Exercise 4

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1 Steady advaction-diffusion equation

1.a Non-dimensional form of the equation and boundary conditions

Starting from the one-dimensional advection-diffusion equation:

$$\rho \left(\frac{\partial \Phi}{\partial t} + U \frac{\partial \Phi}{\partial x} \right) = \alpha \frac{\partial^2 \Phi}{\partial x \partial x} \tag{1}$$

we derive the non-dimensional form of the equation by introducing the following non-dimensional variables:

$$x^* = \frac{x}{L}, \quad t^* = \frac{t}{T}, \quad \Phi^* = \frac{\Phi}{\Phi_L}$$

where L is a characteristic length, $T = \frac{L}{U}$ is the characteristic advection time, and Φ_L is a characteristic value of the variable Φ .

Then we perform the change of the variable for the deivatives:

$$\frac{\partial}{\partial x} = \frac{1}{L} \frac{\partial}{\partial x^*}, \quad \frac{\partial}{\partial t} = \frac{1}{T} \frac{\partial}{\partial t^*}, \quad \frac{\partial^2}{\partial x \partial x} = \frac{1}{L^2} \frac{\partial^2}{\partial x^{*2}}$$

Now we substitute the relations above into the original equation:

$$\rho\left(\frac{\Phi_L}{T}\frac{\partial\Phi^*}{\partial t^*} + U\frac{\Phi_L}{L}\frac{\partial\Phi^*}{\partial x^*}\right) = \alpha\frac{\Phi_L}{L^2}\frac{\partial^2\Phi^*}{\partial x^{*2}}$$

This equation can be simplified by dividing by Φ_L (assuming the quantity is not zero) and observing that $T = \frac{L}{U}$:

$$\rho\left(\frac{U}{T}\frac{\partial\Phi^*}{\partial t^*} + \frac{U}{L}\frac{\partial\Phi^*}{\partial x^*}\right) = \alpha\frac{1}{L^2}\frac{\partial^2\Phi^*}{\partial x^{*2}}$$

now we multiply for $\frac{L}{\rho U}$ and we get the following equation

$$\frac{\partial \Phi^*}{\partial t^*} + \frac{\partial \Phi^*}{\partial x^*} = \frac{\alpha}{\rho U L} \frac{\partial^2 \Phi^*}{\partial x^{*2}}$$

where we can substitute the Peclet number $Pe = \frac{UL}{\alpha}$ to obtain the non-dimensional form of the equation (1):

$$\frac{\partial \Phi^*}{\partial t^*} + \frac{\partial \Phi^*}{\partial x^*} = \frac{1}{Pe} \frac{\partial^2 \Phi^*}{\partial x^{*2}} \tag{2}$$

Now we repeat the same procedure for the boundary condistions, starting from the dimensional ones:

$$\Phi(0,t) = 0, \quad \Phi(L,t) = \Phi_L \tag{3}$$

and performing the change of variable: x = 0 becomes $x^* = 0$ and x = L becomes $x^* = 1$. Thus, the non-dimensional boundary conditions are:

$$\Phi^*(0, t^*) = 0, \quad \Phi^*(1, t^*) = 1 \tag{4}$$

1.b Analytical solution of the steady non-dimensional equation

The steady non-dimensional equation is obtained by setting the time derivative to zero in (2):

$$Pe\frac{\partial \Phi^*}{\partial x^*} = \frac{\partial^2 \Phi^*}{\partial x^{*2}} \tag{5}$$

which represents a second-order ordinary differential equation. The general solution of this equation is:

$$\Phi^*(x^*) = C_1 e^{\lambda_1 x^*} + C_2 e^{\lambda_2 x^*}$$

where λ_1 and λ_2 are the roots of the characteristic equation, which can be found by substituting $\Phi^*(x^*) = e^{\lambda x^*}$ into the ODE, as follows:

$$\lambda^2 e^{\lambda x^*} = Pe\lambda e^{\lambda x^*} \quad \Rightarrow \quad \lambda^2 = Pe\lambda \quad \Rightarrow \quad \lambda = 0, \lambda = Pe$$

