# CFD - Assignment 1.3

Lars Zondag (4095588) Thomas Schiet (4181484)

11 December 2016

## 1 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:

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

$$q(t,x) = \beta^2 \epsilon \cos\beta(x - ut), \quad \alpha = 4\pi, \quad \beta = 2\pi, \tag{2}$$

with solution

$$\phi(t,x) = \cos\beta(x-ut) + e^{-\alpha^2\epsilon t}\cos\alpha(x-ut), \tag{3}$$

for properly chosen boundary and initial conditions. We will use the $\kappa$-scheme:

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

with $\kappa$ 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 $y' = f(t,y)$:

$$y^{n+1} = y^n + \tau\sum_{i=1}^{s} b_i k_i, \tag{5}$$

$$k_i = f\left(t_n + c_i\tau, y_n + \tau\sum_{j=1}^{s} a_{ij}k_j\right), \tag{6}$$

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

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \dots & \dots & \dots & \dots & \dots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array} \qquad \begin{array}{c|ccccc} 0 & & & & & \\ \frac{1}{3} & \frac{1}{3} & & & & \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{6} & & & \\ \frac{1}{2} & \frac{1}{8} & 0 & \frac{3}{8} & & \\ 1 & \frac{1}{2} & 0 & -\frac{3}{2} & 2 & \\ \hline & \frac{1}{6} & 0 & 0 & \frac{2}{3} & \frac{1}{6} \end{array} \tag{7}$$

1. Numerically generate a graph of the stability locus $S$, defined as:

$$S = \{\lambda\tau \in \mathbb{C} | \ |R(\lambda\tau)| = 1\}, \tag{8}$$

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

$$R(\lambda\tau) = 1 + (\lambda\tau) + \frac{1}{2}(\lambda\tau)^2 + \frac{1}{6}(\lambda\tau)^3 + \frac{1}{24}(\lambda\tau)^4 + \frac{1}{144}(\lambda\tau)^5 \tag{9}$$

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

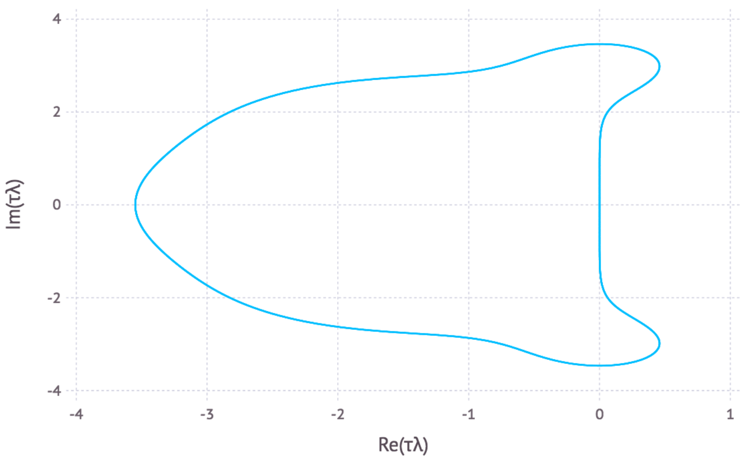



Figure 1: Contourline for $|R(\lambda\tau)| = 1$

2. 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 $\kappa$-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.

Let the one dimensional convection diffusion equation be written as:

$$\frac{\partial \phi}{\partial t} + L\phi = q, \quad L\phi = \left( u\frac{\partial}{\partial x} - \epsilon \frac{\partial^2}{\partial x^2} \right) \phi \tag{10}$$

We can write (with $\kappa$-scheme and CDS): $\tau L_h = C_h + D_h$, with

$$C_h = \frac{1}{4} c \left\{ (1-\kappa)\phi_{j-2} - (5 - 3\kappa)\phi_{j-1} + (3 - 3\kappa)\phi_j + (1+\kappa)\phi_{j+1} \right\} \tag{11}$$

and

$$D_h = \frac{1}{2} d(-\phi_{j-1} + 2\phi_j - \phi_{j+1}), \tag{12}$$

Taking the Fourier transform:

$$\tau \hat{L}_h(\theta) = \hat{C}_h(\theta) + \hat{D}_h(\theta), \tag{13}$$

$$\hat{C}_h(\theta) = \gamma_1(\theta) + i\gamma_2(\theta), \quad \hat{D}_h(\theta) = \delta(\theta) \tag{14}$$

