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Exercise Number 11

Topic: **Models with Distributed Parameters – numerical flow simulation with FDM**

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Introduction

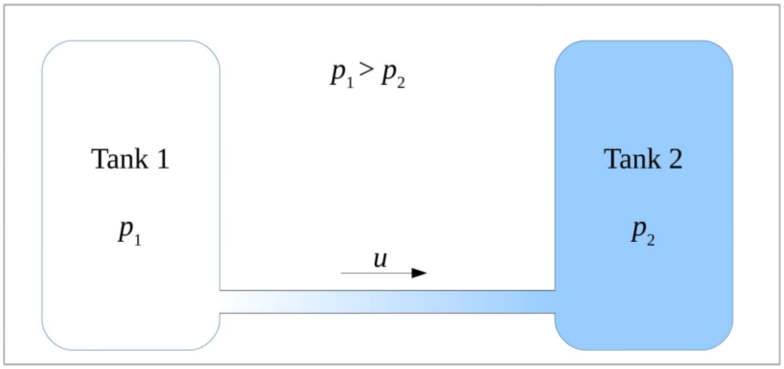
In this exercise, students are introduced to the process of formulating model equations, especially the derivatives, in a way that is applicable with numerical solvers. For that, model equations are discretized by use of the finite difference method (FDM). In a first step, ready-made Matlab codes are to be completed using derivatives that have been presented in the lecture and have been obtained during preceding exercises, respectively. In a second step, students have to evaluate accuracy and stability of the method depending on spatial and temporal discretization by means of parameter variations. This study can efficiently be conducted based on a one-dimensional test case in exercise 1. Exercise 2 demonstrates the significant increase of computational effort when extending the model from one to two dimensions. This is due to an increasing number of mathematical operations to be done, but also due to an intensified dependency on geometrical resolution. The exercises offer an opportunity to gain first-hand experience on how quickly a simulation model can be implemented and on how many parameters have effects on the results.

Exercise 1

1D test case: convection/diffusion equation

The main focus of this exercise is the investigation of the stability limits of the so-called upwind-scheme (UDS) and the central-difference scheme (CDS). In order to enable exact comparison of the quality of numerical solutions, a test case has been selected that also allows for analytical solution. Your objective is to achieve low computation time and reasonably accurate results at the same time.

Under investigation is a one-dimensional flow with a convection (u) in positive x-direction, with a substance of concentration $\phi = 1$ at position $x = L$ and of concentration $\phi = 0$ at position $x = 0$ (Dirichlet boundary conditions for ϕ).
This situation can occur when two containers are connected by a pipe. The length of the pipe is L. If the pressure in container 1 is larger than that in container 2, the fluid will flow from container 1 into container 2. If any substance has been added to the fluid in container 2, but not in container 1, diffusion of that substance will take place from container 2 into container 1.
Imagine a technical problem where the diameter of the connecting pipe and the required pressures inside of the containers (and thus the velocity of the fluid inside the pipe) is to be defined so that none of the substance from container 2 shall get into container 1. As a constraint, the mass flow rate in the connecting pipe shall not be too high, so that only a limited amount of fluid can flow from container 1 into container 2.



The concentration of the substance in the fluid can be described by the following equation:

$$\frac{\partial(\rho u \phi)}{\partial x} = \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right). \tag{1}$$

The exact solution to the problem is:

$$\phi = \frac{e^{x\mathrm{Pe}} - 1}{e^{\mathrm{Pe}} - 1}. \tag{2}$$

with Pe as the Peclet number, which equals the ratio of convective to diffusive forces:

$$\mathrm{Pe} = \frac{\rho u L}{\Gamma}, \tag{3}$$

where Γ is the diffusion coefficient. Throughout this exercise, L = 1 m.

1. Implement the spatial derivatives into the function `MuS_FDM_1d_en.m`:
   - the **first derivative** with backwards-difference scheme (UDS means 'upwind', but in this case the direction of the convection is given, and only the backward variant is to be used) and central-difference scheme (CDS). Please use the variables `phi_uds` and `phi_cds`!
   - the **second derivative** with central-difference scheme (CDS). As the solution variables differ depending on the value of ϕ calculated with UDS and CDS, the identical formulations for `phi_uds` and `phi_cds` have to be implemented.
2. The solutions is to be obtained iteratively. The time-dependent term is to be added to the equation stated above. As the solution converges, this term approaches zero:

$$\frac{\partial \phi}{\partial t} + \frac{\partial(\rho u \phi)}{\partial x} = \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right). \tag{4}$$

   Implement the explicit Euler scheme at the marked position in the file `MuS_FDM_1d_en.m`. Note that you can instantaneously overwrite the previous value with the new value of the variable ϕ at the spatial position i!
3. If a long time step is selected for the solver, the steady state can be reached faster, but the solution can become unstable. The explicit Euler scheme is conditionally stable. The characteristic

diffusion time (D) and the characteristic convection time (CFL, Courant-Friedrichs-Lewy) have to be considered when determining the time step:

$$\mathrm{D} = \frac{\Gamma dt}{\rho (dx)^2} \ \text{ and } \ \mathrm{CFL} = \frac{u}{dx} dt\,. \tag{5}$$

In the code, both numbers are added and calculated as a so-called DCFL variable. This number can serve as a figure of merit when investigating the stability of the computational scheme.