Then we have to find the constants C_1 and C_2 by imposing the boundary conditions (4):

$$\Phi^*(0) = C_1 + C_2 = 0, \quad \Phi^*(1) = C_1 e^0 + C_2 e^{Pe} = 1$$

from which we get:

$$C_1 = -C_2, \quad C_2 = \frac{1}{1 - e^{Pe}}$$

and the final solution is:

$$\Phi^*(x^*) = \frac{e^{x^*Pe} - 1}{e^{Pe} - 1} \tag{6}$$

1.c Discretization of the steady non-dimensional equation

Diffusion term discretization

We discretize the diffusion term with the central finite differencing scheme:

$$\frac{1}{Pe} \frac{\partial^2 \Phi^*}{\partial x^{*2}} \approx \frac{1}{Pe} \frac{\Phi^*_{i+1} - 2\Phi^*_i + \Phi^*_{i-1}}{\Delta x^{*2}}$$
 (7)

Advection term discretization

For the advection term we use different approaches:

• Second-order central differencing:

$$\frac{\partial \Phi^*}{\partial x^*} \approx \frac{\Phi_{i+1}^* - \Phi_{i-1}^*}{2\Delta x^*} \tag{8}$$

• First-order upwind differencing:

$$\frac{\partial \Phi^*}{\partial x^*} \approx \frac{\Phi_i^* - \Phi_{i-1}^*}{\Delta x^*} \tag{9}$$

• Second-order upwind differencing:

$$\frac{\partial \Phi^*}{\partial x^*} \approx \frac{3\Phi_i^* - 4\Phi_{i-1}^* + \Phi_{i-2}^*}{2\Delta x^*} \tag{10}$$

1.d Matrix form of the discretized equation

To obtain the matrix formulations we have to match the discretizations of the the advection term with the one for the diffusion term.

Second-order central differencing for the advection term

$$\frac{1}{Pe} \frac{\Phi_{i+1}^* - 2\Phi_i^* + \Phi_{i-1}^*}{\Delta x^{*2}} = \frac{\Phi_{i+1}^* - \Phi_{i-1}^*}{2\Delta x^*}$$

$$\Phi_{i+1}^* - 2\Phi_i^* + \Phi_{i-1}^* = \frac{Pe\Delta x^*}{2} (\Phi_{i+1}^* - \Phi_{i-1}^*)$$

$$(1 - \frac{Pe\Delta x^*}{2}) \Phi_{i+1}^* - 2\Phi_i^* + (1 + \frac{Pe\Delta x^*}{2}) \Phi_{i-1}^* = 0$$

Then we set the boundary condistions: $\Phi_0 = 0$ and $\Phi_N = 1$ and we obtain the following matrix form:

First-order upwind differencing for the advection term

$$\frac{1}{Pe} \frac{\Phi_{i+1}^* - 2\Phi_i^* + \Phi_{i-1}^*}{\Delta x^{*2}} = \frac{\Phi_i^* - \Phi_{i-1}^*}{\Delta x^*}
\Phi_{i+1}^* - 2\Phi_i^* + \Phi_{i-1}^* = Pe\Delta x^* (\Phi_i^* - \Phi_{i-1}^*)
\Phi_{i+1}^* - (2 + Pe\Delta x^*)\Phi_i^* + (1 + Pe\Delta x^*)\Phi_{i-1}^* = 0$$
(13)

Then we set the boundary condistions: $\Phi_0 = 0$ and $\Phi_N = 1$ and we obtain the following matrix form:

$$\begin{bmatrix} 1 & 0 & & & & & & \\ 1 + Pe\Delta x^* & -(2 + Pe\Delta x^*) & 1 & & & & \\ & 1 + Pe\Delta x^* & -(2 + Pe\Delta x^*) & 1 & & & \\ & & \ddots & & \ddots & & \\ & & & 1 + Pe\Delta x^* & -(2 + Pe\Delta x^*) & 1 \\ & & & & 0 & 1 \end{bmatrix} \begin{bmatrix} \Phi_0 \\ \Phi_1 \\ \vdots \\ \vdots \\ \Phi_{N-1} \\ \Phi_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$
(14)

Second-order upwind differencing for the advection term

$$\frac{1}{Pe} \frac{\Phi_{i+1}^* - 2\Phi_i^* + \Phi_{i-1}^*}{\Delta x^{*2}} = \frac{3\Phi_i^* - 4\Phi_{i-1}^* + \Phi_{i-2}^*}{2\Delta x^*}$$

$$\Phi_{i+1}^* - 2\Phi_i^* + \Phi_{i-1}^* = \frac{Pe\Delta x^*}{2} (3\Phi_i^* - 4\Phi_{i-1}^* + \Phi_{i-2}^*)$$

$$\Phi_{i+1} - (2 + \frac{3}{2}Pe\Delta x^*)\Phi_i + (1 + 2Pe\Delta x^*)\Phi_{i-1} - \frac{Pe}{2}\Delta x^*\Phi_{i-2} = 0$$
(15)

