

Resolution and numerical simulation of a pollution model in a bounded domain of the atmosphere

Research Article

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Abstract: A given environment state of contamination is due to the presence of polluting agents. The earth's atmosphere pollution is a typical issue that has many consequences: climate changes, certain animal species disappearance, the ozone layer gradual destruction, the ice caps melting of ... In addition to environmental damage, atmospheric pollution can also have consequences for human health. These phenomena can be represented by mathematical models. In most cases, these models use a system of partial differential equations for which no analytical solution is sometimes known. Hence, in a given domain, the importance of numerical methods. In this paper, our objective is to numerically solve an air pollution problem in a bounded domain of two-dimensional space. Concerning numerical study, two numerical methods will be used: the finite difference method and the finite element method. The error estimates and numerical simulations of the model will be performed in order to carry out a comparative study of these two methods.

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Keywords: Partial differential equations • Variational methods applied to PDEs • Atmosphere pollution • Numerical analysis • Algorithms with automatic result verification

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1. Introduction

The objective of this work is to analyze a mathematical model of pollution. We propose a numerical approach for this analysis based on two numerical methods. The older one is the finite difference method and the other one is the finite element method, which is very well known and adapted to complex problems. The structure of our article is as follows:

The first part deals with the mathematical analysis of the model problem: This part is divided into two sections. The first is devoted to the presentation of the model object. In the second part we will proceed to the mathematical analysis of the model. We will use the variational formulation of the model in the linear case to establish the existence and the uniqueness of the solutions in spaces that we will determine.

The second part is dedicated to the numerical study: This part includes two sections devoted to the two numerical methods chosen. In each of them, we will first recall the principles and then apply these methods to the model problem. In the first section we will present the different numerical schemes obtained by finite difference method, as well

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as the results of consistencies and stabilities. The second section deals with the finite element approach of the model. The third part will be devoted to numerical simulations: In this part we will present the results of numerical simulations, in particular the estimates of errors obtained by using each of the two methods. This will be done by varying the time step and the number of nodes of the mesh. Finally we will end with a synthesis and a conclusion.

2. Mathematical analysis of the problem

2.1. Model presentation

$\Omega = [0; T] \times C$ is a bounded domain of sufficiently regular boundary. Let us consider the model:

$$\begin{cases} \frac{\partial u}{\partial t} + \text{div}(\alpha u) + \sigma u = \mu \Delta u + f, & \text{on } [0; T] \times C, \\ u = u_1, & \text{in } \partial S, \\ u(r, 0) = u_0 \end{cases} \tag{1}$$

- the initial condition is : $u(r, 0) = u_0$
- C is a circular type domain with boundary S
- r is a point in three-dimensional space with coordinates x_1, x_2 et x_3 .
- $u(r; t)$ is the concentration of the pollutant at the time t and the point r .
- α is the air velocity.
- $\sigma = cte > 0$ is the specific rate of deterioration of the pollutant.
- μ is the horizontal diffusion coefficient where $\mu > 0$
- $f(r; t)$ is the intensity function of the pollution source.

2.2. Theoretical analysis of the problem

2.2.1. Variational formulation of the problem

We assume that the source term $f \in L^2(0, T, H^{-1}(C))$ and $u_0 \in L^2(C)$. Recall that $H^{-1}(C)$ denotes the dual of $H^1(C)$. Consider a test function $v \in H^1(\Omega)$ and $\langle ; \rangle$ the scalar product on $H^1(C)$. The variational formulation is then given by:

$$\int_C \frac{\partial u(r, t)}{\partial t} v dr + \int_C \alpha \nabla u(r, t) v dr + \sigma \int_C u(r, t) v dr = \mu \int_C \Delta u(r, t) v dr + \int_C f v dr$$

Using Green's formula, we obtain:

$$\int_C \frac{\partial u(r, t)}{\partial t} v dr + \int_C \alpha \nabla u(r, t) v dr + \sigma \int_C u(r, t) v dr + \mu \int_C \nabla u(r, t) \nabla v dr = \int_{\partial C} \frac{\partial u(r, t)}{\partial n} v d\epsilon + \int_C f v dr$$

We can put the problem in the form:

$$\begin{cases} \langle \frac{\partial u}{\partial t}(t), v \rangle + a(t, u(t), v) = \langle f(t), v \rangle, & \text{p.p } t \in [0; T] \\ u(0) = u_0 \end{cases} \tag{2}$$

$$\begin{cases} a(t, u; v) = \int_C \alpha \nabla u v dr + \sigma \int_C u v dr + \mu \int_C \nabla u \nabla v dr \\ L(v) = \int_{\partial C} \frac{\partial u}{\partial n} v d\epsilon + \int_C f v dr \end{cases} \tag{3}$$

The previous formulation can be put in the form:

$$\langle \frac{\partial u}{\partial t}(t), v \rangle + a(t, u, v) = L(v) \tag{4}$$

2.2.2. Functional framework of the model

In the very general abstract setting, we can establish the existence and uniqueness of a weak solution by using the J.L.Lions theorem [1, 11] which plays a role comparable to the Lax-Milgram theorem for parabolic problems.

2.2.3. Existence and uniqueness of the solution

Theorem 2.1.

For $f \in L^2(0, T, H^{-1}(C))$ and $u_0 \in L^2(C)$, there exists a unique solution u to the formulation (4) such that:

$$\begin{cases} u \in L^2(0, T; H^1(C)) \cap C(0, T; H^2(C) \cap H^1(C)) \\ \frac{\partial u}{\partial t} \in L^2(0, T; H^1(C)) \end{cases} \quad (5)$$

Proof. We must show that the form $L(\cdot)$ is continuous and the form $a(\cdot; \cdot)$ is bilinear, continuous, coercive:

1. the integral being linear, we can trivially conclude that the form $a(\cdot; \cdot)$ is bilinear,

2. continuity of $a(\cdot; \cdot)$:

$$|a(u; v)| \leq |\alpha| \left| \int_C \nabla u \cdot \nabla v \, dr \right| + \sigma \left| \int_C u v \, dr \right| + \mu \left| \int_C \nabla u \nabla v \, dr \right|$$

Using Hölder's inequality, we deduce that:

$$|a(u; v)| \leq |\alpha| \|\nabla u\|_{L^2(C)} \|v\|_{L^2(C)} + \sigma \|u\|_{L^2(C)} \|v\|_{L^2(C)} + \mu \|\nabla u\|_{L^2(C)} \|\nabla v\|_{L^2(C)}$$

Considering that: $\|u\|_{H^1(C)} = \|u\|_{L^2(C)} + \|\nabla u\|_{L^2(C)}$

$$\|u\|_{L^2(C)} \leq \|u\|_{H^1(C)} \text{ and } \|v\|_{L^2(C)} \leq \|v\|_{H^1(C)}$$

$$\|\nabla u\|_{L^2(C)} \leq \|u\|_{H^1(C)} \text{ and } \|\nabla v\|_{L^2(C)} \leq \|v\|_{H^1(C)}$$

we have: $|a(u; v)| \leq (|\alpha| + \sigma + \mu) \|u\|_{H^1(C)} \cdot \|v\|_{H^1(C)}$

Then we conclude: $|a(u; v)| \leq c \|u\|_{H^1(C)} \|v\|_{H^1(C)}$ with $c = |\alpha| + \sigma + \mu$ and therefore $a(\cdot; \cdot)$ is continuous.

