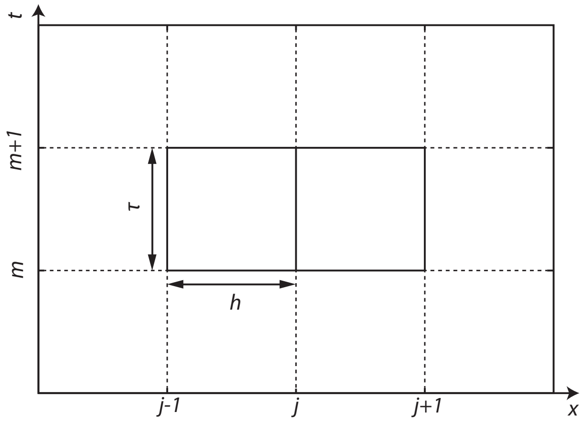

Figure 1: Discretization grid example.

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