With:

$$\gamma_1(\theta) = 2(1-\kappa)cs^2, \quad \gamma_2(\theta) = c\{(1-\kappa)s + 1\}\sin\theta, \quad \delta(\theta) = 2ds \tag{15}$$

where $s = \sin^2 \frac{1}{2}\theta$. If we now make $\kappa = \frac{1}{3}$, we get:

$$\gamma_1(\theta) = \frac{4}{3}cs^2, \quad \gamma_2(\theta) = c\{\frac{2}{3}s + 1\}\sin\theta \tag{16}$$

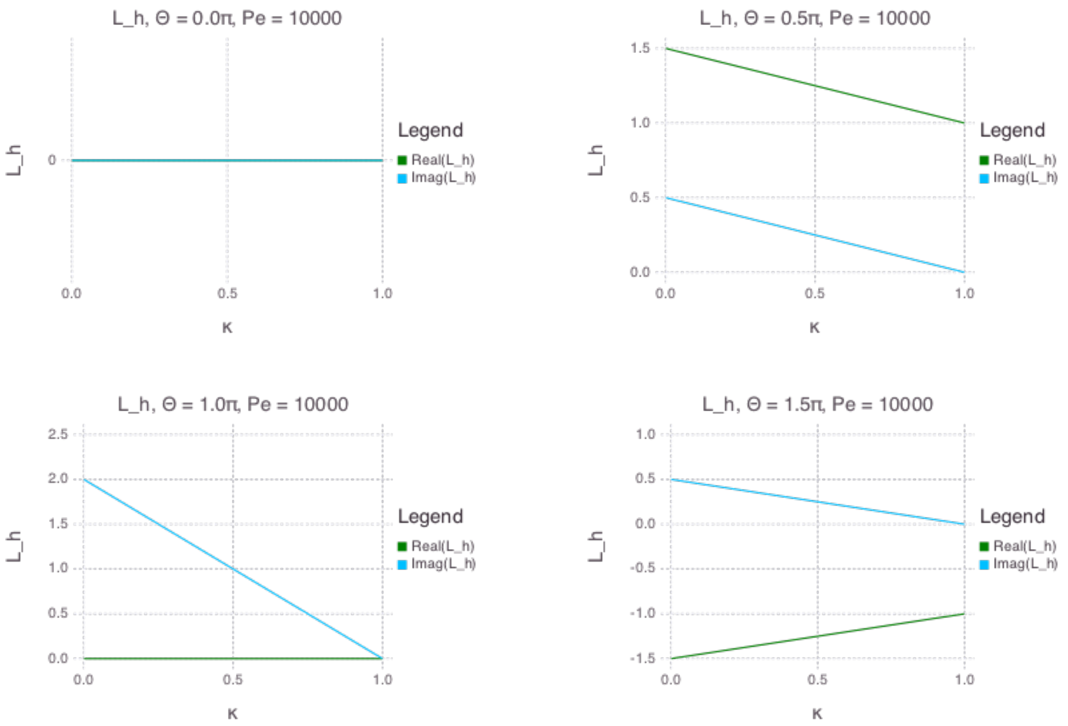
Finally leading to:

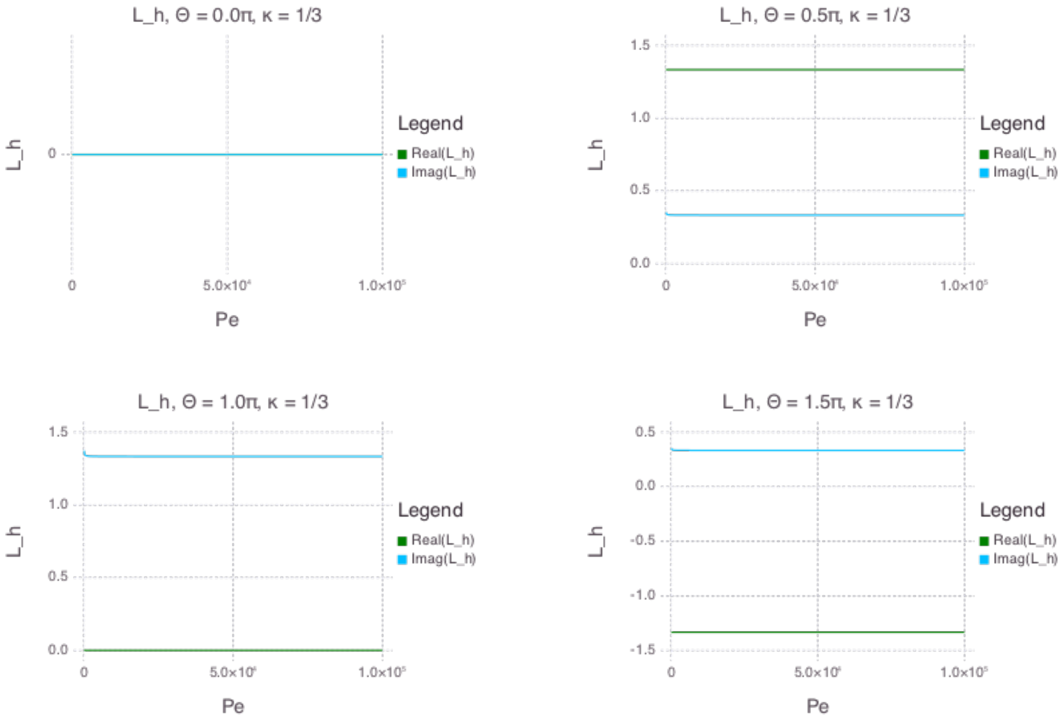
$$\tau\hat{L}(\theta) = \frac{4}{3}cs^2 + 2ds + ic\{\frac{2}{3}s + 1\}\sin\theta \tag{17}$$

3. The symbol $\hat{L}_h$ depends on

$$c = \frac{|u|\tau}{h}, \quad d = \frac{2\epsilon\tau}{h^2}, \text{ and } \kappa, \tag{18}$$

where $c$ is the *Courant-Friedichs-Lewy-number*, $d$ is the diffusion-number and $h$ is the mesh-width. Visualize the dependence of the symbol on the value of $\kappa$ for a fixed high Péclèt number and on the Péclèt number for a fixed $\kappa$.






4. 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 $Pe \gg 1$

---

For this we need to know the values of our constants:

$$c = \frac{|u|\tau}{h}, \quad d = \frac{2\epsilon\tau}{h^2}, \text{ and } \kappa, \tag{19}$$

Let $\tilde{d} = d + (1-\kappa)c = \frac{\tau}{h}\left(|u| + (1-\kappa)\frac{2\epsilon}{h}\right)$. We will now try to let the symbol be contained in a half ellipse. We have chosen this geometry because it resembles the stability locus the best in our view. For the half ellipse we have the following condition:

$$\tilde{d} \leq \frac{a}{2}, \quad \text{and} \quad \frac{2c^2}{b^2} \leq (2-\kappa)^{-2}\left(1 + \sqrt{1 - 4\tilde{d}^2/a^2}\right) \tag{20}$$

Then $S_L$ is contained in the left half of the ellipse given by

$$\left(\frac{v}{a}\right)^2 + \left(\frac{w}{b}\right)^2 = 1, \quad v + iw = z. \tag{21}$$

We estimate that the half ellipse would fit in the stability locus with parameters $a = 3.5$ and $b = 2$. And for our scheme we chose $\kappa = 1/3$. According to Wessling, however, we can take $\sqrt{1 - 4\tilde{d}^2/a^2} = 0$ without losing too much sharpness. Since this simplifies the equation a lot we will apply this step. This means that:

$$\tilde{d} \leq \frac{7}{4}, \quad \text{and} \quad \frac{c^2}{2} \leq \frac{9}{25} \tag{22}$$

$$\frac{\tau}{h}\left(|u| + (1-\kappa)\frac{2\epsilon}{h}\right) \leq \frac{7}{4}, \quad \text{and} \quad \frac{|u|^2\tau^2}{2h^2} \leq \frac{9}{25} \tag{23}$$

When $Pe \gg 1$ our assumption to set $\sqrt{1 - 4\tilde{d}^2/a^2} = 0$ becomes less valid since $\tilde{d}$ decreases with increasing $Pe$. Since the time step is restricted by the minimum of both inequalities, we also see that for higher $Pe$ the complexity increases.