3. continuity of $L(\cdot)$:

From (3), using the Cauchy-Schwarz inequality, we obtain the inequality:

$$|L(v)| \leq \left| \int_C f v \, dr \right| + \left| \int_{\partial C} \frac{\partial u}{\partial n}(u) \, d\epsilon \right|$$

$$|L(v)| \leq \|f\|_{L^2(C)} \|v\|_{L^2(C)} + \left\| \frac{\partial u}{\partial n} \right\|_{L^2(\partial C)} \|\gamma_0 v\|_{H^{1/2}(\partial C)}$$

According to the trace theorems: $\exists c_4 > 0 / \left\| \frac{\partial u}{\partial n} \right\|_{L^2(\partial C)} \leq c_4 \|u\|_{H^2(C)}$

$$\exists c_5 > 0 / \|\gamma_0 v\|_{H^{1/2}(\partial C)} \leq c_5 \|v\|_{H^1(C)}$$

We deduce:

$$|L(v)| \leq \left[\|f\|_{L^2(C)} + c_4 c_5 \|u\|_{H^2(C)} \right] \|v\|_{H^1(C)}$$

This allows us to conclude: $|L(v)| \leq c_6 \|v\|_{H^1(C)}$ with $c_6 = \|f\|_{L^2(C)} + c_4 c_5 \|u\|_{H^2(C)}$

And therefore that L is continuous on $H^2(C) \cap H^1(C)$

4. coercivity of $a(\cdot; \cdot)$:

$$a(u; u) = \int_C \alpha \cdot \nabla u \, dr + \sigma \int_C u^2 \, dr + \mu \int_C (\nabla u)^2 \, dr$$

$u_S \in H^{\frac{1}{2}}(\partial C)$, let's consider the trace application γ_0 . There exists at least one bearing R such that $u_S = \gamma_0(R)$.

Let's say $\bar{u} = u - R$. The problem (4) become:

$$\begin{cases} a(\bar{u}, v) = \int_C \alpha \nabla \bar{u} v \, dr + \sigma \int_C \bar{u} v \, dr + \mu \int_C \nabla \bar{u} \nabla v \, dr \\ L_{u_S}(v) = \int_C f v \, dr - \int_C \alpha \nabla u_S v \, dr - \mu \int_C \nabla u_S \nabla v \, dr \end{cases} \quad (6)$$

Then

$$\begin{cases} \text{Find } \bar{u} \in H_0^1(C) \\ a(\bar{u}, v) = L_{u_S}(v) \end{cases} \quad (7)$$

We took $v_{\partial C} = 0$ (in the vector space associated with the affine space to which u) because $u_{\partial C}$ being known ($= u_S$), we don't need to consider non-zero functions v on ∂C (it is intuitive and it is justified during the "strong problem-weak problem" equivalence). See [26]

We need to control the convection term to establish coercivity.

$$\text{Let's say: } \beta(\bar{u}, v) = \int_C \alpha \cdot \nabla \bar{u} v \, dr$$

$div \alpha = 0$, by integrating by parts we have:

$$\int_C \alpha \cdot \nabla \bar{u} v dr = - \int_C \alpha \nabla v \bar{u} dr + \int_{\partial C} \bar{u} n v d\epsilon = - \int_C \alpha \nabla v \bar{u} dr$$

It can be seen that $\beta(\bar{u}, v)$ is antisymmetric and therefore:

$$\beta(\bar{u}, \bar{u}) = 0$$

$$\text{In addition: } \sigma \int_C \bar{u}^2 dr + \mu \int_C (\nabla \bar{u})^2 dr \geq \min(\mu; \sigma) \times [\int_C |\bar{u}|^2 dr + \int_C |(\nabla \bar{u})|^2 dr]$$

Let's say: $\theta = \min(\mu; \sigma)$

$$\text{We deduce: } a(\bar{u}; \bar{u}) \geq \theta \|\bar{u}\|_{H_0^1(C)}^2$$

Hence the form $a(\cdot, \cdot)$ is coercive on $H_0^1(C)$.

□

3. Numerical resolution of the model

This part is devoted to the numerical solution of the problem. The partial differential equations are solved in an approximate way, using numerical methods.

The problem is discretised by representing functions by a finite number of values, thus passing from a continuous to a discrete framework. In our study, we will use the following two numerical methods:

- the finite difference method [1, 5]
- the finite element method [1, 35]

We will restrict our study to the case of dimension two space.

3.1. The finite difference method

3.1.1. Explicit finite difference scheme in dimension two

The generalization to the two-dimensional case of the explicit scheme gives us:

$$\begin{aligned} \frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} + \alpha_1 \frac{u_{i+1,j}^n - u_{i-1,j}^n}{2\Delta x} + \alpha_2 \frac{u_{i,j+1}^n - u_{i,j-1}^n}{2\Delta y} + \sigma u_{i,j}^n - \mu \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{(\Delta x)^2} \\ - \mu \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{(\Delta y)^2} = f_{i,j}^n \end{aligned} \tag{8}$$

where $\vec{\alpha}$ is the velocity vector of components $(\alpha_1; \alpha_2)$.

If we group the different terms together, we get:

$$\begin{aligned} u_{i,j}^{n+1} = \left[1 - \sigma \Delta t - 2(c_x + c_y) \right] u_{i,j}^n + \left(-\frac{\alpha_1 \Delta t}{2\Delta x} + c_x \right) u_{i+1,j}^n + \left(\frac{\alpha_1 \Delta t}{2\Delta x} + c_x \right) u_{i-1,j}^n \\ + \left(-\frac{\alpha_2 \Delta t}{2\Delta y} + c_y \right) u_{i,j+1}^n + \left(\frac{\alpha_2 \Delta t}{2\Delta y} + c_y \right) u_{i,j-1}^n + \Delta t f_{i,j}^n \end{aligned} \tag{9}$$

With: $c_x = \frac{\mu \Delta t}{(\Delta x)^2}$ et $c_y = \frac{\mu \Delta t}{(\Delta y)^2}$

By reasoning analogously to the case of dimension one space (see [1, 11]), the scheme is consistent and stable in L^∞ norm with the CFL condition:

$$\Delta t \left[\sigma + 2\mu \left(\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right) \right] \leq 1 \tag{10}$$

$$\text{where: } \Delta x \leq \frac{2\mu}{\alpha_1}, \Delta y \leq \frac{2\mu}{\alpha_2}, \sigma \leq \frac{1}{\Delta t}$$

