Ma323–Finite differences

Project : Analysis of the dispersion of a pollutant and application to river modeling

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Teacher : H. El-Otmany

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Rules : *We remind you that when submitting your project on Moodle you must submit a* ***report written*** *only in.pdf format and the* ***Python programs*** *stored in a folder named PyCode. The report should describe the developments analytical facts and illustrate the results obtained with figures generated by Python. It is not necessary to include screenshots and listings of Python programs in the report. Good luck ! ! !*

1 Motivation and mathematical modeling

For a long time, water pollution in free surface flows has been an important topic of interest to many scientific researchers and mankind in general. Consequently, research conducted on the quality of water and its resources is increasing. They respond to a request expressed by specialists in the protection of the environment and humanity against diseases. These researchers are interested in the quality of the water rather than its quantity. Water quality affects on the use that humans make of it, but the reverse is also true. When we use water, we alter its quality instead of its quantity. This vicious circle indicates that the age-old habit of dumping untreated sewage and chemical wastes directly into rivers, streams, and seas for eventual assimilation into the environment is no longer acceptable in order to avoid environmental degradation.

Natural decomposition processes in water bodies are no longer sufficient to deal with these inputs of pollutants. Technology can be used in many cases to reduce or eliminate substances that can harm the environment. But what happens when contaminants are not removed, even by the most modern water treatment methods ? They may be present in minimal quantity only, however, as they are persistent they can accumulate to produce harmful concentrations. In this case, there is only one way to protect future generations and the whole ecosystem, to prevent chemicals in the water system.

In this perspective, digital water quality models reconstruct different mechanisms present in the environment and provide all necessary information. The importance of the velocity field in the transport of pollution makes it necessary to represent it by a very precise mathematical model which takes into account physical phenomena such as diffusion, advection, dispersion, adsorption, desorption, precipitation, sedimentation, evaporation, etc. which depend both on the nature of the material discharged and on the hydrodynamic characteristics intrinsic to the watercourse. With respect to polluting substances governed almost entirely by the mixing of the fluid, the consideration of turbulence is essential.

Despite the extensive research that has been carried out on the numerical modeling of the dispersion of pollutants in waterways, certain phenomena are still taken into account in a very simplified way.

This project involves studying the evolution of a pollutant first spilled into a river, then into the ocean when the river flows into it. The river and the ocean are two environments subject to currents and we seek to observe the effects on the dispersion of the pollutant. We therefore propose to model the evolution of the concentration of pollutant $u = u(t, x)$ at time t and at position $x \in \mathbb{R}^d$, $d = 1,\ 2$, by a convection-diffusion equation

$$\left\{ \begin{array}{rcl} \dfrac{\partial u}{\partial t} + V \cdot \nabla u - \nu \Delta u & = & f \\ u(0, x) & = & u_0(x) \end{array} \right. \tag{1}$$

where V is the convection speed of the pollutant, representing the speed of the current and which can therefore depend on position and time, ν is its diffusion coefficient, f is the source and u_0 is the initial concentration.

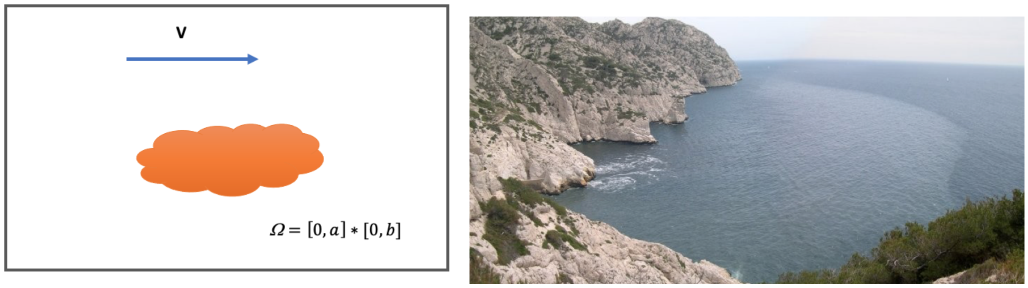

FIGURE 1 – Examples representing the river in the presence of polluting product.

