Exam Numerical Simulation of Differential Equations

Friday, January 28, 2022, Prof. Giovanni Samaey

- The exam is written. You may use the course materials, and handwritten notes, but no other books.
- Write clearly legible and structure your answer. Start a new page for each question.
- The exam takes a maximum of 3 hours.

Good luck!

Vraag 1. Consider 3 methods for the initial value problem $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ with initial condition $\boldsymbol{y}(0) = \boldsymbol{y}_0$:

- **Method 1:**

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

- **Method 2:**

$$\boldsymbol{y}^{k+3} - \frac{18}{11}\boldsymbol{y}^{k+2} + \frac{9}{11}\boldsymbol{y}^{k+1} + \frac{2}{11}\boldsymbol{y}^{k} = \frac{6}{11}\Delta t \boldsymbol{f}(t^{k+3}, \boldsymbol{y}^{k+3}).$$

- **Method 3:**

$$\begin{aligned} \boldsymbol{\xi} &= \boldsymbol{y}^k + \frac{\Delta t}{2}\boldsymbol{f}\left(t^{k+1/2}, \boldsymbol{\xi}\right) \\ \boldsymbol{y}^{k+1} &= \boldsymbol{y}^k + \Delta t \boldsymbol{f}\left(t^{k+1/2}, \boldsymbol{\xi}\right). \end{aligned}$$

Now answer the following three questions:

1. Part I: classification (2 points)
   a) Write the first method in formula form.
   b) One of these methods contains a typo. Find the typo and explain how to notice it. (Simply stating that the method is different in the course notes is not sufficient ...). **In the rest of the question, we pretend that the typo has been corrected.**
   c) Describe and classify each of the methods. Be as clear and precise as possible. Give the order of each method.
   d) Which stability region belongs to each method? Make a sketch illustrating the essential characteristics of each stability region and briefly justify using the theoretical stability properties of the method.
2. Part II: behavior (2 points)
   a) What behavior do you expect for each of the methods for the linear equation $y' = -y$ if you increase the time step size Δt? Explain your answer.
   b) Consider for a moment the different possibilities for the behavior of a system of differential equations, and the corresponding properties we would like to see after time discretization. In our limited catalog here, do we have a method available for every possible case? If so, please note. If not, what kind of method is missing?

3. Part III: application (3 points)

   Now consider a system of M atoms with positions $\boldsymbol{x}(t) = (x_m(t))_{m=1}^M$ and velocities $\boldsymbol{v}(t) = (v_m(t))_{m=1}^M$, satisfying the following system of differential equations:

$$\begin{aligned} \boldsymbol{x}' &= \boldsymbol{v}, \\ \boldsymbol{v}' &= -\nabla V(\boldsymbol{x}), \end{aligned}$$

   with V some potential energy function. (Remark that all atoms have unit mass.)

   a) Which of the above time discretization methods do you recommend for this problem? Why? When in doubt, give your reasoning and the steps you would take to decide which method is most appropriate.

   b) If you choose an implicit method, how would you solve the nonlinear system at each time step? Consider iteration scheme, starting value, and stopping criterion.

   c) If your iterative method requires you to solve linear systems in each iteration: how would you solve those linear systems?

Question 2. Consider the two-dimensional heat equation for the function $u(x, y, t)$,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}.$$

a) We derived an ADI method for this equation. What is the advantage of this method, compared to the explicit Euler method on one hand and the Crank-Nicholson scheme on the other hand? (1 point)

b) Show convergence of this ADI method using the maximum principle. (1.5 point)

Now consider a variation on this classical ADI method, using the notation in Morton and Meyers, as once proposed by D'Yakonov:

$$\begin{aligned} \left(1 - \mu_x \frac{1}{2}\delta_x^2\right) U^{n,*} &= \left(1 + \frac{1}{2}\mu_x \delta_x^2\right)\left(1 + \frac{1}{2}\mu_y \delta_y^2\right) U^n \\ \left(1 - \mu_y \frac{1}{2}\delta_y^2\right) U^{n+1} &= U^{n,*} \end{aligned}$$

with $\mu_x = \Delta t/\Delta x^2$ and $\mu_y = \Delta t/\Delta y^2$.

c) Write out this method explicitly as a finite difference method, and show what the stencil is of both steps. (1 point)

d) What is the order of this method? Prove your claim. (1 point)

e) Analyse the stability of this method. Compare with the classical ADI method. (1.5 point)

Question 3. Briefly answer the following questions. Limit yourself to about half a page per answer. The goal is not to define all concepts in detail, but to use the necessary terms correctly in your answer. If a figure or formula can help, use it. Derivations, proofs, etc., are not necessary unless explicitly asked otherwise.

a) In the finite element method, one of the steps in the derivation is the transition to local coordinates in each element. What is the importance of this step for the finite element method? (What does this transition allow that would not otherwise be possible?) (1 point)

b) Explain why the finite element method is better suited to problems with irregular domains and the associated boundary conditions than the finite difference method. (1.5 points)

c) Show that the Lax-Wendroff method for linear advection can be understood as a forward Euler scheme with central differences in space and artificial diffusion. What goes wrong without this artificial diffusion? (1.5 points)

d) Describe the behavior of characteristics of a hyperbolic conservation law (with constant, space-dependent, or solution-dependent coefficients). (1.5 points)

e) When the linear advection equation is solved by the upwind method, the solution is damped and smoothed. Why? (1.5 points)