To solve the system of evolution of the system, we put the diagram in the form:

$$u_{i,j}^{n+1} = Au_{i,j}^n + Bu_{i+1,j}^n + Cu_{i-1,j}^n + Du_{i,j+1}^n + Eu_{i,j-1}^n + \Delta t f_{i,j}^n \tag{11}$$

with:

$$A = 1 - \sigma \Delta t - 2(c_x + c_y), B = -\frac{\alpha_1 \Delta t}{2\Delta x} + c_x$$

$$C = \frac{\alpha_1 \Delta t}{2\Delta x} + c_x, D = -\frac{\alpha_2 \Delta t}{2\Delta y} + c_y$$

$$E = \frac{\alpha_2 \Delta t}{2\Delta y} + c_y$$

$$i \in [1; I] \text{ et } j \in [1; J]$$

The (Dirichlet) boundary conditions are then: $u_{0;j}, u_{I+1;j}, u_{i;0}, u_{i;J+1}$.

The problem can be put in the form:

$$U^{n+1} = MU^n + V + \Delta t f^n \quad (12)$$

where M is a matrix ($I * J; I * J$). It is a block matrix of the form:

$$M = \begin{pmatrix} M_c & M_d & 0 & \cdots & 0 \\ M_g & M_c & M_d & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & M_g & M_c & M_d \\ 0 & \cdots & 0 & M_g & M_c \end{pmatrix}$$

Each block is of size $J * J$, with:

$$M_g = \begin{pmatrix} C & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & C \end{pmatrix}; M_d = \begin{pmatrix} B & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & B \end{pmatrix}$$

and

$$M_c = \begin{pmatrix} A & D & 0 & \cdots & 0 \\ E & A & D & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & E & A & D \\ 0 & \cdots & 0 & E & A \end{pmatrix}$$

Recall the column vectors:

$$U^n = \begin{pmatrix} u_{1,1} \\ u_{1,2} \\ \vdots \\ u_{1,J} \\ u_{2,1} \\ \vdots \\ u_{2,J} \\ \vdots \\ u_{I-1,J} \\ u_{I,1} \\ \vdots \\ u_{I,J} \end{pmatrix} \text{ and } V = \begin{pmatrix} Cu_{0,1} + Eu_{1,0} \\ Cu_{0,2} \\ \vdots \\ Cu_{0,J} + Du_{1,J+1} \\ Eu_{2,0} \\ 0 \\ \vdots \\ 0 \\ Du_{2,J+1} \\ Eu_{3,0} \\ 0 \\ \vdots \\ 0 \\ Du_{I-1,J+1} \\ Bu_{I+1,1} + Eu_{I,0} \\ Bu_{I+1,2} \\ \vdots \\ Bu_{I+1,J} + Du_{I,J+1} \end{pmatrix}$$

3.1.2. Implicit finite difference scheme in dimension two

The generalization to the two-dimensional case of the implicit scheme gives us:

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} + \alpha_1 \frac{u_{i+1,j}^{n+1} - u_{i-1,j}^{n+1}}{2\Delta x} + \alpha_2 \frac{u_{i,j+1}^{n+1} - u_{i,j-1}^{n+1}}{2\Delta y} + \sigma u_{i,j}^{n+1} - \mu \frac{u_{i+1,j}^{n+1} - 2u_{i,j}^{n+1} + u_{i-1,j}^{n+1}}{(\Delta x)^2} - \mu \frac{u_{i,j+1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j-1}^{n+1}}{(\Delta y)^2} = f_{i,j}^{n+1} \quad (13)$$

After grouping the different terms, we obtain:

$$u_{i,j}^{n+1} \left[1 + \sigma \Delta t + 2(c_x + c_y) \right] + \left(\frac{\alpha_1 \Delta t}{2\Delta x} - c_x \right) u_{i+1,j}^{n+1} + \left(-\frac{\alpha_1 \Delta t}{2\Delta x} - c_x \right) u_{i-1,j}^{n+1} + \left(\frac{\alpha_2 \Delta t}{2\Delta y} - c_y \right) u_{i,j+1}^{n+1} + \left(-\frac{\alpha_2 \Delta t}{2\Delta y} - c_y \right) u_{i,j-1}^{n+1} = u_{i,j}^n + \Delta t f_{i,j}^{n+1} \tag{14}$$

Where $c_x = \frac{\mu \Delta t}{(\Delta x)^2}$ and $c_y = \frac{\mu \Delta t}{(\Delta y)^2}$.

By posing:

$$\theta_x^1 = \frac{\alpha_1 \Delta t}{2\Delta x} - c_x, \theta_x^2 = -\frac{\alpha_1 \Delta t}{2\Delta x} - c_x$$

$$\theta_y^1 = \frac{\alpha_2 \Delta t}{2\Delta y} - c_y \text{ and } \theta_y^2 = -\frac{\alpha_2 \Delta t}{2\Delta y} - c_y$$

we have:

$$u_{i,j}^{n+1} \left[1 + \sigma \Delta t + 2(c_x + c_y) \right] + \theta_x^1 u_{i+1,j}^{n+1} + \theta_x^2 u_{i-1,j}^{n+1} + \theta_y^1 u_{i,j+1}^{n+1} + \theta_y^2 u_{i,j-1}^{n+1} = u_{i,j}^n + \Delta t f_{i,j}^{n+1} \tag{15}$$

Vector formulation

We will match each table of values to $u_{i,j}^n$, the vector $(U_k^n)_{k \in [1,N]}$ defined by:

$$U_k^n = u_{i,j}^n$$

$k \in [1, N]$ (with $N = IJ$) bijectively related to the pair $(i, j) \in [1, I] \times [1, J]$ by :

$$k = i + (j - 1)I$$

We can move on to the vector formulation of the problem (15):

$$U_k^{n+1} [1 + \sigma \Delta t + 2(c_x + c_y)] + \theta_x^1 U_{k+1}^{n+1} + \theta_x^2 U_{k-1}^{n+1} + \theta_y^1 U_{k+I}^{n+1} + \theta_y^2 U_{k-I}^{n+1} = U_k^n + \Delta t f_k^{n+1} \tag{16}$$

we can write the problem in the form:

$$MU_k^{n+1} = U_k^n + \Delta t f_k^{n+1}$$

where $M \in \mathbb{R}^{N \times N}$ is a block tridiagonal matrix:

$$M = \begin{pmatrix} D & F & 0 & \dots & 0 \\ E & D & F & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & E & D & F \\ 0 & \dots & 0 & E & D \end{pmatrix}$$

