Numerical Methods
Bachelor in Physics

Practicum 8: Partial differential equations II: Advanced explicit methods.

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In the previous practical sessions, we have studied the archetype of the parabolic PDE: the diffusion equation. We have seen that it is possible to solve this equation numerically with a simple *marching* method. In this practical session, we will use a number of advanced *marching* methods to solve *hyperbolic* PDEs.

1 The advection equation

1.1 The wave and the advection equation

The archetype of a hyperbolic PDE is the wave equation

$$\frac{\partial^2 A}{\partial t^2} = c^2 \frac{\partial^2 A}{\partial x^2}$$

with amplitude $A(x,t)$, and velocity c. Let's rewrite this equation as a pair of first order PDEs. Let's define

$$P = \frac{\partial A}{\partial t}; \;\; Q = -c\frac{\partial A}{\partial x}$$

Rewriting the wave equation with these definitions yields

$$\frac{\partial P}{\partial t} = -c\frac{\partial Q}{\partial x}; \;\; \frac{\partial Q}{\partial t} = -c\frac{\partial P}{\partial x}$$

or

$$\frac{\partial \mathbf{a}}{\partial t} = -c\mathbf{B}\frac{\partial \mathbf{a}}{\partial x}$$

with $\mathbf{a} = \begin{bmatrix} P \\ Q \end{bmatrix}$ and $\mathbf{B} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

This suggests that the most familiar hyperbolic PDE, the wave equation, is not the most elementary hyperbolic PDE. Because the advection equation

$$\frac{\partial a}{\partial t} = -c\frac{\partial a}{\partial x}$$

is the most rudimentary hyperbolic PDE, we will try to solve this equation instead of the wave equation. (In meteorology, the term *advection* is used for the horizontal transport of air layers.) If we assume that $a(x, t)$ is the temperature at location x and at moment t, the equation reads as

$$\text{(Rate of temperature change in } x \text{)} =$$

$$- \text{ (transport velocity of air)} \times \text{ (the temperature gradient)}$$

The advection equation is the most elementary equation of a continuity equation

$$\frac{\partial p}{\partial t} = -\nabla \cdot \mathbf{F}(p)$$

E.g. for charge density p, and current density F.

1.2 Analytical solution of the advection equation

For the following initial conditions

$$a(x, t = 0) = f_0(x)$$

with an arbitrary function $f_0(x)$, the solution of the advection equation is given by

$$a(x, t) = f_0(x - ct).$$

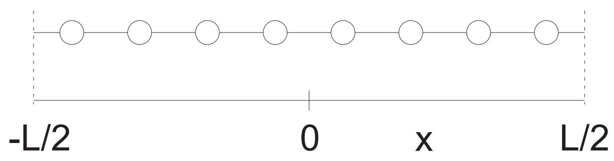
E.g. consider a Gaussian pulse modulated with a cosine

$$a(x, t = 0) = \cos[k(x - x_0)] \exp\left[-\frac{(x - x_0)^2}{2\sigma^2}\right]$$

with width σ and initial location of the peak x_0. The solution is given by

$$\begin{aligned} a(x, t) &= \cos[k((x - ct) - x_0)] \exp\left[-\frac{((x - ct) - x_0)^2}{2\sigma^2}\right] \\ &= \cos[k(x - (x_0 + ct))] \exp\left[-\frac{(x - (x_0 + ct))^2}{2\sigma^2}\right] \end{aligned}$$

Note that the solution preserves its exact shape, but the position of the peak shifts to $x_0 + ct$. Because it is easy to solve the advection equation analytically, it is an ideal hyperbolic PDE to demonstrate numerical methods. We will see that solving hyperbolic PDEs, including the simple advection equation, is far from trivial.



Figuur 1: The chosen grid with PBC. The border lays between the first and the last grid point.

1.3 FTCS method for the advection equation

First, we will try to solve the advection equation with the FTCS method used in the previous practical session. Let's use the central difference approximation for the first time derivative

$$\frac{\partial a}{\partial t} \Rightarrow \frac{a_i^{n+1} - a_i^n}{\tau}$$

and for the spatial derivative

$$\frac{\partial a}{\partial x} \Rightarrow \frac{a_{i+1}^n - a_{i-1}^n}{2h}$$

We will consider periodic boundary conditions (see Fig. 1) and grid size $h = L/N$.

