Computer exercise C1

(15 % of Final Grade)

March 2024

Deadline: see the webpage of the course.
(This is an individual assignment!)

PART A (20 points)

Consider the one-dimensional stationary convection-diffusion model:

$$\begin{cases} -\delta u''(x) + \nu u'(x) = 0, \ x \in [0,1], \ \delta, \nu > 0, \\ u(0) = 0, \quad u(1) = 1. \end{cases} \tag{1}$$

The exact solution reads: $u(x) = \frac{e^{P_e x} - 1}{e^{P_e} - 1}$ with $P_e := \frac{\nu}{\delta}$.

(a) Work out a central difference (for u') and an upwind difference[1] scheme (for u') in equation (1). Write the fully-discretized linear system as: $\mathcal{A}\vec{u} = \vec{f}$, where

$$\mathcal{A} = \frac{1}{(\Delta x)^2} \begin{pmatrix} b & c & 0 & & & & & \\ a & b & c & 0 & & & \emptyset & \\ 0 & a & b & c & 0 & & & \\ & & \cdots & \cdots & \cdots & & & \\ & & & \cdots & \cdots & \cdots & & \\ & & & 0 & a & b & c & 0 \\ & \emptyset & & & 0 & a & b & c \\ & & & & & 0 & a & b \end{pmatrix},$$

and

$$\vec{u} = [u_1, u_2, ..., u_{I-2}, u_{I-1}]^T, \ \vec{f} = [0, 0, ..., 0, f_{I-1}]^T.$$

Find the values a, b, c and f_{I-1}.

(b) Solve the following linear difference equations:

$$a\, u_{i-1} + b\, u_i + c\, u_{i+1} = 0, \quad i = 1, ..., I-1,$$

$$\text{where } a < 0, \ b > 0, \ a + b + c = 0.$$

[hint: use a trial solution of the form: $u_i = \alpha + \beta r^i$ with $u_0 = 0, \ u_I = 1$].

(c) Consider the three cases $c < 0$, $c > 0$ and $c = 0$. Check for the solutions in part (b), whether we can expect positivity-preserving numerical solutions

[1] Approximation: $u'|_{x_i} \approx \frac{u_i - u_{i-1}}{\Delta x}$.

($u_i > 0$) or solutions with non-physical oscillations in the u_i. Conclude that the difference scheme produces no oscillations, if $c \leq 0$.

(d) For the central scheme, we have $c = -1 + \frac{P_e \Delta x}{2}$ and $P_e \Delta x \leq 2$, whereas for the upwind scheme $c = -1$ (unconditionally).
Show, by using Taylor series, that the (local) truncation error for the upwind scheme is $\mathcal{O}(\Delta x)$ (for the original model), but $\mathcal{O}((\Delta x)^2)$ for the so-called modified equation:

$$(-\delta + \frac{\nu \Delta x}{2})u''(x) + \nu u'(x) = 0,$$

where $\frac{\nu \Delta x}{2}$ is a numerical (artificial) diffusion coefficient.

(e) Plot a few relevant numerical solutions (choose specific values for P_e) to support the results from parts (a)-(d). Also compare the results with the exact solution of the model. Discuss the numerical solutions in terms of (unphysical) oscillations and (extra) damping.

PART B (10 points)

(a) Construct a time-integration method for $y'(t) = f(y(t))$ that is consistent, but not *zero-stable*[2].

(b) Determine and plot the stability region in the complex plane of the following linear multistep method:

$$y^{n+2} - y^{n+1} = \Delta t f(y^n).$$

PART C (30 points)

Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{1}{6}\frac{\partial^2 u}{\partial x^2}, \quad x \in [0,1], \quad t \in (0,T],$$

with initial /boundary conditions $u(x,0) = \sin(\pi x)$, $u(0,t) = 0$, $u(1,t) = 0$, The exact solution reads $u(x,t) = \mathrm{e}^{-\frac{\pi^2}{6}t}\sin(\pi x)$.

(a) Write a *computercode* (in Matlab or Python) for the FTCS-scheme when applied to this model. In this code Δx and Δt are input parameters.

(b) Make a table of the maximum (absolute) error at $T = 0.6$ as a function of Δt ($= 10^{-2}, 10^{-3}, ..., 10^{-5}$) and Δx ($=\frac{1}{5}, \frac{1}{10}, ..., \frac{1}{80}$). Is the method *stable* for each combination of Δt and Δx?

[2] It is not allowed to use the examples that are discussed in the exercises or lecture notes.