In such a way that $\forall (i, j) \in [2, I - 1]^2$

$$M_{k,k-I} = \theta_y^2, \tag{17}$$

$$M_{k,k-1} = \theta_x^2, \tag{18}$$

$$M_{k,k} = 1 + 2(c_x + c_y), \tag{19}$$

$$M_{k,k+I} = \theta_y^1, \tag{20}$$

$$M_{k,k+1} = \theta_x^1, \tag{21}$$

$$\tag{22}$$

lets pose $\theta_{x,y} = 1 + \sigma \Delta t + 2(c_x + c_y)$, we finally obtain diagonal blocks D :

$$D = \begin{pmatrix} \theta_{x,y} & \theta_y^1 & 0 & \dots & 0 \\ \theta_y^2 & \theta_{x,y} & \theta_y^1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \theta_y^2 & \theta_{x,y} & \theta_y^1 \\ 0 & \dots & 0 & \theta_y^2 & \theta_{x,y} \end{pmatrix}$$

and the extra-diagonal blocks E et F :

$$E = \begin{pmatrix} \theta_x^2 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \theta_x^2 \end{pmatrix} \text{ and } F = \begin{pmatrix} \theta_x^1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \theta_x^1 \end{pmatrix}$$

The conditions at the edges are as follows:

$$u_{1,j}^n = u_{I,j}^n = u_S(1, y_j), \forall j$$

$$u_{i,1}^n = u_{i,J}^n = u_S(x_i, 1), \forall i$$

The initial data is discretized by:

$$u_{i,j}^0 = u_0(x_i, y_j), \forall i, j$$

3.1.3. Alternate directions

However, it can be seen that the computational cost of the previous scheme is very high on the machine because of the weight of the resulting matrix [1]. This is the reason why the implicit scheme is often replaced by a generalization to several space dimensions of one-dimensional schemes obtained by a technique of alternating directions (also called splitting of operators). The idea is to solve, instead of the two-dimensional equation, alternately the two one-dimensional equations [1]:

$$\frac{\partial u}{\partial t} + \alpha_1 \frac{\partial u}{\partial x} + \sigma u - \mu \frac{\partial^2 u}{\partial x^2} = \frac{f}{2}$$

and

$$\frac{\partial u}{\partial t} + \alpha_2 \frac{\partial u}{\partial y} + \sigma u - \mu \frac{\partial^2 u}{\partial y^2} = \frac{f}{2}$$

$$\left(\vec{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \right)$$

the average of which gives the two-dimensional equation.

For example, by using a Crank-Nicholson scheme in each direction for a $\Delta t/2$ time step, we obtain the Peaceman-Rachford inspired alternating directions scheme:

$$\begin{aligned} \frac{u_{i,j}^{n+\frac{1}{2}} - u_{i,j}^n}{\Delta t} + \alpha_1 \frac{u_{i+1,j}^{n+\frac{1}{2}} - u_{i-1,j}^{n+\frac{1}{2}}}{8\Delta x} + \alpha_1 \frac{u_{i,j+1}^n - u_{i,j-1}^n}{8\Delta y} + \frac{\sigma}{4} u_{i,j}^{n+\frac{1}{2}} + \frac{\sigma}{4} u_{i,j}^n - \mu \frac{u_{i+1,j}^{n+\frac{1}{2}} - 2u_{i,j}^{n+\frac{1}{2}} + u_{i-1,j}^{n+\frac{1}{2}}}{4(\Delta x)^2} \\ - \mu \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{4(\Delta y)^2} = \frac{f_{i,j}^{n+\frac{1}{2}}}{2} \end{aligned} \quad (23)$$

$$\begin{aligned} \frac{u_{i,j}^{n+1} - u_{i,j}^{n+\frac{1}{2}}}{\Delta t} + \alpha_2 \frac{u_{i,j+1}^{n+1} - u_{i,j-1}^{n+1}}{8\Delta y} + \alpha_2 \frac{u_{i+1,j}^{n+\frac{1}{2}} - u_{i-1,j}^{n+\frac{1}{2}}}{8\Delta x} + \frac{\sigma}{4} u_{i,j}^{n+1} + \frac{\sigma}{4} u_{i,j}^{n+\frac{1}{2}} - \mu \frac{u_{i+1,j}^{n+\frac{1}{2}} - 2u_{i,j}^{n+\frac{1}{2}} + u_{i-1,j}^{n+\frac{1}{2}}}{4(\Delta x)^2} \\ - \mu \frac{u_{i,j+1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j-1}^{n+1}}{4(\Delta y)^2} = \frac{f_{i,j}^{n+\frac{1}{2}}}{2} \end{aligned} \quad (24)$$

It is easy to verify that this scheme is precise of order 2 in space and 1 in time and unconditionally stable . It is therefore convergent [1, 31].

Each of the two steps (23) and (24) consists of solving a tridiagonal system, which is done by direct elimination using a given algorithm.

The two systems to be solved will be written in the following general form:

$$A_{i,j} u_{i-1,j}^{n+\frac{1}{2}} + B_{i,j} u_{i,j}^{n+\frac{1}{2}} + C_{i,j} u_{i+1,j}^{n+\frac{1}{2}} = D_{i,j} u_{i,j-1}^n + E_{i,j} u_{i,j}^n + F_{i,j} u_{i,j+1}^n + G_{i,j}, \quad (25)$$

$$A'_{i,j} u_{i,j-1}^{n+1} + B'_{i,j} u_{i,j}^{n+1} + C'_{i,j} u_{i,j+1}^{n+1} = D'_{i,j} u_{i-1,j}^{n+\frac{1}{2}} + E'_{i,j} u_{i,j}^{n+\frac{1}{2}} + F'_{i,j} u_{i+1,j}^{n+\frac{1}{2}} + G'_{i,j}, \quad (26)$$

The first tridiagonal system is to be solved for each row. The second is to be solved for each column. For a point A inside the domain, we have for the first system:

$$A_{i,j} = -\frac{\alpha_1}{8\Delta x} - \frac{\mu}{4(\Delta x)^2}, \tag{27}$$

$$B_{i,j} = \frac{1}{\Delta t} + \frac{\sigma}{4} + \frac{\mu}{2(\Delta x)^2}, \tag{28}$$

$$C_{i,j} = \frac{\alpha_1}{8\Delta x} - \frac{\mu}{4(\Delta x)^2}, \tag{29}$$

$$D_{i,j} = \frac{\alpha_1}{8\Delta y} + \frac{\mu}{4(\Delta y)^2}, \tag{30}$$

$$E_{i,j} = \frac{1}{\Delta t} + \frac{\sigma}{4} - \frac{\mu}{2(\Delta y)^2}, \tag{31}$$

$$F_{i,j} = -\frac{\alpha_1}{8\Delta y} + \frac{\mu}{4(\Delta y)^2}, \tag{32}$$

$$G_{i,j} = \frac{f_{i,j}^{n+\frac{1}{2}}}{2}, \tag{33}$$

and for the second:

$$A'_{i,j} = -\frac{\alpha_2}{8\Delta y} - \frac{\mu}{4(\Delta y)^2}, \tag{34}$$

$$B'_{i,j} = \frac{1}{\Delta t} + \frac{\sigma}{4} + \frac{\mu}{2(\Delta y)^2}, \tag{35}$$

