EXERCISE WEEK 4:
PRACTICAL COURSE
MODELING, SIMULATION, OPTIMIZATION

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We consider the water tank in Figure 1 of $L_x = 0.3$ [m] by $L_y = 0.5$ [m] by $H = 0.1$ [m]. The water tank contains an inlet at the area

$$A_{\text{in}} = \{0\} \times [0.7L_y, 0.9L_y] \times [0, H],$$

and an outlet at the area

$$A_{\text{out}} = [0.5L_x, 0.8L_x] \times \{0\} \times [0, H].$$

At time $t = 0$, the water tank contains a certain distribution of Chlorine. We want to compute how this distribution evolves due to the combined effects of 1) diffusion and 2) the advective transport due to the flow of the water. We use a two-dimensional model in which the Chlorine density $\rho = \rho(t, x, y)$ [mg/l] and the velocity field for the water in the tank $\mathbf{v} = [v_x(x, y), v_y(x, y)]^\top$ [m/s] do not depend on the z-coordinate.

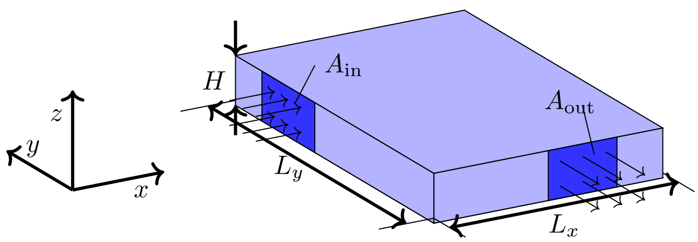

FIGURE 1. The considered water tank

The velocity field $\mathbf{v}(x, y)$ is given. The (two components of the) velocity field $\mathbf{v}(x, y) = [v_x(x, y), v_y(x, y)]^\top$ are zero on the boundary except at the inlet and outlet. We focus only on the computation of the mass density $\rho = \rho(t, x, y)$. Chlorine does not enter the tank through the inlet and the outlet. We therefore assume that $\rho(t, x, y)$ is zero at the inlet and outlet. The initial condition is

$$\rho(0, x, y) = c_0 \exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{a^2}\right)$$

where $c_0 = 10$ [mg/l], $x_0 = 0.1L_x$ [m], $y_0 = 0.7L_y$ [m], and $a = 0.03L_y$ [m]. The diffusivity of Chlorine in water is given by $\kappa = 1.25 \cdot 10^{-5}$ [m^2/s].

a. (3pts) Write down the initial value problem for the mass density of Chlorine $\rho(t, x, y)$ in the water tank. Do not use the unit normal $\mathbf{n}$ in the boundary conditions. Hint: Except for the inlet and outlet, the mass flux of Chlorine must be zero at the boundary.

b. (5pts) Simulate the evolution of the mass density of Chlorine $\rho(t, x, y)$ during the time interval $[0, T_{\text{sim}}]$, where $T_{\text{sim}} = 8$ [minutes] (= 480 [s]), by completing the missing parts in the file `Week4_exercise`. The following observations might be helpful:
   i. Note that the spatial grid and the velocity field in the grid points are given in the file `Week4_velocity_field.mat`.
   ii. Because the given velocity field is position dependent, you could use the chain rule and the fact that the given velocity field is divergence free (i.e. $\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0$) to find the equations for the spatial discretization by finite differences, but there are other correct solutions possible.
   iii. You can use any time-discretization scheme you want, but recall that the Forward Euler scheme can be unstable.

c. (2pts) What happens when you make the velocity field four times larger? Can you spot any strange effects in the simulation?
Hint: Can you estimate the mesh Péclet number?