Finite Difference Methods
Assignments

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Assignment 1: A one-dimensional heat equation

Subtask 1

a) Use the forward Euler scheme to solve the one-dimensional heat problem

$$\begin{cases} u_t &= \lambda u_{xx} \qquad 0 < x < 1, \quad t > 0 \\ u(x,0) &= f(x) \\ u(0,t) &= u(1,t) = 0 \end{cases} \tag{1}$$

where

$$f(x) = \sin \pi x + 0.3 \sin 2\pi x - 0.1 \sin 3\pi x$$

$$\lambda = 0.1, \quad h = 0.1, \quad k = 0.05$$

Compute and plot the values u_j^n for $n = 0, 10, 20, 30, 40, 50$.

b) The same problem as in a) but with $k = 0.1$. Make comments on the results.

c) Solve the same problem as in a) but with $\lambda = 0.05$. Choose k as large as possible but keep $\lambda k/h^2 \leq 1/2$. Plot the results and compare them with a). How does reduction in the value of the parameter λ affect the results? Make experiments with different values of λ.

d) Solve the same problem as in a) with the backward Euler method. This gives a system of equations with $N-1$ unknowns at every time step. The resulting system is a tridiagonal system and can be solved with MATLAB routines. Begin by considering the coefficient matrix. Verify by experiments the unconditional stability of the scheme.

e) Solve the same problem as in d) but with the Crank–Nicolson method.

Subtask 2

Our simple model problem (1) can be generalized in different ways.

a) Change the *boundary values* to

$$u(0,t) = g_1(t) \quad \text{and} \quad u(1,t) = g_2(t)$$

where g_1 and g_2 are chosen in a proper way and compute the solution with the forward Euler scheme.

b) Let λ be a function of x and/ or t. Try with $\lambda = e^x, \quad \lambda = e^t, \quad \lambda = e^{-x+t}$ and others values in combination with backward Euler. Are there any computational complications in comparison with the case when λ constant?

c) Let $\lambda = 2/(2+u^2(x,t))$ i.e. let λ depend on the temperature u and compute the solution with the forward Euler method.

d) Try with $\lambda = -1$. What happens?

e) Try with $u_t = \lambda u_{xx} + au_x + bu + f$ and replace u_x with $(u^n_{j+1} - u^n_{j-1})/2h$ in forward Euler and similarly for backward Euler and Crank–Nicolson.

Assignment 2: A two-dimensional heat equation

Now we have the equation $u_t = \lambda_1 u_{xx} + \lambda_2 u_{yy}$ in the region $0 < x, y < 1,\ t > 0$. The constants λ_1 and λ_2 are both positive.

Suppose we have the initial temperature

$$u(x, y, 0) = f(x, y), \qquad \text{e.g.} \quad = \sin \pi x \sin \pi y$$

and that $u(x, y, t) = 0$ on the boundary.

a) Define forward Euler, implement it and compute the solution for some combination of $h_x, h_y,$ and k. Try to find a stability condition for $\lambda_1 = \lambda_2$.

b) Implement the backward Euler method. How many unknowns do we get on each time level?

c) Try the ADI-method (ADI=Alternating Direction Implicit) given by

$$\frac{u^{n+1/2}_{ij} - u^n_{ij}}{k/2} = \lambda_1 \frac{u^{n+1/2}_{i+1,j} - 2u^{n+1/2}_{ij} + u^{n+1/2}_{i-1,j}}{h_x^2} + \lambda_2 \frac{u^n_{i,j+1} - 2u^n_{ij} + u^n_{i,j-1}}{h_y^2}$$
$$\frac{u^{n+1}_{ij} - u^{n+1/2}_{ij}}{k/2} = \lambda_1 \frac{u^{n+1/2}_{i+1,j} - 2u^{n+1/2}_{ij} + u^{n+1/2}_{i-1,j}}{h_x^2} + \lambda_2 \frac{u^{n+1}_{i,j+1} - 2u^{n+1}_{ij} + u^{n+1}_{i,j-1}}{h_y^2}$$

Here we have used an extra time level with time index $n + 1/2$. Instead of solving one very large linear system we solve a number of smaller systems.

