Computer Exercise C1B

Numerical Methods for PDEs

10% of Final Grade

Deadline: See the course webpage.

Individual Work: This is an indvidual assignment.

Submission: Send your report and all MATLAB (or Python) code to: `numpde2025ATgmail.com`.

PART A (40 points)

Consider the one-dimensional advection equation:

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x}, \quad x \in (0,1),\ t \in (0,10), \tag{1}$$

with the initial condition:

$$u(x,0) = u_0(x) = \begin{cases} e^{-200(x-\frac{3}{10})^2}, & \text{for } x < \frac{1}{2}, \\ 0, & \text{for } \frac{1}{2} \le x \le \frac{3}{5} \text{ or } x \ge \frac{4}{5}, \\ 1, & \text{for } \frac{3}{5} < x < \frac{4}{5}. \end{cases}$$

The equation is subject to periodic boundary conditions:

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

(a) Show that the following quantity is conserved for PDE (1):

$$M_m(t) = \frac{1}{m}\int_0^1 [u(x,t)]^m \, dx, \quad m \in \mathbb{N}\backslash\{0\}.$$

We define the Courant number as $\sigma = \frac{\Delta t}{\Delta x}$. The following finite-difference schemes are used to numerically approximate solutions of PDE (1):

FTFS: $u_j^{n+1} = u_j^n + \sigma(u_{j+1}^n - u_j^n)$,

FTCS: $u_j^{n+1} = u_j^n + \frac{\sigma}{2}(u_{j+1}^n - u_{j-1}^n)$,

FTBS: $u_j^{n+1} = u_j^n + \sigma(u_j^n - u_{j-1}^n)$,

BTCS: $u_j^{n+1} = u_j^n + \frac{\sigma}{2}(u_{j+1}^{n+1} - u_{j-1}^{n+1})$,

Lax-Friedrichs: $u_j^{n+1} = \frac{u_{j+1}^n + u_{j-1}^n}{2} + \frac{\sigma}{2}(u_{j+1}^n - u_{j-1}^n)$,

Lax-Wendroff: $u_j^{n+1} = u_j^n + \frac{\sigma}{2}(u_{j+1}^n - u_{j-1}^n) + \frac{\sigma^2}{2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$.

For each of these six methods, answer the following questions:
Hint: For the BTCS method, first rewrite the finite-difference equation into a suitable form.
Hint: Do not be alarmed if some methods turn out to be unconditionally unstable.

(b) Take $\Delta x = \frac{1}{100}$ as fixed. Perform several numerical simulations with different values of the Courant number σ to illustrate the properties of each method. Comment on aspects such as accuracy, stability, numerical diffusion, numerical dispersion and/or oscillations. If applicable, determine values for Δt that result in stable and accurate numerical solutions. Compare your numerical results with the analytical solution, given by:

$$u(x,t) = u_0\big((x+t) \bmod 1\big).$$

(c) Plot relevant numerical solutions to support your answer to part (b). Compare with the exact solution at $t = 0$ and $t = T = 10$.

(d) Verify whether the numerical solution preserves the conserved quantities derived in part (a) for the following cases:

$$m = 1: \quad \mathcal{M}(t) = \int_0^1 u(x,t)\, dx, \qquad \text{momentum}$$

and

$$m = 2: \quad \mathcal{E}(t) = \frac{1}{2}\int_0^1 [u(x,t)]^2\, dx, \qquad \text{energy.}$$

Hint: The degree of conservation may depend on the choice of time step Δt

PART B (30 points)

In phase-field theory, the propagation of domain walls in liquid crystals can be modeled by the following *sixth-order* time-dependent PDE:

$$\frac{\partial u}{\partial t} = \delta \frac{\partial^6 u}{\partial x^6} + \gamma \frac{\partial^4 u}{\partial x^4} + \epsilon \frac{\partial^2 u}{\partial x^2} + u - u^3, \tag{2}$$

where $\epsilon, \delta, \gamma \in \mathbb{R}$, and $x \in [0, L],\ t \in [0, T]$. The initial condition is given by:

$$u(x, 0) = u_0(x).$$

We consider two special cases:

Case I: Extended Fisher-Kolmogorov Equation

Parameters: $\delta = 0,\ \gamma = -1,\ \epsilon = -2$. **Domain:** $L = 100,\ T = 10$. **Initial Condition:** $u_0(x) = \cos\left(\frac{\pi x}{20}\right)$. **Boundary Conditions:**

$$u(0,t) = 1, \quad u_x(0,t) = 0,$$
$$u(L,t) = -1, \quad u_x(L,t) = 0.$$

(Hint: The corresponding solutions are sometimes called “Batman ears”.)