$$C'_{i,j} = \frac{\alpha_2}{8\Delta y} - \frac{\mu}{4(\Delta y)^2}, \tag{36}$$

$$D'_{i,j} = \frac{\alpha_2}{8\Delta x} + \frac{\mu}{2(\Delta x)^2}, \tag{37}$$

$$E'_{i,j} = \frac{1}{\Delta t} + \frac{\sigma}{4} - \frac{\mu}{2(\Delta x)^2}, \tag{38}$$

$$F'_{i,j} = -\frac{\alpha_2}{8\Delta x} + \frac{\mu}{2(\Delta x)^2}, \tag{39}$$

$$G'_{i,j} = \frac{f_{i,j}^{n+\frac{1}{2}}}{2}, \tag{40}$$

A Dirichlet boundary condition on the point (i, j) is written:

$$A_{i,j} = 0, \tag{41}$$

$$B_{i,j} = 1, \tag{42}$$

$$C_{i,j} = 0, \tag{43}$$

$$D_{i,j} = 0, \tag{44}$$

$$E_{i,j} = 0, \tag{45}$$

$$F_{i,j} = 0, \tag{46}$$

$$G_{i,j} = u_s, \tag{47}$$

3.2. Finite element method - Lagrangian triangular finite elements of degree one: P1 finite elements

3.2.1. Approximation space description

In the finite element method, the construction of the discrete subspace requires the prior discretisation of the Ω domain into simple geometric elements.

Let Ω be an open of \mathbb{R}^2 and let us consider a $\bar{\Omega}$ mesh formed by K triangles checking the following criteria:

- the $K \subset \bar{\Omega}$ elements of the mesh must cover the domain, that means their union is equal to $\bar{\Omega}$
- the intersection of two distinct elements must satisfy:

$$K \cap K' = \begin{cases} \emptyset, \\ a \text{ corner}, \\ a \text{ side}. \end{cases}$$

We denote by Γ_h the set of all these elements; Γ_h is called triangular mesh or triangulation of $\bar{\Omega}$

- $S = S_1, \dots, S_N$ is a finite set of N distinct points of K
- P is a finite-dimensional vector space of real functions defined on K , and such that S is P -unisolvent (so $\dim P = N$).

A finite Lagrange element is a triplet (K, S, P)

Let (K, S, P) be a finite Lagrangian element. The local basis functions of the element are the N functions $p_i (i = 1, \dots, N)$ of P such that

$$p_i(a_{ij}) = \delta_{ij}, 1 \leq i, j \leq N.$$

We call the interpolation operator (or P -interpolation) on S the operator π_K which, to any function v defined on K , associates the function $\pi_K v$ of P defined by :

$$\pi_K v = \sum_{i=1}^N v(a_i) p_i$$

$\pi_K v$ is therefore the only element of P that takes the same values as v on the points of S [8, 18, 30].

3.3. Application to the model problem

The study area considered is: $L^2(0, T; H^1(C)) \cap C(0, T; H^2(C) \cap H^1(C))$, then:
 $r = (x, y) \in H^2(\Omega) \cap H^1(\Omega) \subset H^1(\Omega)$

3.3.1. Semi-discretization in space

Consider $V_h \cap V$ ($V = \bigcup_h V_h$ with $\dim V_h = N_h$) and $\Omega = I \cup J$ where $J = \partial\Omega$. We introduce a simple auxiliary function taking the values imposed on the edge: $u_{1/\partial\Omega} = u_S$ and by posing $u = u_h + u_S$, we have:

$$\begin{aligned} \int_V \frac{\partial u_h}{\partial t} v dr + \int_V \bar{\alpha} \nabla u_h v dr + \sigma \int_V u_h v dr + \mu \int_V \nabla u_h \nabla v dr = \\ \int_V f v dr - \int_V \bar{\alpha} \nabla u_S v dr - \sigma \int_V u_S v dr - \mu \int_V \nabla u_S \nabla v dr \end{aligned}$$

where $u_h = \sum_{i \in I} u_i \phi_i$ et $u_{1,h} = u_S = \sum_{i \in J} u_S(x_i, y_i) \phi_i$. Let's pose $v = \phi_j$ we obtain

$$\begin{aligned} \sum_{i \in I} \left[\left(\int_{V_h} \phi_i \phi_j dr \right) u_i'(t) + \left(\int_{V_h} \bar{\alpha} \nabla \phi_i \phi_j dr + \sigma \int_{V_h} \phi_i \phi_j dr + \mu \int_{V_h} \nabla \phi_i \nabla \phi_j dr \right) u_i(t) \right] = \\ \int_{V_h} f \phi_j dr - \sum_{i \in J} \left[\int_{V_h} \bar{\alpha} \nabla \phi_i \phi_j dr - \sigma \int_{V_h} \phi_i \phi_j dr - \mu \int_{V_h} \nabla \phi_i \nabla \phi_j dr \right] u_S(x_i, y_i) \end{aligned}$$

This leads to the system:

$$\begin{cases} MU'(t) + RU(t) = B \\ U(0) = U_0 \end{cases} \quad (48)$$

$$M_{i,j} = \int_{V_h} \phi_i \phi_j dr$$

$$R_{i,j} = \int_{V_h} \bar{\alpha} \nabla \phi_i \phi_j dr + \sigma \int_{V_h} \phi_i \phi_j dr + \mu \int_{V_h} \nabla \phi_i \nabla \phi_j dr$$

$$B_j = \int_{V_h} f \phi_j dr - \sum_{i \in J} \left[\int_{V_h} \bar{\alpha} \nabla \phi_i \phi_j dr + \sigma \int_{V_h} \phi_i \phi_j dr + \mu \int_{V_h} \nabla \phi_i \nabla \phi_j dr \right] u_S(x_i, y_i)$$

Let Γ be a triangulation or lattice corresponding to V and $K \subset \Gamma$, on an element K of the mesh we have:

$\phi_{i/K}(x, y) = \lambda_i^K(x, y)$ and therefore:

$$M_{i,j}^K = \int_K \lambda_i^K \lambda_j^K dr$$

$$R_{i,j}^K = \int_K \bar{\alpha} \nabla \lambda_i^K \lambda_j^K dr + \sigma \int_K \lambda_i^K \lambda_j^K dr + \mu \int_K \nabla \lambda_i^K \nabla \lambda_j^K dr$$

$$B_j^K = \int_K f \lambda_j^K dr - \sum_{i \in J} \left[\int_K \bar{\alpha} \nabla \lambda_i^K \lambda_j^K dr + \sigma \int_K \lambda_i^K \lambda_j^K dr + \mu \int_K \nabla \lambda_i^K \nabla \lambda_j^K dr \right] u_S(x_i, y_i)$$

Let us then determine these three matrices:

- For the mass matrix $M_{i,j}^K$

Let us recall the exact integration formulas:

$$\int_K \lambda_i^K dr = \frac{|K|}{3}$$

$$\int_K [\lambda_i^K]^2 dr = \frac{|K|}{6}$$

$$\int_K \lambda_i^K \lambda_j^K dr = \frac{|K|}{12}$$

$$\int_K (\lambda_i^K)^{\alpha_1} (\lambda_j^K)^{\alpha_2} (\lambda_r^K)^{\alpha_3} dr = |K| \frac{\alpha_1! \alpha_2! \alpha_3!}{(2 + \alpha_1 + \alpha_2 + \alpha_3)!}$$

where $|K|$ is the area of the triangle K. We then deduce the matrix:

$$M_{i,j}^K = \frac{|K|}{12} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \tag{49}$$

- For the stiffness matrix $R_{i,j}^K$:

We can write: $R_{i,j}^K = N_{i,j}^K + \sigma M_{i,j}^K + \mu A_{i,j}^K$

1. Let's determine $A_{i,j}^K$:

Consider the triangle K with corners $S_1(x_1, y_1)$, $S_2(x_2, y_2)$ et $S_3(x_3, y_3)$

Using the change of variables: $(x, y)^T = F_K(\hat{x}, \hat{y})$, we obtain:

$$\lambda_i^K(x, y) = \lambda_i^K(F_K(\hat{x}, \hat{y})) = \hat{\lambda}_i(\hat{x}, \hat{y})$$

and

$$\begin{aligned} \nabla \lambda_i^K &= \begin{pmatrix} \frac{\partial \lambda_i^K}{\partial x} \\ \frac{\partial \lambda_i^K}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial \lambda_i^K}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial x} + \frac{\partial \lambda_i^K}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial x} \\ \frac{\partial \lambda_i^K}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial y} + \frac{\partial \lambda_i^K}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial x} + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial x} \\ \frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial y} + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial y} \end{pmatrix} \\ &= \frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \nabla \hat{x} + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \nabla \hat{y} \end{aligned}$$

we deduce:

$$\nabla \lambda_i^K \nabla \lambda_j^K = \frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \frac{\partial \hat{\lambda}_j}{\partial \hat{x}} |\nabla \hat{x}|^2 + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \frac{\partial \hat{\lambda}_j}{\partial \hat{y}} |\nabla \hat{y}|^2 + \left(\frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \frac{\partial \hat{\lambda}_j}{\partial \hat{y}} + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \frac{\partial \hat{\lambda}_j}{\partial \hat{x}} \right) \nabla \hat{x} \nabla \hat{y} \tag{50}$$

on the other hand:

$$\nabla \hat{x} = \frac{1}{2|K|} \begin{pmatrix} y_3 - y_1 \\ x_1 - x_3 \end{pmatrix} \text{ et } \nabla \hat{y} = \frac{1}{2|K|} \begin{pmatrix} y_1 - y_2 \\ x_2 - x_1 \end{pmatrix}.$$

So:

$$|\nabla \hat{x}|^2 = \frac{1}{4|K|^2} [(y_3 - y_1)^2 + (x_1 - x_3)^2] = \frac{1}{4|K|^2} |\overrightarrow{S_1 S_3}|^2 \tag{51}$$

$$|\nabla \hat{y}|^2 = \frac{1}{4|K|^2} [(y_1 - y_2)^2 + (x_2 - x_1)^2] = \frac{1}{4|K|^2} |\overrightarrow{S_1 S_2}|^2 \tag{52}$$

and

$$\nabla \hat{x} \nabla \hat{y} = -\frac{1}{4|K|^2} [(y_3 - y_1)(y_2 - y_1) + (x_3 - x_1)(x_2 - x_1)] = \frac{1}{4|K|^2} \overrightarrow{S_1 S_3} \cdot \overrightarrow{S_1 S_2} \tag{53}$$

Substituting (51), (52) and (53) into (50), we obtain:

$$\nabla \lambda_i^K \nabla \lambda_j^K = \frac{1}{4|K|^2} \left(\frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \frac{\partial \hat{\lambda}_j}{\partial \hat{x}} |\overrightarrow{S_1 S_3}|^2 + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \frac{\partial \hat{\lambda}_j}{\partial \hat{y}} |\overrightarrow{S_1 S_2}|^2 - \frac{1}{4|K|^2} \left(\frac{\partial \hat{\lambda}_i}{\partial \hat{x}} \frac{\partial \hat{\lambda}_j}{\partial \hat{y}} + \frac{\partial \hat{\lambda}_i}{\partial \hat{y}} \frac{\partial \hat{\lambda}_j}{\partial \hat{x}} \right) \overrightarrow{S_1 S_3} \cdot \overrightarrow{S_1 S_2} \right) \tag{54}$$

$\hat{\lambda}_i$ ($i = 1, 2, 3$) designating the base functions on the reference element, after integration we obtain the elements $a_{i,j}^K$ of the matrix $A_{i,j}^K$. Finally we have:

$$A_{i,j}^K = \frac{1}{4|K|} \begin{pmatrix} \frac{|\overrightarrow{S_2 S_3}|^2}{S_1 S_3 S_3 S_2} & \frac{\overrightarrow{S_1 S_3} \cdot \overrightarrow{S_3 S_2}}{S_1 S_3 S_2 S_1} & \frac{\overrightarrow{S_1 S_2} \cdot \overrightarrow{S_2 S_3}}{S_1 S_3 S_2 S_1} \\ \frac{\overrightarrow{S_1 S_3} \cdot \overrightarrow{S_3 S_2}}{S_1 S_3 S_2 S_1} & \frac{|\overrightarrow{S_1 S_3}|^2}{S_1 S_3 S_2 S_1} & \frac{\overrightarrow{S_1 S_3} \cdot \overrightarrow{S_2 S_1}}{S_1 S_3 S_2 S_1} \\ \frac{\overrightarrow{S_1 S_2} \cdot \overrightarrow{S_2 S_3}}{S_1 S_3 S_2 S_1} & \frac{\overrightarrow{S_1 S_3} \cdot \overrightarrow{S_2 S_1}}{S_1 S_3 S_2 S_1} & \frac{|\overrightarrow{S_1 S_2}|^2}{S_1 S_3 S_2 S_1} \end{pmatrix}. \tag{55}$$