Obtain the roughly highest possible stable time step for the following set of parameters:

- nx=11; Pe=2 with rho=1 *kg/m³*; u0=2 *m/s*; gamma=1 *kg/ms*;
- nx=11; Pe=2 with rho=1 *kg/m³*; u0=20 *m/s*; gamma=10 *kg/ms*;
- nx=11; Pe=40 with rho=1 *kg/m³*; u0=4 *m/s*; gamma=0.1 *kg/ms*;
- nx=31; Pe=40 with rho=1 *kg/m³*; u0=4 *m/s*; gamma=0.1 *kg/ms*;

Please state your observations!

Important Note

When varying the time step, take the maximum number of time steps and the computational time into account!
If the maximum number of time steps is set too low, the steady state might not be reached in the computation. If set it too high, the duration of the simulation might get too long. Make sure the solver has reached the steady state before considering the output as the solution!

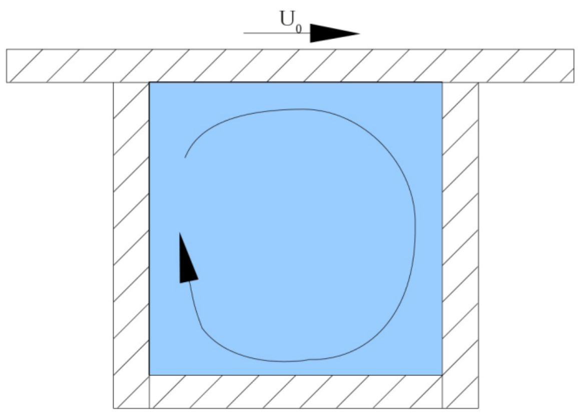
Comprehension questions

- How would you distribute the grid nodes for higher Peclet numbers?
- Why is the stability limit at larger time step for CDS and at lower one for UDS?
- Would you use a different initialization? For which Peclet numbers is this better?
- Which spatial resolution gives a reasonable accurate solution for Pe=40 for UDS, and which one for CDS?

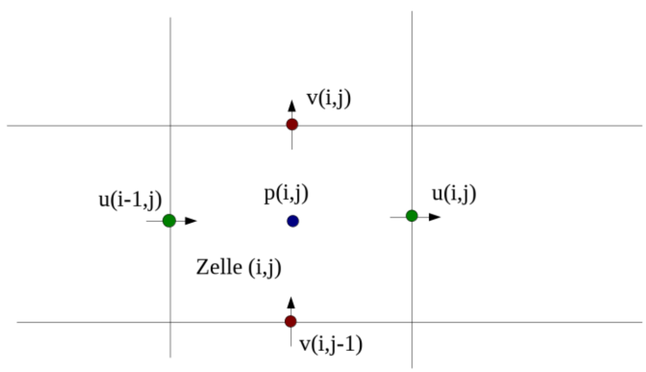
Exercise 2 (optional)

2D test case: lid-driven cavity flow

In this example, a flow that is confined by four walls is to be simulated. The flow is driven by a wall moving at constant velocity through in its plane. This test case has long been used as a test or validation case for new codes or new solution methods.



Background to the implemented numerical scheme
In order to prevent an oscillating solution of the finite difference scheme, a staggered arrangement of the variables is used in this case. The velocities are stored at the cell boundaries, whereas the pressure in the center of the cells. The derivation of the velocities is done with central-differences at the center of the cells, which is why you will find only expressions of u(i) - u(i-1) instead of u(i+1) - u(i-1).



The convective terms are discretized with a combination of central-differences and a modified upwind scheme to increase numerical stability.
The effect of the weighting coefficient gamma is stated in the code.

- Read the function `MuS_FDM_2d_en.m` and try to identify the relevant derivatives!
- Compare length and complexity of the code with the one of Exercise 1.
- Vary the wall velocity, the time step, the spatial discretization, the density, the viscosity, and gamma!
- Compare the duration to complete a simulation to the one of the 1D test case above.
- Are flows with lower of higher Reynolds number more or less complicated to simulate?