WI4011
Computational Fluid Dynamics
Assignment 1.3 2016-2017

The completion of Assignment 1.3 is required to pass the exam for WI4011. Provide clear and motivated answers to the questions. Try to use the information available in the book of Prof. Wesseling and the lecture notes. Assignment 1.3 should be handed in (by email or in hard copy) before December 11, 23:59. You are advised but not obliged to work in pairs of two students. If you work in a pair, please state both your names clearly on your work. Preferably use LaTeX. Only well-organised hand-written reports are accepted.

The unsteady convection-diffusion equation in one dimension.

We will investigate the accuracy of the time-step constraints that result from the application of the method of Wesseling for the one-dimensional linear scalar unsteady convection-diffusion equation:

$$\frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} - \varepsilon\frac{\partial^2 \varphi}{\partial x^2} = q, \quad u, \varepsilon > 0, \quad \varepsilon << 1, \quad 0 < x < 1, \quad 0 < t \leq T \ , \tag{1}$$

$$\begin{gathered} q(t,x) = \beta^2 \varepsilon \cos\beta(x - ut) \ , \ \alpha = 4\pi, \ \beta = 2\pi, \\ \text{with solution:} \\ \varphi(t,x) = \cos\beta(x-ut) + e^{-\alpha^2\varepsilon t}\cos\alpha(x-ut), \end{gathered} \tag{2}$$

for properly chosen boundary and initial conditions. We will use the κ-scheme:

$$(u\phi)\big|_{j+\frac{1}{2}} = u\left(\frac{\phi_j + \phi_{j+1}}{2} + \frac{1-\kappa}{4}\left(-\phi_{j-1} + 2\phi_j - \phi_{j+1}\right)\right), \tag{3}$$

with κ equal to $\frac{1}{3}$ to discretize the convective part of the spatial differential operator and a second order central approximation for the diffusive part. The temporal discretisation will be done using *Merson's method*, as illustrated for the general ordinary differential equation $y' = f(t,y)$:

$$y^{n+1} = y^n + \tau \sum_{i=1}^{s} b_i k_i, \tag{4}$$

$$k_i = f\left(t_n + c_i\tau, y_n + \tau \sum_{j=1}^{s} a_{ij} k_j\right), \tag{5}$$

where the coefficients a_{ij}, b_i, c_j are given in the following *Butcher array*:

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ \dots & \dots & \dots & \dots & \dots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array} \qquad \begin{array}{c|ccccc} 0 & & & & & \\ \frac{1}{3} & \frac{1}{3} & & & & \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{6} & & & \\ \frac{1}{2} & \frac{1}{8} & 0 & \frac{3}{8} & & \\ 1 & \frac{1}{2} & 0 & -\frac{3}{2} & 2 & \\ \hline & \frac{1}{6} & 0 & 0 & \frac{2}{3} & \frac{1}{6} \end{array}. \tag{6}$$

- Numerically generate a graph of the stability locus S, defined as:

  $$S = \{\lambda\tau \in \mathbb{C} |\ |R(\lambda\tau)| = 1\}, \tag{7}$$

  of Merson's method, given the fact that the stability polynomial of the time integration method is given by:

  $$R(\lambda\tau) = 1 + (\lambda\tau) + \tfrac{1}{2}(\lambda\tau)^2 + \tfrac{1}{6}(\lambda\tau)^3 + \tfrac{1}{24}(\lambda\tau)^4 + \tfrac{1}{144}(\lambda\tau)^5. \tag{8}$$

  Hint: use MATLAB contour to generate the single contourline $|R(\lambda\tau)| = 1$.

- Determine the symbol $\hat{L}_h = e^{-i\theta} L_h e^{i\theta}$ for the spatial discretisation of the convection-diffusion equation based on the combination of a κ-scheme with $\kappa = \frac{1}{3}$ and a central approximation for the convective and diffusive part of the spatial differential operator, respectively. Do not derive the symbol from scratch, but use the results presented in the book of Wesseling.

- The symbol $\hat{L}_h$ depends on

  $$c = \frac{|u|\tau}{h}, \quad d = \frac{2\epsilon\tau}{h^2}, \text{ and } \kappa, \tag{9}$$

where c is the *Courant-Friedichs-Lewy-number*, d is the *diffusion-number* and h is the meshwidth. Visualize the dependence of the symbol on the value of κ for a fixed high Péclèt number and on the Péclèt number for a fixed κ.

- Select one of the geometric shapes, as described by Wesseling to contain the symbol, and to be fit in the stability locus of the proposed time-integration method. Discuss your choice and consider complexity of the resulting restriction on the time step and the accuracy of the predicted threshold for stability when $Pe \gg 1$.

- Determine the appropriate restriction on the timestep.

- Solve the one dimensional convection-diffusion equation (1) on a cell centered grid on the unit interval using the above spatial discretisation and demonstrate the validity of the constraint on the time step for two values of the Péclèt number: $Pe = 200$ and $Pe = 400$. Impose periodic boundary conditions and use the exact solution to impose the initial condition.

  Adapt the program from Blackboard, or write your own. If you leave κ as a parameter in your discretisation you can compare your numerical solution with the original program in `convectiondiffusion.tar`: First change the spatial discretisation and leave the time integration unchanged. When you are sure the spatial discretisation is correct proceed with adapting the time integration. It is also recommended to separately verify the implementation for your time integration method for a simple ODE, e.g. $y' = \cos(t)$.