Then we set the boundary condistions: $\Phi_0 = 0$ and $\Phi_N = 1$ and we obtain the following matrix form:

$$\begin{bmatrix} 1 & 0 & & & & & & & \\ 1 + 2Pe\Delta x^* & -(2 + \frac{3}{2}Pe\Delta x^*) & 1 & & & & & \\ -\frac{Pe}{2}\Delta x^* & 1 + 2Pe\Delta x^* & -(2 + \frac{3}{2}Pe\Delta x^*) & 1 & & & & \\ & \ddots & & \ddots & & \ddots & & \\ & & -\frac{Pe}{2}\Delta x^* & 1 + 2Pe\Delta x^* & -(2 + \frac{3}{2}Pe\Delta x^*) & 1 & \\ & & 0 & 1 & \end{bmatrix} \begin{bmatrix} \Phi_0 \\ \Phi_1 \\ \vdots \\ \vdots \\ \Phi_{N-1} \\ \Phi_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$
(16)

2 Numerical solution of the steady advection-diffusion equation

2.a L^2 norm

As suggested by the assignment, to analyze the accuracy of the numerical discretizations described in the previous task, we implemented the three methods and computed the L^2 norm of the error between the analytical solution and the numerical solution. The error was plotted in a log-log scale against Δx , as shown in the convergence plot below.

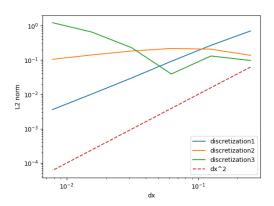


Figure 1: Convergence plot of the L^2 norm of the error

The results show different convergence behaviors for the three methods. The second-order central differencing scheme (Discretization1) shows a trend of second-order accuracy. This can be seen by the fact that the slope of the L^2 norm follows the one of Δx^2 in the log-log plot. This behavior aligns with the theoretical expectation.

In contrast, the first-order upwind differencing method (Discretization 2) shows a much slower convergence: the error remains nearly constant for smaller Δx values. This result may suggest that numerical diffusion dominates the solution, and further grid refinement does not improve accuracy. First-order schemes like upwind differencing are stable but suffer from significant numerical dissipation, especially for advection-dominated problems or at high Peclet numbers.

The second-order upwind method (Discretization 3) displays improved accuracy compared to the first-order upwind method, with the error reducing more significantly as Δx decreases. However, the convergence behavior is less smooth, with some variability observed at intermediate grid sizes. This may result from the interplay between truncation errors and the Peclet number, which affects the balance between advection and diffusion.

2.b Comparison for different Peclet numbers

To further investigate the impact of the Peclet number on the accuracy of the numerical solutions, we repeated the convergence analysis for different values of Pe, as indicated by the assignment.

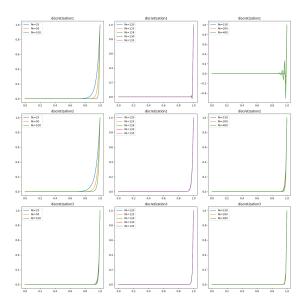


Figure 2: Solutions for different Peclet numbers

From the picture above, we can observe that CDS discretization shows an oscillatory behavior for high Peclet numbers in particular for the region where the solution varies rapidly, while it provides high accuracy in regions where the solution varies smoothly. This behavior may be due to the fact that the CDS is not a suitable method when the advection term is dominant, since it is not capturing the upwind information.

Focusing on the first-order upwind discretization, we can see that the solution is stable for all Peclet numbers, but for small Peclet values it is making the function smoother than it should be, because of the numerical dissipation.

In the end we can see that the second-order upwind discretization is able to capture the correct behavior of the solution, providing a good approximation and stability for all Peclet numbers.

All the three methods are described by sparse matrices, which reflects the local nature of the finite difference approximations, but the second-order upwind scheme, which provides the highest accuracy, requires more memory due to the larger stencil size.

