Numerical Analysis [WI4014TU]
Assignment 3

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We want to model the spread of a polluting gas, such as NO_2, in the atmosphere. 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:

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

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.

Solution:

$$\begin{aligned}
\nabla \cdot \mathbf{w} &= \left\langle \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right\rangle \cdot \langle w_x, w_y \rangle \\
&= \frac{\partial w_x}{\partial x} + \frac{\partial w_y}{\partial y} \\
&= \frac{\partial}{\partial x}\left[B - \frac{y}{\sqrt{x^2+y^2}}\right] + \frac{\partial}{\partial y}\left[\frac{x}{\sqrt{x^2+y^2}}\right] \\
&= -y\left[\frac{-1}{2}\frac{1}{\sqrt{(x^2+y^2)^3}}2x\right] + x\left[\frac{-1}{2}\frac{1}{\sqrt{(x^2+y^2)^3}}2y\right] \\
&= -\frac{xy}{\sqrt{(x^2+y^2)^3}} + \frac{xy}{\sqrt{(x^2+y^2)^3}} \\
&= 0
\end{aligned}$$

$\because \nabla \cdot \mathbf{w} = 0$ therefore, the flow is incompressible.
Now, for the third term of the equation;

$$\begin{aligned}
\nabla \cdot (u\mathbf{w}) &= u \cdot \nabla\mathbf{w} + \mathbf{w} \cdot \nabla u \\
&= \mathbf{w} \cdot \nabla u \qquad [\because \nabla \mathbf{w} = 0]
\end{aligned}$$

   (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.

Solution: The boundary value problem to be solved is:

$$\frac{\partial u}{\partial t} - D\Delta u + \mathbf{w} \cdot \nabla u = f, \quad t > 0, \quad (x, y) \in \Omega \tag{4}$$

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

Boundary condition(s):

$$u(x, y, t) = 0, \qquad (x, y) \in \partial\Omega, \qquad t \geq 0 \tag{5}$$

and, Initial condition:

$$u(x, y, 0) = 0, \qquad (x, y) \in \Omega, \qquad t \geq 0 \tag{6}$$

(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).

Solution: Applying Backward Euler Time Integration to the equation (4):

$$\begin{aligned}
&\implies \frac{\partial u}{\partial t} = f + D\Delta u - \mathbf{w} \cdot \nabla u \\
&\implies u(x, y, t_{k+1}) = u(x, y, t_k) + h[f(x, y, t_{k+1}) + D\Delta u(x, y, t_{k+1}) \\
&\qquad\qquad - \mathbf{w}(x, y, t_{k+1}) \cdot \nabla u(x, y, t_{k+1})] \\
&\implies u^{k+1} = u^k + h(f^{k+1} + D\Delta u^{k+1} - \mathbf{w}^{k+1} \cdot \nabla u^{k+1})
\end{aligned}$$

Recurrence relation dictates that once u^{k+1} or $u(t_k + h)$ is found, $u^{k+2} = u(t_k + h + h)$ can be obtained using by iterating over the same procedure.

Properties of the Backwards Euler Time Integration method:

- It is an implicit method
- It is convergent and locally of order $\mathcal{O}(h^2)$ and globally $\mathcal{O}(h)$
- It is unconditionally stable for any $h > 0$

(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.

Solution: Time discretised FEM equation is given by:

$$u^{k+1} - u^k - h(f^{k+1} + D\Delta u^{k+1} - \mathbf{w}^{k+1} \cdot \nabla u^{k+1}) = 0$$

$$\text{B.C:} \qquad u(x, y, t) = 0, \qquad (x, y) \in \partial\Omega$$

Step 1: Introduce 2 function spaces:
Solution space: $U(\Omega) : \{\text{'smooth' } u | u(x, y, t) = 0 \forall (x, y) \in \partial\Omega\}$
Test space: $V(\Omega) : \{\text{'smooth' } v | v(x, y, t) = 0 \forall (x, y) \in \partial\Omega\}$

Step 2: Apply du-Bois Reymond Lemma to find $u \in U(\Omega)$ such that:

$$\int_\Omega \left[u^{k+1} - u^k - h(f^{k+1} + D\Delta u^{k+1} - \mathbf{w}^{k+1} \cdot \nabla u^{k+1})\right] v d\Omega = 0 \tag{7}$$