This project is divided into two parts :
The first part deals with the one-dimensional case ($d = 1$) of the flow problem when the pollutant flows in a river modeled in $1D$.
The second part is dedicated to the two-dimensional case ($d = 2$), when the pollutant is discharged at the mouth of the river into an ocean modeled as a medium $2D$.
In order to correctly implement the numerical resolution of the continuous problem (1), we proceed in several steps. First, we focus on the discretization of the Laplacian operator, for which we consider mixed (non)homogeneous Dirichlet/Neumann conditions. After that, we study a discretization by finite difference of the convective-advective term, and finally we finish by looking at the discretization aspects in time.

2 Variation in the concentration of pollutant in the river

This involves simulating the evolution of a pollutant spilled into a watercourse via finite difference diagrams. In order to observe the behavior of different schemes, we first study the convection equation of which we can easily calculate explicit solutions.

2.1 Convection phenomenon in 1D

To better understand this phenomenon, we simplify the problem by neglecting the terms of diffusion and source ($\nu = 0$ and $f = 0$), as well as by considering the constant and positive velocity, $V > 0$. The convection model problem becomes

$$\left\{ \begin{array}{rcl} \dfrac{\partial u}{\partial t} + V\dfrac{\partial u}{\partial x} & = & 0, \forall\, x \in \mathbb{R}, \forall\, t > 0 \\ u(0, x) & = & u_0(x), \forall\, x \in \mathbb{R}. \end{array} \right. \tag{2}$$

Suppose now that the initial condition u_0 is of class $\mathcal{C}^1$ on $\mathbb{R}$. So, we can explicitly solve the equation (2) via the method of characteristics. Indeed, we are looking for a function $X(t)$ such that u is constant along the characteristic curves $t \longmapsto (t, X(t))$. For u solution of (2) we then set $\Phi(t) = u(t, X(t))$.

1. Calculate the derivative of Φ and deduce the shape of the characteristic curves. What can we deduce about the existence and uniqueness of solutions of the model problem ?

In the following, we will therefore be able to compare the exact solutions with numerical solutions obtained by the finite difference method. To solve this continuous problem numerically, we restrict an interval of space $[0,\ a]$ ($a > 0$) and time $[0,\ T]$ ($T > 0$), with an initial support condition in $[0,\ a]$ and we note

— $N > 0$ the number of interior points in space ;
— τ the discretization step in time ;
— $h := \frac{a}{N+1}$ the discretization step in space ;
— $t_n = n\tau$ and $x_i = ih$ the coordinates of the points of the discretization ;
— u_i^n the approximation of the function $u(t_n, x_i)$;
— $U_n = (u_i^n)_{1 \leqslant i \leqslant n}$ the approximate vector $u(t_n, \cdot)$.

We first impose the Dirichlet boundary conditions $u_0^n = u_{N+1}^n = 0$ for all $n \in \mathbb{N}$.

In the following questions, we can perform the numerical applications with : $a = 50,\ T = 5,\ V = 1, \nu = 1,\ h = 0.1,\ \tau = 0.0025$ and the initial condition

$$u_0(x) = f_{x_e,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - x_e)^2}{2\sigma^2}\right)$$

1. Write the centered explicit scheme for the continuous problem (2) and verify that U_{n+1} is given by the recurrence relation
$$U^{n+1} = (I_N - \tau M)U^n, \quad \forall\, n \in \mathbb{N}.$$
Test this numerical scheme with the numerical data and draw an animation of U as a function of time t. Comment on the phenomenon observed.
2. Write the Crank-Nicolson scheme and verify that U^{n+1} is given by
$$\left(I_N + \frac{V\tau}{2} M\right) U^{n+1} = \left(I_N - \frac{V\tau}{2} M\right) U^n, \quad \forall\, n \in \mathbb{N}.$$
Show that this scheme is unconditionally stable in L^2 norm and specify its order. Numerically test this diagram using the numerical data above.
3. Implement a Python function that gives the convergence orders of the upstream offset and Crank-Nicolson schemes. Observe these convergence orders numerically by imposing $\frac{V\tau}{h} = 0.25$.