2. $M_{i,j}^K$ is known, it remains to determine $N_{i,j}^K$:

$$N_{i,j}^K = \int_K \vec{\alpha} \nabla \lambda_i^K \lambda_j^K dx dy$$

we pose $\vec{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$, knowing that: $\nabla \lambda_i^K = \frac{\partial \widehat{\lambda}_i}{\partial \widehat{x}} \nabla \widehat{x} + \frac{\partial \widehat{\lambda}_i}{\partial \widehat{y}} \nabla \widehat{y}$, we deduce:

$$\vec{\alpha} \nabla \lambda_i^K = \alpha_1 \left[\frac{\partial \widehat{\lambda}_i}{\partial \widehat{x}} (y_3 - y_1) + \frac{\partial \widehat{\lambda}_i}{\partial \widehat{y}} (y_1 - y_2) \right] + \alpha_2 \left[\frac{\partial \widehat{\lambda}_i}{\partial \widehat{x}} (x_1 - x_3) + \frac{\partial \widehat{\lambda}_i}{\partial \widehat{y}} (x_2 - x_1) \right] = \tau_i$$

$$\text{hence } \int_K \vec{\alpha} \nabla \lambda_i^K \lambda_j^K dx dy = \tau_i \int_K \lambda_j^K dx dy = \frac{|K|}{3} \tau_i$$

after determination of the elements $n_{i,j}^K$ of the matrix $N_{i,j}^K$, we have:

$$N_{i,j}^K = \frac{|K|}{3} \begin{pmatrix} \tau_1 & \tau_1 & \tau_1 \\ \tau_2 & \tau_2 & \tau_2 \\ \tau_3 & \tau_3 & \tau_3 \end{pmatrix}.$$

hence:

$$N_{i,j}^K = \frac{|K|}{3} \begin{pmatrix} \alpha_1(y_2 - y_3) + \alpha_2(x_3 - x_2) & \alpha_1(y_2 - y_3) + \alpha_2(x_3 - x_2) & \alpha_1(y_2 - y_3) + \alpha_2(x_3 - x_2) \\ \alpha_1(y_3 - y_1) + \alpha_2(x_1 - x_3) & \alpha_1(y_3 - y_1) + \alpha_2(x_1 - x_3) & \alpha_1(y_3 - y_1) + \alpha_2(x_1 - x_3) \\ \alpha_1(y_1 - y_2) + \alpha_2(x_2 - x_1) & \alpha_1(y_1 - y_2) + \alpha_2(x_2 - x_1) & \alpha_1(y_1 - y_2) + \alpha_2(x_2 - x_1) \end{pmatrix}. \quad (56)$$

On the triangle T of vertices $S_1^0(0,0)$, $S_2^0(1,0)$ et $S_3^0(0,1)$ (reference triangle) we find:

$$M_{i,j}^T = \frac{1}{2} \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{pmatrix}. \quad (57)$$

$$A_{i,j}^T = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}. \quad (58)$$

$$N_{i,j}^T = \frac{1}{6} \begin{pmatrix} -(\alpha_1 + \alpha_2) & -(\alpha_1 + \alpha_2) & -(\alpha_1 + \alpha_2) \\ \alpha_1 & \alpha_1 & \alpha_1 \\ \alpha_2 & \alpha_2 & \alpha_2 \end{pmatrix}. \quad (59)$$

Recall that:

$$R_{i,j}^T = N_{i,j}^T + \sigma M_{i,j}^T + \mu A_{i,j}^T$$

• Let's determine B_j

$$\begin{aligned} B_j^K &= \int_K f \lambda_j^K dr - \sum_{i \in J} \left[\int_K \vec{\alpha} \nabla \lambda_i^K \lambda_j^K dr + \sigma \int_K \lambda_i^K \lambda_j^K dr + \mu \int_K \nabla \lambda_i^K \nabla \lambda_j^K dr \right] u_S(x_i, y_i) \\ &= F_1 - \sigma F_2 - F_3 - \mu F_4 \end{aligned}$$

1. It is assumed that f is analytically known and sufficiently simple:

$$F_1 = \int_K f_i \lambda_i^K \lambda_j^K dx dy$$

hence:

$$F_1 = f_i M_{i,j}^K \quad (60)$$

2.

$$F_2 = \sum_{i \in J} \int_K \lambda_i^K \lambda_j^K dx dy u_S(x_i, y_i)$$

we find the coefficients already calculated for the matrix $M_{i,j}^K$. For a triangle (I, J, K_{int}) whose side IJ belongs to the edge and whose corner K_{int} is inside the domain, we obtain a unique contribution to the K_{int} component:

$$F_2 = (m_{ik_{int}}, m_{jk_{int}}, m_{kk_{int}}) \begin{pmatrix} u_{S,I} \\ u_{S,J} \\ 0 \end{pmatrix}. \tag{61}$$

where i, j, k_{int} are the internal numbers of the triangle corresponding to the indices I, J, K_{int} .

3.

$$F_3 = \sum_{i \in J} \int_K \vec{\alpha} \nabla \lambda_i^K \lambda_j^K dx dy u_S(x_i, y_i)$$

based on the previous reasoning, we find:

$$F_3 = (n_{ik_{int}}, n_{jk_{int}}, n_{kk_{int}}) \begin{pmatrix} u_{S,I} \\ u_{S,J} \\ 0 \end{pmatrix}. \tag{62}$$

4.

$$F_4 = \sum_{i \in J} \int_K \nabla \lambda_i^K \nabla \lambda_j^K dx dy u_S(x_i, y_i)$$

we have:

$$F_4 = (a_{ik_{int}}, a_{jk_{int}}, a_{kk_{int}}) \begin{pmatrix} u_{S,I} \\ u_{S,J} \\ 0 \end{pmatrix}. \tag{63}$$

3.3.2. Complete discretization in space and time

We will apply the time schemes already presented in the case of finite difference discretization to obtain a complete discretization of the problem.

The explicit Euler scheme, whose stability depends on a very severe condition on the time step, is not adapted to our problem. We will then adopt the implicit scheme since it is unconditionally stable.

This leads to the scheme:

$$M \frac{U^{n+1} - U^n}{\Delta t} + RU^{n+1} = B$$

Either

$$(M + \Delta t R)U^{n+1} = MU^n + \Delta t B \tag{64}$$

4. Numerical simulation

We will consider the case where the source term does not have a fixed position in the domain in dimension two of space which will be of rectangular type with $L=1$ for our case. We will consider an analytical solution from which we can generate the source term, the edge conditions and the initial condition, while being careful to respect the regularity rules and the working space established during the mathematical analysis of the problem.

Considering the homogeneous case, in order to search for solutions verifying the boundary conditions, we first determine the diffusion eigenmodes by using the method of variable separations. The eigenmodes are the following functions [12]:

$$u_{p,q}(t; x; y) = \sin\left(\frac{(2p+1)\pi}{2} \frac{x}{L}\right) \sin\left(\frac{(2q+1)\pi}{2} \frac{y}{L}\right) e^{-\left(\left(\frac{(2p+1)\pi}{2L}\right)^2 + \left(\frac{(2q+1)\pi}{2L}\right)^2\right)\mu + \sigma)t} \tag{65}$$

which verify the homogeneous boundary conditions.

The general diffusion solution is then a linear combination of these modes.