(c) Make a few relevant plots as an illustration of the numerical experiments (don't forget to plot the exact solution as well).

(d) Explain your numerical results in terms of accuracy and stability.

(e) Next, take the special ratio $\frac{\Delta t}{(\Delta x)^2} = 1$ and $\Delta t = 10^{-2}, ..., 10^{-4}$. What happens with the maximum absolute error as a function of Δt? Can you explain this theoretically?

(f) Send the Matlab (or Python) code(s) to: P.A.Zegeling@uu.nl.

PART D (40 points)

In phase-field theory the propagation of domain walls in liquid crystals may be modelled by the following *sixth*-order time-dependent PDE model:

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

with $\epsilon, \delta, \gamma \in \mathbb{R},\ x \in [0, L],\ t \in [0, T]$ and initial condition $u(x, 0) = u_0(x)$.

We consider three special cases[3]:

Case I (Fisher/Huxley)

$\delta = \gamma = 0,\ \epsilon = 1,\ L = 100,\ T = 30,\ u_0(x) = e^{-\frac{x^2}{16}},\ u(0,t) = 1,\ u(L,t) = 0.$
("a monotone travelling wave solution")

Case II (extended Fisher-Kolmogorov)

$\delta = 0,\ \gamma = -1, \epsilon = -2,\ L = 100,\ T = 10,\ u_0(x) = \cos(\frac{\pi x}{20}),\ u(0,t) = 1,\ u_x(0,t) = 0,\ u(L,t) = -1,\ u_x(L,t) = 0.$
("Batman-ear" solutions)

Case III (pattern formation in phase transitions)

$\delta = 0.12,\ \gamma = -0.5,\ \epsilon = 1,\ L = 300,\ T = 120,\ u_0(x) = e^{-\frac{x^2}{16}},\ u(0,t) = 1,\ u_x(0,t) = 0,\ u_{xx}(0,t) = 0,\ u(L,t) = 0,\ u_x(L,t) = 0,\ u_{xx}(L,t) = 0.$
("travelling oscillatory waves")

[3] You need to pay extra attention to the boundary conditions!

(*a*) First, numerically approximate the spatial derivatives in model (2).

(*b*) Then, apply an explicit time-integration method (EF, RK2, RK4, ...) or a standard time-integrator of Matlab or Python.

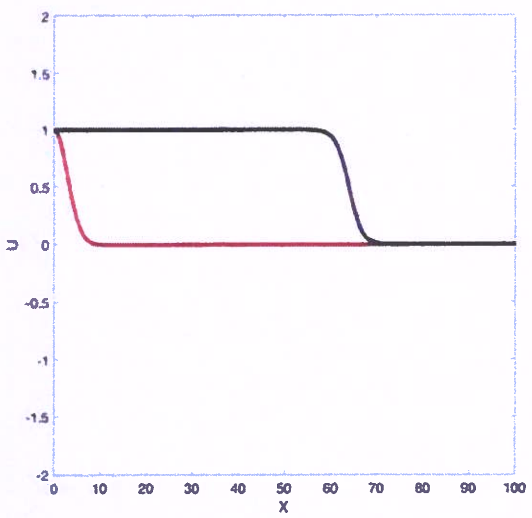
(*c*) Motivate the validity of your results qualitatively. (check the accuracy and explain!)[4]

(*d*) Illustrate your report with graphs at $t = 0$ and $t = T$.

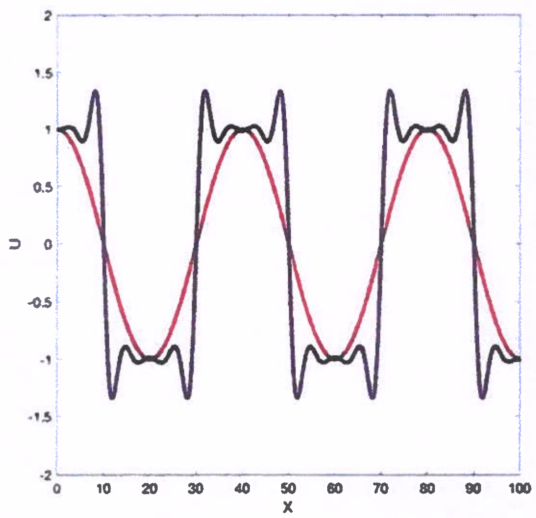
(*e*) Send the Matlab (or Python) code(s) to: P.A.Zegeling@uu.nl.

[4] You may consult the next page for accurately computed solutions.

Case I



Case II



Case III