Step 3: Reduce order of the highest order partial derivative, i.e. reduce the order of;

$$\int_\Omega -hD\Delta u^{k+1} v d\Omega = -hD \int_\Omega \Delta u^{k+1} v d\Omega$$

Now,

$$\begin{aligned} \nabla(\nabla u v) &= \nabla \cdot \nabla u v + \nabla u \nabla v \\ &= \Delta u v + \nabla u \nabla v \\ \implies \Delta u v &= \nabla(\nabla u v) - \nabla u \nabla v \end{aligned}$$

Using this result, we get;

$$\begin{aligned} -hD \int_\Omega \Delta u^{k+1} v d\Omega &= -hD \int_\Omega \nabla(\nabla u^{k+1} v) d\Omega + hD \int_\Omega \nabla u^{k+1} \nabla v d\Omega \\ &\text{using Green's Theorem:} \\ &= -hD \int_{\partial\Omega} (\nabla u^{k+1} v) \cdot \mathbf{n} d\Gamma + hD \int_\Omega \nabla u^{k+1} \nabla v d\Omega \\ &\text{since } v = 0 \text{ on } \partial\Omega \\ \implies -hD \int_\Omega \Delta u^{k+1} v d\Omega &= hD \int_\Omega \nabla u^{k+1} \nabla v d\Omega \end{aligned}$$

Substituting this result into equation (7), and separating the known and unknown terms, we get;

$$\int_\Omega \left[u^{k+1} v + hD\nabla u^{k+1} \nabla v - h\mathbf{w}^{k+1} \cdot \nabla u^{k+1} v\right] d\Omega = \int_\Omega (u^k + hf^{k+1}) v d\Omega \tag{8}$$

The LHS of equation (8) is a bilinear since it is linear in u and v separately. The RHS of this equation is linear in v.

(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.

Solution: The program employs Backward Euler Time Integration and therefore should be stable for any time-step $h > 0$. Spatial discretisation could be a source of numerical errors which can be dealt with by increasing the number of cells in $x-$ and $y-$ direction.

2. Implementation in FEniCSx and numerical experiments.

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.

(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.

Solution:

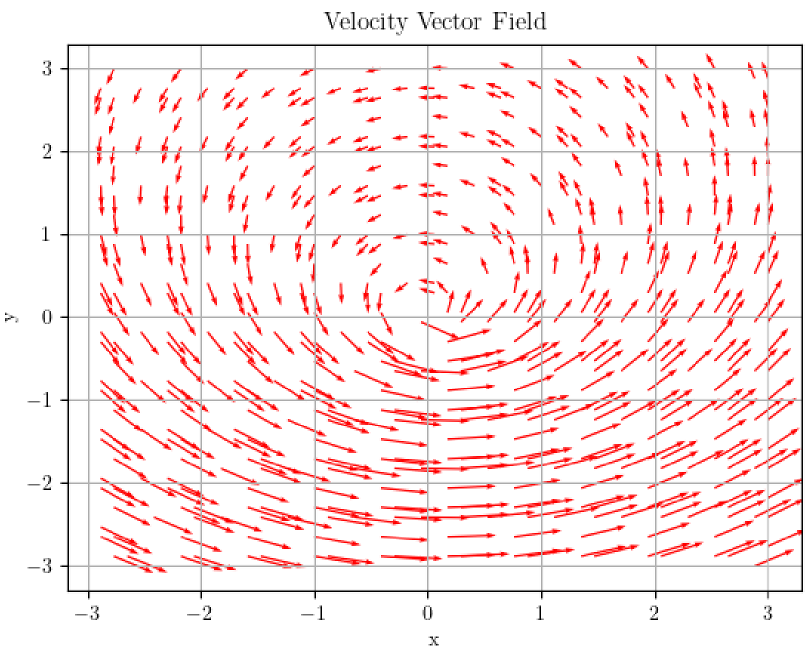

Figure 1: Plot of velocity vector $\mathbf{w}$ at nx = 51 and ny = 51

Missing parts of the code is completed– assigning values to variable, defining source function, components of velocity vector, the bi-linear and linear form of the Galerkin method to be solved by the code, and plotting the velocity vector field $\mathbf{w}$. The plot is attached in Figure 1. For better visualisation, only every 5th vector is plotted in the figure.

(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.