2.2 Phenomenon of convection-diffusion in $1D$

We are interested in the finite difference approximation of the convection-diffusion equation in $1D$:

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) + V\dfrac{\partial u}{\partial x}(t,x) - \nu\dfrac{\partial^2 u}{\partial x^2}(t,x) = 0, & \forall\, x \in \mathbb{R}, \forall\, t > 0, \\ \\ u(0,x) = u_0(x) & \forall\, x \in \mathbb{R}. \end{cases}$$

Using the same conditions as the previous section, the Crank-Nicolson scheme is written as

$$\frac{u_j^{n+1} - u_j^n}{\tau} + \frac{V}{2}\left(\frac{u_{j+1}^n - u_{j-1}^n}{2h} + \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2h}\right)$$
$$-\frac{\nu}{2}\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} + \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}\right) = 0.$$

1. Write the matrix A for which U^{n+1} can be obtained by the recurrence relation
$$\left(I_N + \frac{V\tau}{2} M - \frac{\nu\tau}{2} A\right) U^{n+1} = \left(I_N - \frac{V\tau}{2} M + \frac{\nu\tau}{2} A\right) U^n$$
for all $n \in \mathbb{N}$.

2. Numerically test the scheme for $\nu = 1$. What do we observe if we resume this simulation with $T = 10$.

3. In some situations, the behavior observed at the output $(x = a)$ is not the expected behavior for a solution set to $\mathbb{R}$. One thus chooses to use in $x = a$ conditions of the homogeneous Neumann type which amount to imposing
$$\frac{u_{N+1} - u_N}{h} = 0$$
Modify the M and A matrices to take into account these new conditions and perform the numerical simulations once these modifications have been made.

4. In order to simulate the action of a factory discharging a pollutant, we assume that the concentration of pollutant at $t = 0$ is zero and we introduce a source term $f(t, x)$.
$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) + V\dfrac{\partial u}{\partial x}(t,x) - \nu\dfrac{\partial^2 u}{\partial x^2}(t,x) = f(t,x), & \forall\, x \in \mathbb{R}, \forall\, t > 0, \\ \\ u(0,x) = 0 & \forall\, x \in \mathbb{R}. \end{cases}$$
Using the discretization $f_j^n = f(t_n, x_j)$ of f, rewrite the Crank-Nicolson scheme of the question to take the term into account and perform the numerical tests for the defined source term by :
$$f(t,x) = f_{x_e,\sigma}(x).$$

5. To simulate the action of a factory dumping the chemical product (orange, see figure 1) and operating only during the day, numerically test the preceding diagram with
$$f(t,x) = \begin{cases} f_{x_e,\sigma}(x) & \text{if } \lfloor t \rfloor \text{ is even },\\ 0 & \text{if } \lfloor t \rfloor \text{ is odd.} \end{cases}$$
Propose an operating time and a pause time so as to ensure that the concentration of $x = a$ does not exceed $\frac{4}{10}$ once steady state is reached.

3 Variation in pollutant concentration in the ocean

As soon as the polluted water of the river reaches the ocean, mathematical modeling in $1D$ is no longer suitable for describing the environment, but we can still neglect the depth of the ocean and study the phenomenon of convection diffusion in $2D$ to understand the evolution of the pollutant concentration. We always seek to use Crank-Nicolson type schemes for their good properties but their implicit character imposes preliminary work on us. In order to understand and correctly implement the resolution of the $2D$ problem, we proceed in several steps. First, we focus on the approximation of the Laplacian operator using mixed Dirichlet/Neumann (non)homogeneous conditions. Then, we discretize the two-dimensional convection-diffusion equation by the finite differences by looking at the discretization aspects in time. Finally, we are interested in the objective of the project which consists in observing the effects of the ocean current on the dispersion, in particular when this one depends on the position like near the mouth of a river.