Case II: Pattern formation in phase transitions

Parameters: $\delta = 0.12,\ \gamma = -0.5,\ \epsilon = 1$. **Domain:** $L = 300,\ T = 120$. **Initial Condition:** $u_0(x) = e^{-\frac{x^2}{16}}$. **Boundary Conditions:**

$$u(0,t) = 1, \quad u_x(0,t) = 0, \quad u_{xx}(0,t) = 0,$$
$$u(L,t) = 0, \quad u_x(L,t) = 0, \quad u_{xx}(L,t) = 0.$$

(Hint: The corresponding solutions are sometimes called "travelling oscillatory waves".)

For both cases, answer the following questions:

(a) Numerically approximate the spatial derivatives in model (2) using central finite difference schemes.

(b) Determine the numerical boundary conditions. *(Hint: There are 4 boundary conditions for Case I and 6 for Case II.)*

(c) Apply the forward Euler method to derive an expression for u_i^{n+1} in terms of u_j^n for $j \in \{1, 2, \ldots, I\}$.

(d) Compute the local truncation error and verify that the error is of order $\mathcal{O}((\Delta t)^2, \Delta t \cdot (\Delta x)^2)$.

(e) Generate and plot accurate numerical solutions at $t = 0$ and $t = T$.

PART C (30 points)

Consider the following *infinite-order* PDE in one spatial dimension:

$$\frac{\partial u}{\partial t} = \alpha \sum_{k=0}^{\infty} \frac{\partial^k u}{\partial x^k}, \quad u(x, \cdot) \in \mathcal{C}^{\infty}(\mathbb{R}), \ t > 0, \ 0 < x < L, \ \alpha \in \mathbb{R}. \tag{3}$$

(a) Show that the solution $u(x,t)$ of PDE (3) must satisfy the *finite-order* PDE:

$$u_t = \alpha u + u_{xt}. \tag{4}$$

(b) We impose the boundary condition:

$$u_t(0,t) = u_t(L,t).$$

Apply the first step of the Method of Lines to PDE (4): use a central difference approximation for the spatial derivative and approximate the model as a system of ODEs in the form:

$$\dot{\vec{u}} = \mathcal{M}\vec{u}.$$

(c) Let $x \in [0,1]$, $t \in [0,20]$, and the initial condition be $u(x,0) = \sin(2\pi x)$. Using the second step of the Method of Lines, solve the system using the **Implicit Euler method** for $\alpha = -1$. Plot the numerical solutions for various step sizes Δx and Δt. Assess the numerical accuracy by comparing the approximations with the exact solution:

$$u(x,t) = e^{-\beta t}\left[-\sin(2\beta\pi t)\cos(2\pi x) + \cos(2\beta\pi t)\sin(2\pi x)\right],$$

where $\beta = \frac{1}{1+4\pi^2}$.

(d) Plot the eigenvalues of the matrix $\mathcal{M}$ and the stability region of the Implicit Euler method for $\Delta x = 0.05$. Do all eigenvalues fall within the stability region?

(e) Repeat parts (c) and (d) using the **Explicit Euler method**.

(f) Explain why both the Explicit and Implicit Euler methods are inappropriate for $\alpha = 1$.

(g) Derive an exact solution for the case $\alpha = 1$ using the Fourier Transform Method. Compare this solution with the analytical solution for $\alpha = -1$ and describe the key difference. You may use without proof that:

$$\lim_{x \to \pm\infty} u_t(x,t) = 0.$$