The program `advect.m` solves the advection equation with the FTCS method, among others. The initial condition is a Gaussian pulse modulated with a cosine. Since the speed of the wavefront is equal to c, the wave will cover a distance h in time $t_w = h/c$. This reveals the characteristic time scale τ of this problem. A translation over a distance L means that the pulse is again at its starting position. For this translation, one needs $L/(c\tau)$ iterations.

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Study the program `advect.m`, especially the implementation of the boundary conditions. Run the FTCS scheme for different time steps τ. What do you notice?

1.4 Lax method for the advection equation

The FTCS scheme is unconditionally unstable (for every time step τ). Luckily, there is an easy solution: the Lax method, defined by following scheme

$$a_i^{n+1} = \frac{1}{2}(a_{i+1}^n + a_{i-1}^n) - \frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n)$$

The Lax method replaces the a_i^n term in the FTCS scheme with the average of the values in the adjacent grid points. This method is stable if $\frac{c\tau}{h} \leq 1$. The maximal value for τ is $\tau_{\max} = \frac{h}{c} = t_w$. This condition is known as the *Courant-Friedrichs-Lewy* (CFL) condition and is often used in numerical methods to solve PDEs.

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Study the implementation of the Lax method in advect.m and solve the advection equation with this method. First, choose $\tau = \tau_{\max} = t_w$. Decrease the time step subsequently. What do you notice.

The Lax method has an interesting property. For values $\tau > \tau_{\max}$, the method is not stable. However, for time steps smaller than $\tau_{\max}$, the solution is also wrong! After all, in that case, we find that the pulse extinguishes. One gets the best result if $\tau = \tau_{\max}$. This is an example of a method for which a smaller step size does not yield a better result.

When we use the average value of the two adjacent grid points, we introduce an artificial diffusion which is inversely proportional to time step τ. If the time step is too large, then the artificial diffusion will be to weak to stabilize the solution. On the other hand, if τ is too small, then the artificial diffusion is too strong, and the solution will extinguish. Many schemes used for solving hyperbolic PDEs introduce some form of diffusion in order to stabilize the solution.

1.5 Lax-Wendroff scheme

Finally, let's derive a second order difference method, the Lax-Wendroff scheme. We start from the following Taylor expansion

$$a(x, t+\tau) = a(x,t) + \tau \left(\frac{\partial a}{\partial t}\right) + \frac{\tau^2}{2}\left(\frac{\partial^2 a}{\partial t^2}\right) + O(\tau^3)$$

We can rewrite the term linear in τ using the advection equation:

$$\frac{\partial a}{\partial t} = -c\frac{\partial a}{\partial x}.$$

Analogously, we can write

$$\frac{\partial^2 a}{\partial t^2} = c^2\frac{\partial^2 a}{\partial x^2}.$$

We find that

$$a(x, t+\tau) \approx a(x,t) - c\tau\frac{\partial a}{\partial x} + \frac{c^2\tau^2}{2}\frac{\partial^2 a}{\partial x^2}.$$

And after discretizing:

$$a_i^{n+1} = a_i^n - \frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n) + \frac{c^2\tau^2}{2h^2}(a_{i+1}^n + a_{i-1}^n - 2a_i^n)$$

Note that the last term is a second derivative of $a(x,t)$. This term is the artificial diffusion needed to stabilize the solution. One can prove that the CFL condition is the correct stability criterion for this scheme. Also, note that the Lax-Wendroff scheme reduces to the Lax scheme if $\tau = \tau_{\text{max}} = h/c$.

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Run the Lax-Wendroff scheme for different time steps τ

1.6 Tasks

1. Implement the following Dirichlet boundary conditions in `advect.m`:

$$\begin{aligned} a(x = -L/2, t) &= \sin(\omega t) \\ a(x = L/2, t) &= 0 \end{aligned}$$

   Run the program (without the Gaussian pulse) for a sufficient amount of time (the wave should arrive on the other side). Test the FTCS, Lax and Lax-Wendroff scheme for $\omega = 10\pi$.

2. The combination of the advection and diffusion equation gives the transport equation:

$$\frac{\partial T}{\partial t} = -c\frac{\partial T}{\partial x} + \kappa\frac{\partial^2 T}{\partial x^2}$$

   Write a program that solves this PDE, using a FTCS. Use periodic boundary conditions and a normalized Gaussian pulse, with standard deviation $2h$, as initial condition. Check empirically that the solution is stable if

$$\left(\frac{c\tau}{h}\right)^2 \le \frac{2\kappa\tau}{h^2} \le 1$$

   Experiment with different values for c and κ.