2.c Comparison of the different methods

For advection-dominated problems with medium to high Peclet numbers, the second-order upwind scheme is generally the best choice as it balances stability and accuracy effectively, avoiding any kind of oscillation. For high Peclet values, we can also consider to use the first-order upwind scheme, since it is stable and does not show oscillations, it is also easier to implement and computationally cheaper than the second-order upwind scheme. For problems in which we have a Peclet number close to 1 the CDS scheme is a viable option.

3 Stability of the unsteady advection-diffusion equation

3.a Discretization of of the unsteady one-dimensional advection-diffusion equation

We start with the one-dimensional advection-diffusion equation:

$$\rho\left(\frac{\partial\Phi}{\partial t}+U\frac{\partial\Phi}{\partial x}\right)=\alpha\frac{\partial^2\Phi}{\partial x^2}.$$

We use central finite differencing in space and explicit Euler in time. The terms are discretized as follows:

$$\bullet \ \frac{\partial \Phi}{\partial t} \approx \frac{\Phi_i^{n+1} - \Phi_i^n}{\Delta t}$$

$$\bullet \quad \frac{\partial \Phi}{\partial x} \approx \frac{\Phi_{i+1}^n - \Phi_{i-1}^n}{2\Delta x}$$

$$\bullet \ \frac{\partial^2 \Phi}{\partial x^2} \approx \frac{\Phi_{i+1}^n - 2\Phi_i^n + \Phi_{i-1}^n}{\Delta x^2}$$

Substituting these approximations into the original equation, we get:

$$\rho\left(\frac{\Phi_i^{n+1} - \Phi_i^n}{\Delta t}\right) + \rho U\left(\frac{\Phi_{i+1}^n - \Phi_{i-1}^n}{2\Delta x}\right) = \alpha\left(\frac{\Phi_{i+1}^n - 2\Phi_i^n + \Phi_{i-1}^n}{\Delta x^2}\right).$$

Multiplying through by Δt :

$$\rho\Phi_i^{n+1} - \rho\Phi_i^n + \rho U\Delta t \left(\frac{\Phi_{i+1}^n - \Phi_{i-1}^n}{2\Delta x}\right) = \alpha \Delta t \left(\frac{\Phi_{i+1}^n - 2\Phi_i^n + \Phi_{i-1}^n}{\Delta x^2}\right).$$

Rearranging to isolate Φ_i^{n+1} on the left-hand side:

$$\rho \Phi_i^{n+1} = \rho \Phi_i^n - \rho U \Delta t \left(\frac{\Phi_{i+1}^n - \Phi_{i-1}^n}{2\Delta x} \right) + \alpha \Delta t \left(\frac{\Phi_{i+1}^n - 2\Phi_i^n + \Phi_{i-1}^n}{\Delta x^2} \right).$$

Dividing through by ρ :

$$\Phi_i^{n+1} = \Phi_i^n - c \left(\frac{\Phi_{i+1}^n - \Phi_{i-1}^n}{2} \right) + d \left(\Phi_{i+1}^n - 2\Phi_i^n + \Phi_{i-1}^n \right), \tag{17}$$

where:

$$c = \frac{U\Delta t}{\Delta x}, \quad d = \frac{\alpha \Delta t}{\rho (\Delta x)^2}.$$

The parameter c represents the Courant number and quantifies the influence of advection in the simulation. For stability and accuracy in explicit schemes, c should typically be small to satisfy the Courant-Friedrichs-Lewy condition that requires $c \le 1$. If c is too large, the simulation may become unstable or inaccurate because the flow travels across more than one grid cell per time step. The parameter d measures the contribution of diffusion to the simulation and it should typically be small to ensure numerical stability. The diffusion stability condition generally requires $d \le 1/2$ to ensure that diffusion does not dominate excessively or destabilize the solution.

3.b Stability Analysis Using Von Neumann Method

Given the discretized convection-diffusion equation (17), we can perform a Von Neumann stability analysis to determine the stability conditions for the explicit scheme.

This is made possible due to the linear nature of such equation and by not considering the imact of boundary conditions. We will consider the domain as periodic in x, allowing the solution and the error to be expressed using a Fourier series with a period of length 2L.

Assuming a disturbance of the form:

$$\epsilon(x,t) = V(t)e^{ikx}$$

where $\theta = k\Delta x$ is the phase angle.