3.1 Approximation of Laplace's equation

This is to study the spatial approximation via the finite differences of the Laplace equation in 2D on the domain $\Omega =]0,a[\times]0,b[$ with $a = b$ and homogeneous Dirichlet-type boundary conditions :

$$\begin{cases} -\Delta u = f(x,y), & \forall\,(x,y) \in \Omega =]0,a[\times]0,b[, \\ u(x,y) = 0 & \forall\,(x,y) \in \partial\Omega. \end{cases}$$

To solve this equation numerically, we then use

— $h = h_x = h_y$ the step of discretization in space common to the two directions ;

— $N = N_y = N_x = \frac{a}{h} - 1$ the number of interior points in the discretization ;

— $x_i = ih$ et $y_j = jh$ the coordinates of the points of the discretization, $0 \leqslant i,j \leqslant N+1$;

— $u_{i,j}$ the approximation of $u\,(x_i, y_j)$ on point (x_i, y_j) ;

— $f_{i,j} = f\,(x_i, y_j)$ the approximation of f at the discretization points.

1. at y_j fixed, show that

$$-\frac{\partial^2 u}{\partial x^2}\,(x_i, y_j) = \frac{2u\,(x_i, y_j) - u\,(x_{i-1}, y_j) - u\,(x_{i+1}, y_j)}{h^2} + \mathcal{O}\left(h^2\right).$$

   Deduce an approximation to order 2 of $-\frac{\partial^2 u}{\partial x^2}\,(x_i, y_j)$ and of $-\frac{\partial^2 u}{\partial y^2}\,(x_i, y_j)$.

2. Write the finite difference scheme consisting of order 2 at a point (x_i, y_j) not belonging to the boundary.

3. Write the discrete homogeneous Dirichlet conditions on the boundary $\partial\Omega$ and put this scheme in the form $MU = F$ with U the vector of size N^2 which is given by the concatenation of the rows of the matrix $(u_{i,j})_{1 \leqslant i,j \leqslant N}$:

$$U_{(i-1)N+j} = u_{i,j} \text{ pour } 1 \leqslant i,j \leqslant \mathbb{N}.$$

4. Use this system to numerically solve Laplace's equation with a well chosen source term f allowing to compare the numerical resolution and the exact solution for different values of $(n,k) \in \mathbb{N}^*$, the function $u_{n,k}(x,y) = \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{k\pi y}{b}\right)$. Show in particular that the approximation error converges well when you refine your discretization.

5. By introducing on $\Gamma_1 = \{(a,y) \mid y \in [0,b]\}$ of domain Ω the Neumann condition

$$\begin{cases} -\Delta u = & f \text{ in } \Omega, \\ u = & 0 \text{ on } \partial\Omega \setminus \Gamma_1, \\ \dfrac{\partial u}{\partial n} = & 0 \text{ on } \Gamma_1. \end{cases}$$

   Show that we have

$$\frac{\partial u}{\partial x}(a,y) = \frac{4u\,(a-h,y) - u\,(a-2h,y) - 3u(a,y)}{2h} + \mathcal{O}\left(h^2\right).$$

6. Deduce the modification to be made on M to take into account this Neumann condition on Γ_1 and perform numerical simulations to verify your results using the solution $u(x,y) = \sin\left(\frac{\pi y}{b}\right)\left(\cos\left(\frac{\pi x}{a}\right) - 1\right)$.

3.2 Phenomenon of convection-diffusion in $2D$

So far, we can simulate the behavior of the pollutant concentration when it is discharged into the ocean by the river by modeling its evolution by the diffusion reaction equation on a bounded domain $\Omega =]0, a[\times]0, b[$ with $a = b$ and Dirichlet conditions at the boundary :

$$\begin{cases} \dfrac{\partial u}{\partial t} + V^x \dfrac{\partial u}{\partial x} + V^y \dfrac{\partial u}{\partial y} - \nu \dfrac{\partial^2 u}{\partial x^2} - \nu \dfrac{\partial^2 u}{\partial y^2} = 0, & \forall\,(x, y) \in \Omega, \forall\, t > 0, \\ u(0, x, y) = u_0(x, y), & \forall\,(x, y) \in \Omega, \\ u(t, x, y) = 0, & \forall\,(x, y) \in \partial\Omega, \forall\, t > 0. \end{cases} \tag{3}$$

To write the finite difference method, we introduce the following notations :

— τ the discretization step in time ;
— $t^n = n\tau$ the temporal discretization coordinates ;
— $u^n_{i,j}$ the approximation of $u\,(t_n, x_i, y_j)$;
— $V^x_{i,j} = V^x\,(x_i, y_j)$ and $V^y_{i,j} = V^y\,(x_i, y_j)$ the discretization of $V = (V^x, V^y) \in \mathbb{R}^2$;
— U^n a vector of size N^2 given by the concatenation of the rows of the matrix $\left(u^n_{i,j}\right)_{1\leqslant i,j\leqslant N}$, for eache $n \in \mathbb{N}$.