Assignment 3: A hyperbolic problem

Subtask 1

We study the PDE-problem

$$\begin{cases} u_t = u_x & 0 < x < 1,\ 0 < t \\ u(x,0) = f(x) = \sin 2\pi x \\ u(x,t) = u(x+1,t) \end{cases}$$

which has the solution $u(x,t) = f(x+t)$

a) Use the "leap-frog scheme"

$$\frac{u_j^{n+1} - u_j^{n-1}}{2k} = \frac{u_{j+1}^n - u_{j-1}^n}{2h}$$

and try the following combinations of h and k

1) $h = 0.1, \quad k = 0.049$
2) $h = 0.1, \quad k = 0.098$
3) $h = 0.05, \quad k = 0.0245$
4) $h = 0.05, \quad k = 0.049$
5) $h = 0.1, \quad k = 0.1$

Use the exact solution for $t = k$. Compare the computed solution with the correct solution. Try to find how the quality depends on the value of $\lambda = k/h$.

In cases of instability, on which time level is it first observed? For which x? Make observations of the propagation of perturbations.

Subtask 2

a) We change the boundary condition to $u(1,t) = 0$. The PDE-problem is still well posed and has the solution

$$u(x,t) = \begin{cases} f(x+t) & \text{for } x+t \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$

But the leap-frog scheme needs a boundary condition also on the left. Choose simple extrapolation $u_0^{n+1} = 2u_1^n - u_2^{n-1}$. Which effects does this "numerical boundary condition" have?

b) To reduce the perturbations we change the difference scheme to

$$u_j^{n+1} = u_j^{n-1} + 2k\frac{u_{j+1}^n - u_{j-1}^n}{2h} - \delta(u_{j+2}^{n-1} - 4u_{j+1}^{n-1} + 6u_j^{n-1} - 4u_{j-1}^{n-1} + u_{j-2}^{n-1})$$

This is "leap-frog with a dissipative term" and it can be applied in $x_2,\ x_3, \dots,$ x_{N-2}. In x_1 and x_{N-1} the simple leap-frog scheme is used. Use $h = 0.05$ and $k = 0.04$ and choose different values of δ between 0 and 0.2 and try to find an optimal value of δ.

Assignment 4: A gas flow problem

One dimensional gas flow can be described by the hyperbolic system

$$\begin{pmatrix} \rho \\ m \\ e \end{pmatrix}_t + \begin{pmatrix} m \\ \rho u^2 + p \\ (e+p)u \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{2}$$

Here ρ is the density of the gas, m the momentum, and e the total energy. The velocity is $u = m/\rho$. Under the assumption that we have an ideal gas, the pressure is given by

$$p = 0.4(e - \frac{1}{2}m^2/\rho).$$

The system can be written in the form $U_t + F(U)_x = 0$, where the vectors U and $F(U)$ can be identified in (2).

The initial state is

$$U(0,x) = \begin{pmatrix} 0.445 \\ 0.311 \\ 8.928 \end{pmatrix} \quad \text{for } x < 0 \quad \text{and} \quad U(0,x) = \begin{pmatrix} 0.5 \\ 0 \\ 1.4275 \end{pmatrix} \quad \text{for } x > 0$$

Subtask 1

Implement and solve the problem in the interval $-2 < x < 2$ up to $t = 0.6$. Use the "leap-frog with a dissipative term" and approximately 400 grid points in space. Try different values of δ to find a solution with as few oscillations as possible. To obtain stability Δt should be chosen such that $\Delta t \leq 0.2\Delta x$.

In Figure 1 the solution, at a time $t > 0$ (not $t = 0.6$), is shown. Note that such a good resolution cannot be obtained with the methods used in this assignment.