We can insert the error function epsilon(x,t) into the discretized differential equation and estimate the temporal behaviour of the amplitude by evaluation the amplification factor G. This can be directly applied to the solution, by exploiting the linearity of the equation so that:

$$\phi_i^n = V^n e^{I\theta i}, \quad \phi_{i+1}^n = V^n e^{I\theta(i+1)}, \quad \phi_{i-1}^n = V^n e^{I\theta(i-1)}.$$

Substituting into the discretized equation:

$$V^{n+1} = V^n \left(1 - \frac{c}{2} (e^{I\theta} - e^{-I\theta}) + d(e^{I\theta} - 2 + e^{-I\theta}) \right).$$

By considering the Euler relation $e^{I\theta} = \cos \theta + I \sin \theta$, we can simplify the equation to:

$$V^{n+1} = V^n \left(1 - Ic\sin\theta + 2d(\cos\theta - 1) \right).$$

The amplification factor G, which can be computed for subsequent steps, is the following:

$$G = 1 - ic\sin\theta + 2d(\cos\theta - 1).$$

To obtain stability, by remembering that the amplification factor should damp the error to obtain stability, we require that the absolute value of G is less than or equal to 1:

$$|G| \leq 1$$
.

We then compute $|G|^2$ to find the stability condition on the real domain:

$$|G|^2 = (1 + 2d(\cos\theta - 1))^2 + (c\sin\theta)^2.$$

For stability, we need to find the values of c and d that satisfy the condition:

$$|G|^2 < 1.$$

We can solve this with variable substitution and trigonometric identities to find the stability condition for the explicit scheme. We get the following disequation:

$$t^{2}(1 - \frac{c^{2}}{4d^{2}}) + t(\frac{1}{d} - 2) + 1(1 - \frac{1}{d} + \frac{c^{2}}{4d^{2}}) \le 0.,$$

where $t = \cos \theta$.

We can thus solve it by applying the general quadratic formula to find the stability condition:

$$\frac{\frac{1}{d} - 2 - \sqrt{(\frac{1}{d} - 2)^2 - 4(1 - \frac{c^2}{4d^2})(1 - \frac{1}{d} - \frac{c^2}{4d^2})}}{2(1 - \frac{c^2}{4d^2})} \le t \tag{18}$$

$$t \le \frac{\frac{1}{d} - 2 + \sqrt{(\frac{1}{d} - 2)^2 - 4(1 - \frac{c^2}{4d^2})(1 - \frac{1}{d} - \frac{c^2}{4d^2})}}{2(1 - \frac{c^2}{4d^2})}$$
(19)

We can now substitute the values of c and d to find the stability condition for the explicit scheme. We recall that $c=\frac{U\Delta t}{\Delta x}$ and $d=\frac{\alpha \Delta t}{\rho(\Delta x)^2}$. By substituting this in the disequation we get:

$$\frac{\frac{\alpha\Delta t}{\rho(\Delta x)^2} - 2 - \sqrt{\left(\frac{\alpha\Delta t}{\rho(\Delta x)^2} - 2\right)^2 - 4\left(1 - \frac{U^2\Delta t^2}{4\alpha\Delta x^2}\right)\left(1 - \frac{\alpha\Delta t}{\rho(\Delta x)^2} - \frac{U^2\Delta t^2}{4\alpha\Delta x^2}\right)}}{2\left(1 - \frac{U^2\Delta t^2}{4\alpha\Delta x^2}\right)} \le t$$
(20)

$$t \le \frac{\frac{\alpha \Delta t}{\rho(\Delta x)^2} - 2 + \sqrt{\left(\frac{\alpha \Delta t}{\rho(\Delta x)^2} - 2\right)^2 - 4\left(1 - \frac{U^2 \Delta t^2}{4\alpha \Delta x^2}\right)\left(1 - \frac{\alpha \Delta t}{\rho(\Delta x)^2} - \frac{U^2 \Delta t^2}{4\alpha \Delta x^2}\right)}}{2\left(1 - \frac{U^2 \Delta t^2}{4\alpha \Delta x^2}\right)}$$
(21)

Given the complexity of the disequation, it is beneficial to analyze the two extreme cases: $\theta = 0$ and $\theta = \pi$.