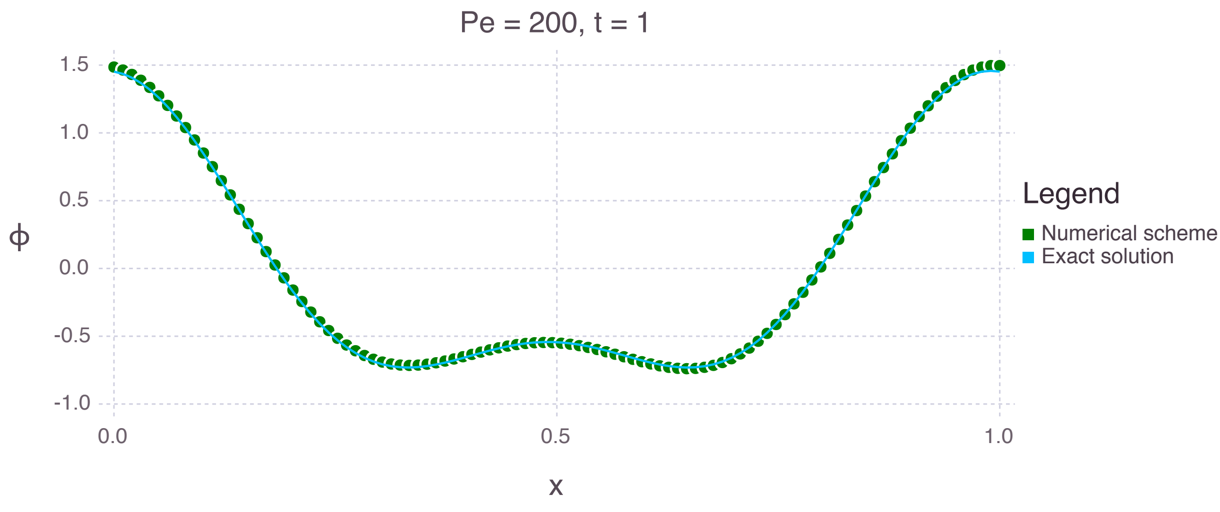
5. Determine the appropriate restriction on the timestep.

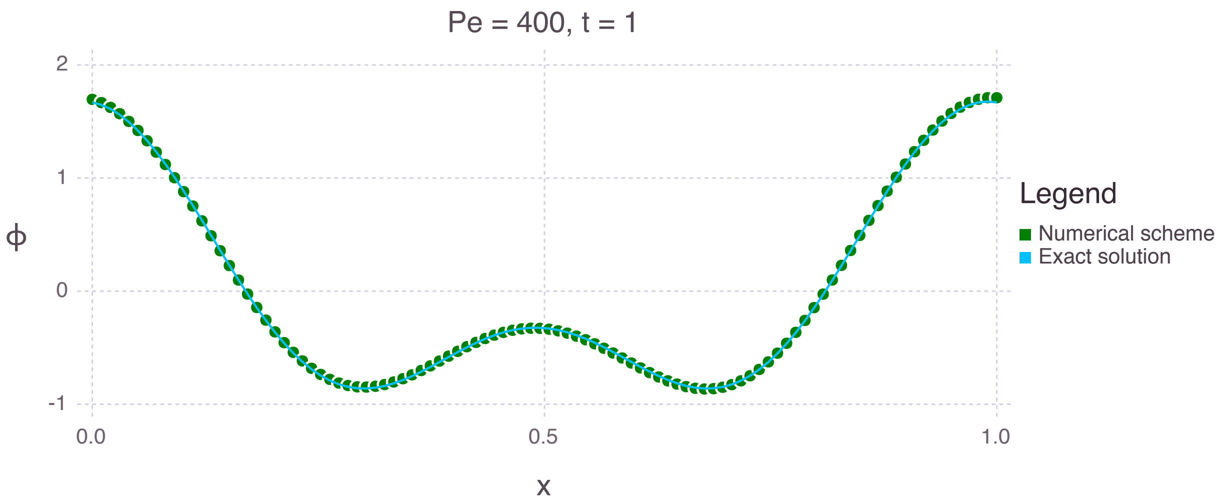
The appropriate restriction on the timestep is:

$$\tau \leq \min\left\{\frac{7}{4}\left(|u| + (1-\kappa)\frac{2\epsilon}{h}\right)^{-1}, \frac{3h}{5|u|}\sqrt{2}\right\} \tag{24}$$

Although, as mentioned before, for very high values of $Pe$ the second restriction may no longer be valid.

6. 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 $\kappa$ 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. $y' = \cos(t)$.






The used code can be found at `https://github.com/thomasschiet/CFD/tree/master/HW3`. N.B. the solution ex. 6 is found in timeintegration.jl