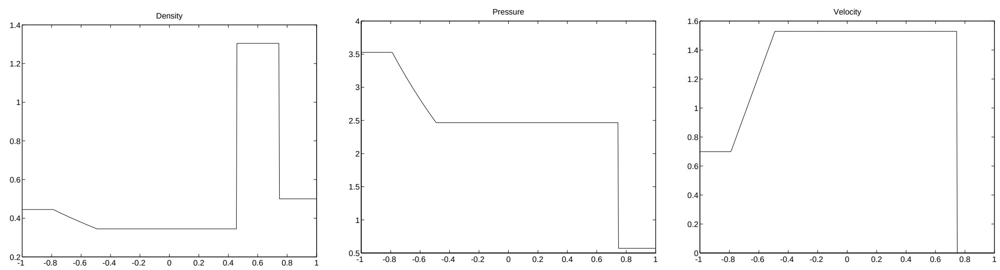

Figure 1: The solution of the gas flow example (2)

Subtask 2

Explain how the upper limit of Δt is found. The limit has something to do with the spectral radius of the Jacobian, $\partial F/\partial U$, which is around 4.7.

Assignment 5: An elliptic problem

Subtask 1

A simple elliptic PDE-problem is

$$\begin{cases} u_{xx} + u_{yy} = f(x,y) & 0 < x, y < 1 \\ u(x,y) = g(x,y) & \text{on the boundary} \end{cases}$$

This is the Dirichlet problem for Poisson's equation. The step lengths are $\Delta x = \Delta y = 1/N$ and the most natural difference approximation is the five-point formula

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = f(x_i, y_j)$$

When this is applied we get a linear system which is sparse, i.e. most of the elements of the coefficient matrix are zeros.

a) First, find the linear system for $N = 4$ and then do the same for a general value of N.

   How is the coefficient matrix changed if $\Delta x \neq \Delta y$?

b) Compute the solution and plot it for $N = 10, 20, 30$. Make own choices of $f(x, y)$ and $g(x, y)$.

Assignment 6: Air Quality Modeling and the Advection Diffusion Equation I

Introduction

An important area in modern Environmental Engineering is the study of various air pollutants. The concentrations of these pollutants are described by *air quality models* which are often formulated as partial differential equations. With the use of models the hope is to predict how peak concentrations will change in response to predefined changes in the source of pollution.

Consider now the concentration $u(x, y, z, t)$ of a gaseous compound. If we have knowledge of the concentration at time $t = 0$, we would like to be able to predict future concentrations. Let, for instance, u be the concentration of a noxious gas formed at an industrial plant. At $t = 0$ a concentrated cloud of the pollutant is released into the air surrounding the plant. Of great importance is the knowledge of how concentrated the gas will be when it reaches the nearby residential areas.

To model the air quality (i.e. the concentration of u) we use the continuity equation,

$$\frac{\partial u}{\partial t} = -\nabla \cdot \overline{J} \tag{3}$$

where ∇ is the nabla operator, $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$. Equation (3) states that the time development of u is related to the flux $\overline{J}$ (amount per area and time) of the gas. The total flux is made up of two terms. First we have the dispersive effect of *diffusion*, given by Fick's first law, $\overline{J}_{\text{diffusion}} = -D \cdot \nabla u$, where D denotes the diffusion constant. In addition to diffusion the gas is transported by the wind through a process called *advection*. This leads to a flux, $\overline{J}_{\text{advection}} = \overline{v} \cdot u$, where $\overline{v}$

is the wind vector. If we now combine the expressions for the flux with equation (3) we get *the advection diffusion equation*,

$$\frac{\partial u}{\partial t} = D \cdot \Delta u - \nabla \cdot (\overline{v} \cdot u) \tag{4}$$

where Δ is the Laplace operator, $\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$. In some special cases equation (4) can be solved analytically. However, in most cases, we have to rely on numerical methods.