Solution:

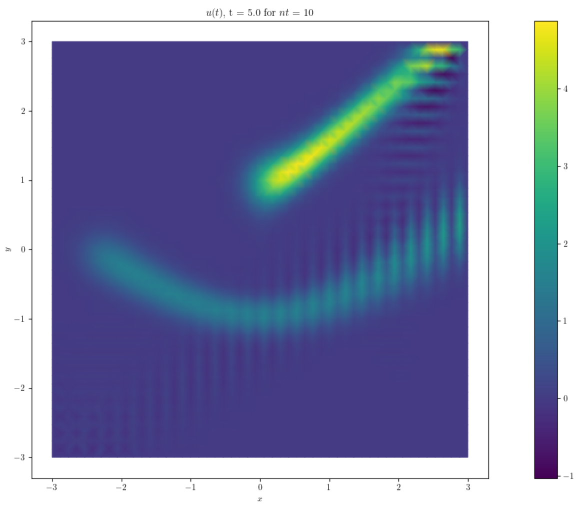

Figure 2: Heat Map of $u(x, y, T)$ at nx = 51, ny = 51 and nt = 10

The heat map of $u(x, y, T)$ given in Figure 2 shows the concentration of the pollutant NO_2 at $T = 5$. The accumulation of numerical errors are clearly seen from the 'fringe' patterns in the domain, which is indicative of dispersive errors.
The column bar displays the lowest concentration of NO_2 in the domain to be negative, i.e. $u(x, y, T) \approx -1$ at some locations. This condition is unrealistic since no sink (or dissipation) terms were incorporated into the mathematical model, moreover, the lowest possible concentration of a pollutant realistically would be $= 0$. Therefore, higher spatial resolution is required to capture the details of the problem.

(c) Refine the spatial discretization by changing `nx` and `ny` until you are satisfied with the calculated result. 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`.

Solution:

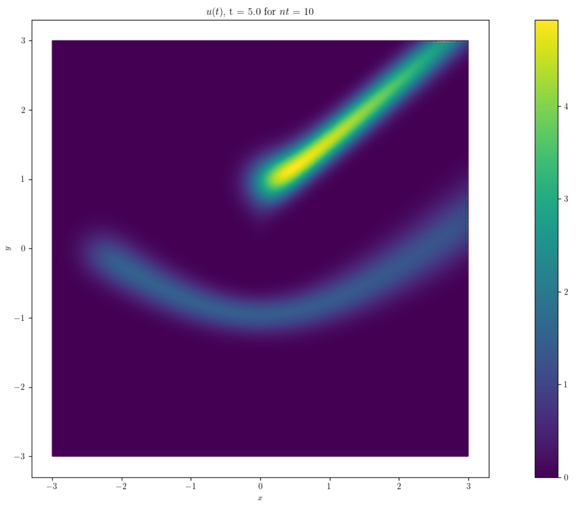

Figure 3: Heat Map of $u(x, y, T)$ at nx = 301, ny = 301 and nt = 10

From Figure 3, we can observe that the numerical errors in the previous case (Figure 2 have largely disappeared– except at locations very close to the boundary of the domain. Solution at grid sizes `nx = nt = 51, 101, 151, 201, 301, 501` was obtained to gauge the change in errors with grid refinement. It was observed that at `nx = 501` (Figure 4), the numerical error did not change and was same as that for `nx = 301`. Therefore a spatial discretisation of `nx = ny = 301` was chosen.

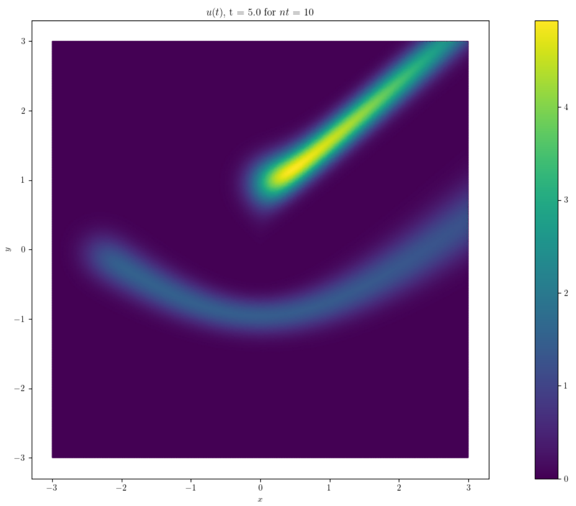

Figure 4: Heat Map of $u(x, y, T)$ at nx = 501, ny = 501 and nt = 10

(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?