The Crank-Nicolson scheme corresponding to this continuous problem is written as follows

$$\begin{aligned} \frac{u^{n+1}_{i,j} - u^n_{i,j}}{\tau} + \frac{V^x_{i,j}}{2} & \left(\frac{u^n_{i+1,j} - u^n_{i-1,j}}{2h} + \frac{u^{n+1}_{i+1,j} - u^{n+1}_{i-1,j}}{2h} \right) \\ & + \frac{V^y_{i,j}}{2} \left(\frac{u^n_{i,j+1} - u^n_{i,j-1}}{2h} + \frac{u^{n+1}_{i,j+1} - u^{n+1}_{i,j-1}}{2h} \right) \\ & - \frac{\nu}{2} \left(\frac{u^n_{i+1,j} - 2u^n_{i,j} + u^n_{i-1,j}}{h^2} + \frac{u^{n+1}_{i+1,j} - 2u^{n+1}_{i,j} + u^{n+1}_{i-1,j}}{h^2} \right) \\ & - \frac{\nu}{2} \left(\frac{u^n_{i,j+1} - 2u^n_{i,j} + u^n_{i,j-1}}{h^2} + \frac{u^{n+1}_{i,j+1} - 2u^{n+1}_{i,j} + u^{n+1}_{i,j-1}}{h^2} \right) = 0. \end{aligned}$$

1. Suppose initially that the convection speed of the pollutant is constant such that $V = (1, 1)$. Calculate the matrices for which we have the recurrence relation

$$\left(I_N - \frac{\nu\tau}{2} A + \frac{\tau}{2} \left(M^x + M^y \right) \right) U^{n+1} = \left(I_N + \frac{\nu\tau}{2} A - \frac{\tau}{2} \left(M^x + M^y \right) \right) U^n, \quad \forall\, n \in \mathbb{N}.$$

2. Numerically test the scheme to calculate an approximation of the solution of the continuous problem (3) on $[T_{\min}, T_{\max}]$. We will perform the simulations with $\nu = 1,\ a = b = 50,\ T_{\min} = 0,\ T_{\max} = 5,\ h = 0.5,\ \tau = 0.1$ whose initial condition is given by

$$u(t = 0, x, y) = u_0 = f_{x_e, y_e, \sigma}(x, y) := \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - x_e)^2 + (y - y_e)^2}{2\sigma^2} \right)$$

where $x_e = y_e = \frac{a}{2}$ et $\sigma = 1$.

3. To model the dispersion and dumping of the pollutant (object in orange, see figure 1) in the ocean, modify the diagram to take into account the participation of the source term f. To take into account

the change in scale of the problem, test the diagrams numerically with the following data : $\nu = 0.1, a = b = 50$, $T_{\max} = 5$, $h = 0.5$, $\tau = 0.1$ and the source term f is a two-variable function defined by $f := f_{x_e,y_e,\sigma}$ where $x_e = 25$, $y_e = 0$ and $\sigma = 1$ where (x_e, y_e) are the coordinates of the mouth of the river in Ω.

4. To carry forward the ultimate goal of this project of predicting the effects of ocean current on dispersion when it depends on position such as near a river mouth, write the matrices M^x and M^y to take into account the dependence of the speed of the pollutant V on the position.
5. Perform numerical tests of the new scheme with the data from the previous question, for convection velocity $V(x, y) = (V^x, V^y)$ where

$$V^x = \cos\left(\frac{i\pi y}{b}\right)\sin\left(\frac{j\pi x}{a}\right), \quad V^y = \cos\left(\frac{j\pi x}{a}\right)\sin\left(\frac{i\pi y}{b}\right), \quad (x, y) \in \Omega, (i, j) \in \mathbb{N}.$$

   which are always parallel to the edge of the domain $\partial\Omega$, and visualize the evolution of the concentration over larger time intervals with $T_{\max} = 50, 100, 200, 500$.