Assignment 4

Modeling atmospheric pollution with the Finite-Element Method

Numerical Analysis For PDE's (WI4014TU)

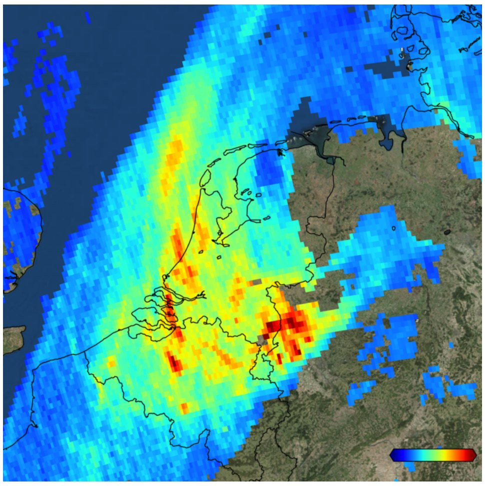

Figure 1: TROPOMI image of the atmospheric pollution above the Netherlands. The TROPOspheric Monitoring Instrument (TROPOMI) is an instrument on board the Copernicus Sentinel-5 Precursor satellite, launched on 13 October 2017. It provides daily data with 5 km spatial resolution about various pollutants: aerosoles, carbon monoxide, formaldehyde, methane, nitrogen dioxide, ozone, and sulfur dioxide.

We want to model the spread of a polluting gas, such as NO_2, in the atmosphere, see Figure 1 for an illustration. The computational domain Ω is a $(L_x \times L_y)$ rectangle with the lower-left corner at (x_c, y_c). The time interval of interest is $t \in [0, T]$. The gas is emitted by two localized sources. The emission rate density is given by the function:

$$f(x,y,t) = \begin{cases} 0, & t < 0; \\ \sum_{i=1}^{2} A \exp\left(-\alpha(x-x_i)^2 - \alpha(y-y_i)^2\right), & t \geq 0. \end{cases} \tag{1}$$

The horizontal transport of the pollutant $u(x,y,t)$ in the atmosphere is described by the advection-diffusion equation:

$$\frac{\partial u}{\partial t} - D\Delta u + \nabla \cdot (u\mathbf{w}) = f, \quad t > 0, \quad (x, y) \in \Omega, \tag{2}$$

where D is the effective diffusivity characterizing the (approximately) diffusive transport of gas caused by the atmospheric turbulence, and $\mathbf{w}(x, y, t) = \langle w_x, w_y \rangle$ is the vector field of the mean wind velocity with its components given by:

$$\begin{aligned} w_x(x, y, t) &= B - \frac{y}{\sqrt{x^2 + y^2}}, \quad t \geq 0, \\ w_y(x, y, t) &= \frac{x}{\sqrt{x^2 + y^2}}, \quad t \geq 0, \end{aligned} \tag{3}$$

where B is a constant. We assume that no pollutant was present in Ω prior to the emission by the sources.

1. Formulation of the problem and its weak form

   (a) Is this compressible or incompressible flow? To find out, calculate $\nabla \cdot \mathbf{w}$ (show intermediate steps) and simplify the third term of the equation (2), if possible.

   (b) Assuming that the concentration of pollutant at the boundary of Ω is zero at all times, write down, in formal mathematical terms, the *boundary value problem* to be solved.

   (c) Apply the Backward-Euler time integration method to your PDE, writing down the recurrence relation. State the mathematical properties of the chosen time integration method (without proofs).

   (d) Derive the standard weak form of the Galerkin Finite-Element Method for your time-discretized problem, showing intermediate steps. Clearly indicate the bi-linear and linear forms. Define the solution and test function-spaces.

   (e) Briefly discuss what stability and other numerical issues can be expected when solving these types of problems, and how you intend to deal with these issues.

2. Implementation in FEniCSx and numerical experiments.

   (a) The FEniCSx code structure for this is provided in the file `Assignment4-code-strycture.py`. Some of the code parts have been written explicitly, others are missing. Finish the code by implementing the missing parts. You can use the tutorial at `https://jsdokken.com/dolfinx-tutorial/chapter2/heat_equation.html`

variable	value
L_x	6
L_y	6
T	5
A	5
B	1.5
α	10
(x_c, y_c)	$(-3, -3)$
(x_1, y_1)	$(-2.4, 0)$
(x_2, y_2)	$(0, 1)$
(x_t, y_t)	$(0, -1)$
D	0.0025

Table 1: Problem parameters.

(b) Set the problem parameters as in Table 1 and run the code with `nt = 10` and `nx = 51`, `ny = 51`. Insert the figure with the calculated $u(x, y, T)$ in your report and discuss it.

(c) Refine the spatial discretization by changing `nx` and `ny` until you are satisfied with the calculated result. Due to the mathematical structure of the wind function, you should work with `nx = 51, 61, 71, ...` etc. Insert the figure of $u(x, y, T)$ at the final appropriate spatial resolution and explain what criterion did you use to settle on these values of `nx` and `ny`.

(d) Calculate the numerical approximation of $u(x, y, T)$ at the appropriate spatial resolution and with the time discretization set as `nt = 10, 12, 15, 20, 50, 100,` recording the value of $u(x, y, T)$ obtained with different `nt` at the point (x_t, y_t), see Table 1, using the provided function `get_value()` for this purpose. Plot the value of the solution $u(x_t, y_t, T)$ as a function of `nt` and discuss it. What is a practical value of `nt` that can be used in this case?

(e) Set $B = 0.5$ and run the code with the appropriate spatial resolution established in the previous steps and with `nt = 50`. Insert the figure of the calculated $u(x, y, T)$ in your report. Find a simple and visual way to explain the difference between the $B = 1.5$ and $B = 0.5$ cases.