Task 1

To start off gently we can simplify equation (4) in the following way. First we leave out the diffusion term (i.e. $D = 0$). If in addition to this we only let the wind blow in the x-direction ($\overline{v} = (v, 0, 0)$) we get the following equation:

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}(v \cdot u)$$

which can be expanded into

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} - u\frac{\partial v}{\partial x} \tag{5}$$

Finally, if v is the same for all x, then equation (5) turns into

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} \tag{6}$$

To solve equation (6) numerically the following explicit finite difference scheme [1] can be used:

$$\frac{u_j^{n+1} - u_j^n}{k} = -v\frac{u_j^n - u_{j-1}^n}{h}$$

Use the scheme above and the initial condition

$$u_0(x) = \begin{cases} 5 & |x| < 1 \\ 0 & \text{otherwise} \end{cases}$$

to solve (6) for the area defined by

$$\begin{cases} |x| \leq 15 \\ 0 < t \leq 4 \end{cases}$$

[1] Standard notation is used in all the schemes. This means that j and n are indices for space and time, respectively, h and k are step lengths for space and time, respectively.

Let $v = 1$ and choose $h = 0.1$ and $k = 0.05$ for the step lengths.

Plot the concentration profile at $t = 4$ together (in the same figure as shown in figure (2 B)) with the profiles you obtain in Task 2 and 3.

Explain the concentration profile at $t = 4$. Is this what you would expect with only advection with a constant wind velocity? The exact solution of 6 is $u(x,t) = u_0(x - vt)$ (shown in figure(2 A) . Does your numerical solution differ from it?

Note that the problem above (equation (6) together with the initial condition) is not *a well-posed problem. To make it a well-posed problem we have to add boundary conditions. Here, and in the other tasks we will use natural constraints assuming that the solution is constant outside a predefined interval. If we solve the problem using a large enough region, like $|x| \leq 15$, this won't lead to any complications.*

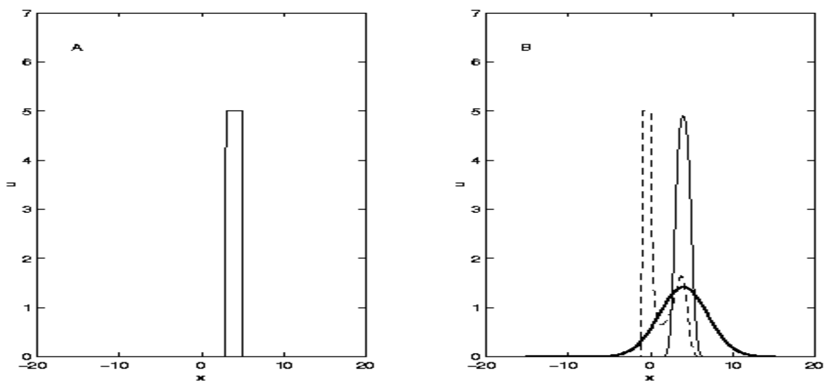

Figure 2: A *The exact solution to equation (6).* B *Numerical solutions to Task 1, 2 and 3.*

Task 2

If we now complicate the situation given in Task 1 somewhat by letting the wind (still just blowing in the x-direction) be a function of x but still ignoring diffusion, then our concentration u can be described by equation (5), given above. An explicit scheme for this problem is:

$$\frac{u_j^{n+1} - u_j^n}{k} = -v_j \frac{u_j^n - u_{j-1}^n}{h} - u_j^n \frac{v_j - v_{j-1}}{h} \tag{7}$$

a) Deduce the order of accuracy for the scheme (7).

b) Use the same step lengths, initial condition and region as in Task 1 to solve equation (5) with the scheme (7). Let the wind velocity be defined as:

$$v(x) = \begin{cases} x^2/(1+x^2) & x > 0 \\ 0 & \text{otherwise} \end{cases}$$

Plot the concentration profile at $t = 4$ together (in the same figure) with the profiles of Task 1 and 3.