Solution:

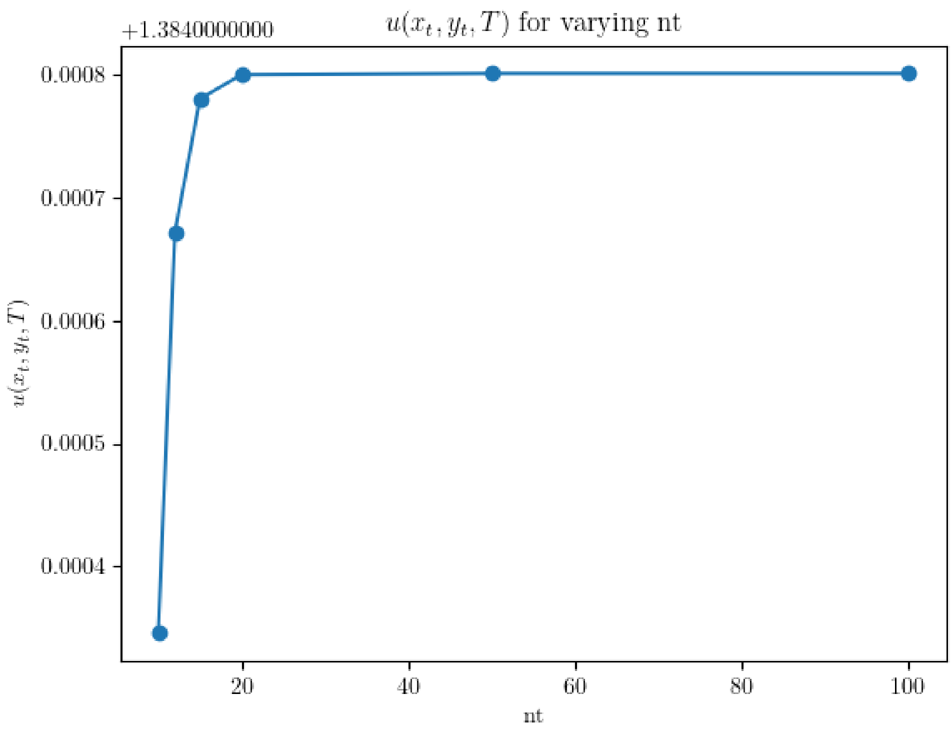

Figure 5: $u(x_t, y_t, T)$ vs nt

From the plot, we can concur that the upper limit of temporal discretisation for this problem statement is at `nt = 20`. For the first three cases, i.e. `nt = 10, 12, 15`, the value of $u(x_t, y_t, T)$ changes significantly until `nt = 20`, following which it stagnates and there is no significant change.

(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.

Solution: The constant B describes the velocity of wind– an important factor to consider in meteorological measurements and especially so in the given problem statement where we model the spread of pollutant in the atmosphere in a certain pre-defined domain. Lower values of B, as in Figure 6, lead to higher concentration of NO_2 in the region, whereas higher values, here $B = 1.5$ in Figure 3, shows how wind could influence the concentration of a pollutant in a certain region and reduces it over time.

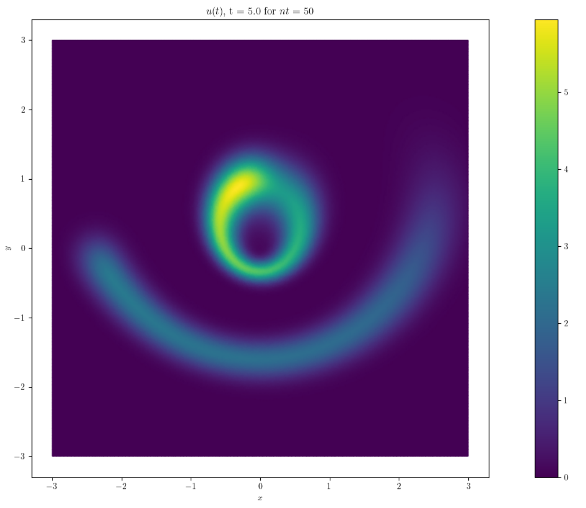

Figure 6: Heat Map of $u(x, y, T)$ at nx = 301, ny = 301 and nt = 10 for $B = 0.5$