1. Case 1: $\theta = \pi$ (Maximum Frequency)

At $\theta = \pi$, we have:

$$\cos \pi = -1, \quad \sin \pi = 0.$$

Substitute into the expression for G:

$$G = 1 + 2d(-1 - 1) = 1 - 4d$$
.

The magnitude is:

$$|G|^2 = (1 - 4d)^2.$$

For instability, we need:

$$\left(1 - 4d\right)^2 > 1.$$

Taking the square root:

$$|1 - 4d| > 1$$
.

This gives two conditions:

$$1 - 4d > 1$$
 or $1 - 4d < -1$.

Solving these inequalities:

- (a) $1 4d > 1 \implies d < 0$ (not physically meaningful),
- (b) $1 4d < -1 \implies d > \frac{1}{2}$.

Thus, instability occurs at $\theta = \pi$ when $d > \frac{1}{2}$. Substituting $d = \frac{\alpha \Delta t}{\rho(\Delta x)^2}$ into the instability condition $d > \frac{1}{2}$:

$$\frac{\alpha \Delta t}{\rho(\Delta x)^2} > \frac{1}{2}.$$

Rearranging to find the relationship between Δx and Δt :

$$\Delta t < \frac{\rho(\Delta x)^2}{2\alpha}.$$

This inequality provides the stability condition for the explicit scheme in terms of the time step Δt and the spatial step Δx . For the scheme to be stable, the time step must be sufficiently small relative to the square of the spatial step.

2. Case 2: $\theta \approx 0$ (Low Frequencies)

For small θ , we use the Taylor expansions:

$$\sin \theta \approx \theta, \quad \cos \theta \approx 1 - \frac{\theta^2}{2}.$$

Substitute into the expression for G:

$$G \approx 1 - d\theta^2 - ic\theta$$
.

Compute $|G|^2$:

$$|G|^2 \approx (1 - d\theta^2)^2 + (c\theta)^2.$$

Neglecting terms of order θ^4 , we get:

$$|G|^2 \approx 1 - 2d\theta^2 + c^2\theta^2.$$

For instability, we need:

$$1 - 2d\theta^2 + c^2\theta^2 > 1.$$

Canceling the 1:

$$-2d\theta^2 + c^2\theta^2 > 0,$$

or:

$$(c^2 - 2d)\theta^2 > 0.$$

For instability, this implies:

$$c^2 > 2d$$
.

Substituting $c = \frac{U\Delta t}{\Delta x}$ and $d = \frac{\alpha \Delta t}{\rho(\Delta x)^2}$ into the instability condition $c^2 > 2d$:

$$\left(\frac{U\Delta t}{\Delta x}\right)^2 > 2\left(\frac{\alpha \Delta t}{\rho(\Delta x)^2}\right).$$

Simplifying:

$$\frac{U^2(\Delta t)^2}{(\Delta x)^2} > \frac{2\alpha \Delta t}{\rho(\Delta x)^2}.$$

Multiplying both sides by $(\Delta x)^2$:

$$U^2(\Delta t)^2 > \frac{2\alpha \Delta t}{\rho}.$$

Dividing both sides by Δt :

$$U^2 \Delta t > \frac{2\alpha}{\rho}.$$

Rearranging to find the relationship between Δx and Δt :

$$\Delta t < \frac{2\alpha}{\rho U^2}.$$

Thus, the stability condition for the explicit scheme, considering both advection and diffusion, is:

$$\Delta t < \min\left(\frac{\rho(\Delta x)^2}{2\alpha}, \frac{2\alpha}{\rho U^2}\right).$$

4 Stability region

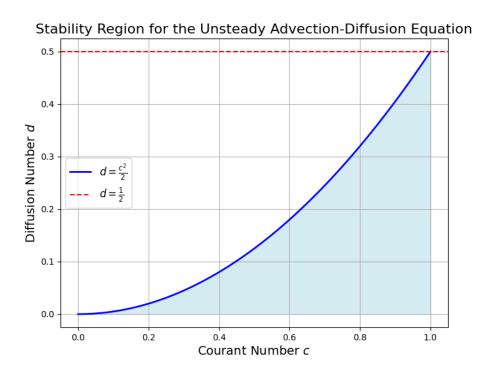


Figure 3: Stability region for the explicit scheme.

References

[1] CFD Repository, Available at: https://github.com/GiuseppePisante/CFD.git

[2] GitHub Copilot, GitHub. Available at: https://github.com/features/copilot