Task 3

If we enter diffusion into equation (6), we obtain the following equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} \tag{8}$$

which can be solved using the scheme,

$$\frac{u_j^{n+1} - u_j^n}{k} = D\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} - v\frac{u_j^n - u_{j-1}^n}{h} \tag{9}$$

a) Solve equation (8), using the same initial condition, region and the same wind as in Task 1. Use $h = 0.1$, $k = 0.004$ and $D = 1$.

Plot the concentration profile at $t = 4$ together (in the same figure) with the profiles you obtained in Task 2 and 3. Explain the differences between the three profiles.

b) The stability conditions for the finite difference schemes can be examined using, for example, the Fourier method. The stability condition for the scheme (9) is

$$\frac{k}{h^2}(2D + vh) \leq 1$$

The choice of step lengths in Task 3a therefore gives a stable difference scheme. Now, solve the same problem as in Task 3a but use the step lengths ($h = 0.1$, $k = 1/210$) and ($h = 0.1$, $k = 1/209$). With these choices of step-lengths it is not possible to find the solution at exactly $t = 4$, however, you can still study the phenomenon of unstable difference schemes. Explain the results.

Assignment 7: Air Quality Modeling and the Advection Diffusion Equation II

Task 1

In assignment 6 we have only looked at cases where the concentration depends on one space variable and time, $u = u(x,t)$. Let's now study what happens if the wind vector has two components, $\overline{v} = (v_1, v_2, 0)$. If we set $D = 0$ the general advection diffusion equation (4) turns into:

$$\frac{\partial u}{\partial t} = -v_1 \frac{\partial u}{\partial x} - v_2 \frac{\partial u}{\partial y} - u \frac{\partial v_1}{\partial x} - u \frac{\partial v_2}{\partial y} \tag{10}$$

Equation (10) can be solved using a generalization of the scheme (7):

$$\begin{aligned} \frac{u^{n+1}(i,j) - u^n(i,j)}{k} = & - v_1(i,j)\frac{u^n(i,j) - u^n(i-1,j)}{h} \\ & - v_2(i,j)\frac{u^n(i,j) - u^n(i,j-1)}{h} \\ & - u^n(i,j)\frac{v_1(i,j) - v_1(i-1,j)}{h} \\ & - u^n(i,j)\frac{v_2(i,j) - v_2(i,j-1)}{h} \end{aligned} \tag{11}$$

Use this scheme to solve (10) with the following specifications. Solve for $|x| \leq 30$, $|y| \leq 30$, $t \leq 15$, step lengths $h = 0.5$, $k = 0.1$ and the initial condition:

$$u_0(x,y) = \begin{cases} 50(1 + \cos\frac{\pi r}{4}) & r \leq 4 \\ 0 & otherwise \end{cases}$$

where

$$\begin{cases} r^2 = (x - x_0)^2 + (y - y_0)^2 \\ (x_0, y_0) = (0, -20) \end{cases}$$

The wind is defined by

$$\begin{cases} R = \sqrt{x^2 + y^2} \\ \overline{v} = (-(y + 0.5x)/R, (x - 0.5y)/R) \end{cases}$$

Make plots of the solution at $t = 0$, $t = 5$, $t = 10$, and $t = 15$. Make a velocity plot of the wind, i.e. plot arrows indicating the wind direction (use *quiver* in matlab). Try to explain your results. Change the step size to $k = 0.01$. What happens?

Task 2

Add the dissipation term with $D = 1.0$. Approximate the Laplace operator with second order centered differences. Re-do the calculations with $h = 0.5$ and $k = 0.01$. Compare with task 1 and explain both the physical and the numerical behavior.

Task 3

Suggest a better numerical method for this problem and motivate your choice, (possibly by showing that it works better).