We can then represent the eigenmode for $p = 0, q = 0$ and $L = 1$ by adapting it to our problem by generating the source term f . Let then be the model problem on the domain $\Omega \times [0; T]$ where $\Omega = [0; 1] \times [0; 1]$

Let's consider the solution:

$$u(t; x; y) = \sin\left(\frac{\pi}{2} x\right) \sin\left(\frac{\pi}{2} y\right) e^{-\left(\frac{\pi^2}{2}\right)\mu + \sigma)t}$$

the source term is given by:

$$f(x, y, t) = \left[\frac{\pi}{2} (\alpha_1 \cos \frac{\pi}{2} x \sin \frac{\pi}{2} y + \alpha_2 \sin \frac{\pi}{2} x \cos \frac{\pi}{2} y) \right] e^{-\left(\frac{\pi^2}{2} \mu + \sigma\right) t}$$

with the initial condition: $u(x, y, 0) = u(x, y, t) = \sin \frac{\pi}{2} x \sin \frac{\pi}{2} y$

and the conditions at the edges:

$$u(0, y, t) = 0$$

$$u(x, 0, t) = 0$$

$$u(1, y, t) = \sin \frac{\pi}{2} y e^{-\left(\frac{\pi^2}{2} \mu + \sigma\right) t}$$

$$u(x, 1, t) = \sin \frac{\pi}{2} x e^{-\left(\frac{\pi^2}{2} \mu + \sigma\right) t}$$

We will use Matlab software to perform finite difference and finite element simulations.

4.1. Error Estimates

The CFL condition is given by:

$$\Delta t \left[\sigma + 2\mu \left(\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right) \right] \leq 1 \quad (66)$$

It can be seen that this condition is very strict regarding the choice of the different discretization steps. We will consider the following values: $\alpha_1 = 5$, $\alpha_2 = 10$, $\mu = 0.5$, $\sigma = 1$.

4.1.1. When the CFL condition is satisfied

1. By the finite difference method: Euler explicit

Table 1. Table of error estimates for $N = 650$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	0.0032	0.0032	0.0027	0.0026	0.0024	0.0022
$L^\infty\mathbf{E}$	0.0276	0.0259	0.0208	0.0196	0.0185	0.0174

Table 2. Table of error estimates for $N = 700$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	0.0032	0.0032	0.0028	0.0026	0.0025	0.0023
$L^\infty\mathbf{E}$	0.0277	0.0260	0.0209	0.0197	0.0186	0.0176

Table 3. Table of error estimates for $N=750$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	0.0032	0.0032	0.0028	0.0027	0.0025	0.0024
$L^\infty\mathbf{E}$	0.0278	0.0261	0.0209	0.0198	0.0187	0.0177

Table 4. Table of error estimates for $N = 800$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	0.0032	0.0032	0.0028	0.0027	0.0026	0.0025
$L^\infty\mathbf{E}$	0.0279	0.0262	0.0210	0.0199	0.0188	0.0178

2. With finite elements

Under the same conditions we have the following error tables:

Table 5. Table of error estimates for $N = 650$

M^2	100	121	225	256	289	394
$L^2\mathbf{E}$	7.8840e-5	7.7118e-5	6.9223e-5	6.7598e-5	6.5523e-5	6.3405e-5
$L^\infty\mathbf{E}$	8.8640e-4	8.8608e-4	8.3587e-4	8.2137e-4	8.0619e-4	7.9039e-4

Table 6. Table of error estimates for $N = 700$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	6.9680e-5	6.8159e-5	6.1541e-5	5.9755e-5	5.7922e-5	5.6049e-5
$L^\infty\mathbf{E}$	7.9367e-4	7.8671e-4	7.4306e-4	7.3041e-4	7.1715e-4	7.0333e-4

Table 7. Table of error estimates for $N = 750$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	6.1701e-5	6.0326e-5	5.4429e-5	5.2840e-5	5.1209e-5	4.9540e-5
$L^\infty\mathbf{E}$	7.0787e-4	7.0003e-4	6.6173e-4	6.5060e-4	6.3892e-4	6.2672e-4

Table 8. Table of error estimates for $N = 800$

M^2	100	121	225	256	289	324
$L^2\mathbf{E}$	5.4664e-5	5.3418e-5	4.8123e-5	4.6699e-5	4.5277e-5	4.3740e-5
$L^\infty\mathbf{E}$	6.3067e-4	3.2374e-4	5.8887e-4	5.8000e-4	5.6963e-4	5.5879e-4

–

4.1.2. If the CFL condition is not satisfied

In this case we have the following conditions:

$$M^2 \geq \frac{N-\sigma}{4\mu} \text{ or } N \leq \sigma + 4\mu M^2.$$

By setting the smallest value of N to 300, we have $M^2 \leq 150.5$.
We vary the number of nodes M^2 from 225 to 1600.

1. By the finite difference method: Euler explicit

Table 9. Table of error estimates for $N = 300$

M^2	225	400	625	900	1225	1600
$L^2\mathbf{E}$	2.1906e-4	0.1173	8.5897e+04	8.9762e+13	8.5315e+24	2.0578e+37
$L^\infty\mathbf{E}$	0.0070	0.1630	199.1878	7.9483e+06	2.6602e+12	4.2928e+18

Table 10. Table of error estimates for $N = 400$

M^2	225	400	625	900	1225	1600
$L^2\mathbf{E}$	6.9170e-04	1.3595e-04	2.7236	1.0938e+07	2.3131e+16	2.1657e+27
$L^\infty\mathbf{E}$	0.0109	0.0090	0.7777	2.3090e+03	1.2711e+08	4.2002e+13

2. With finite elements

Table 11. Table of error estimates for $N = 300$

M^2	225	400	625	300	1225	1600
$L^2\mathbf{E}$	2.3754e-04	1.5003e-04	1.1797e-04	9.0410e-05	6.7562e-05	2.1820e-05
$L^\infty\mathbf{E}$	0.0028	0.0019	0.0016	0.0013	0.0011	0.0009

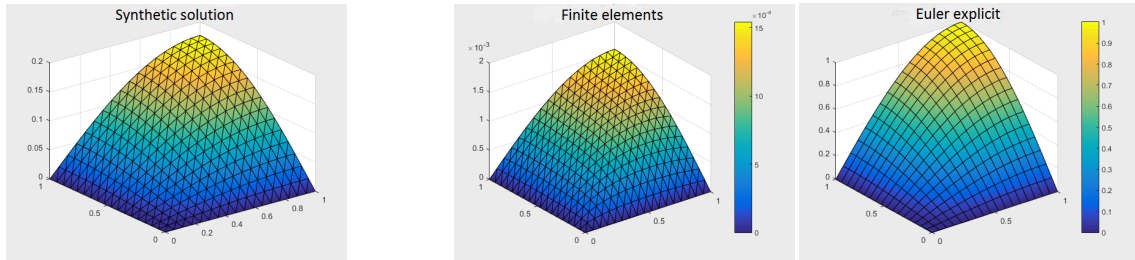
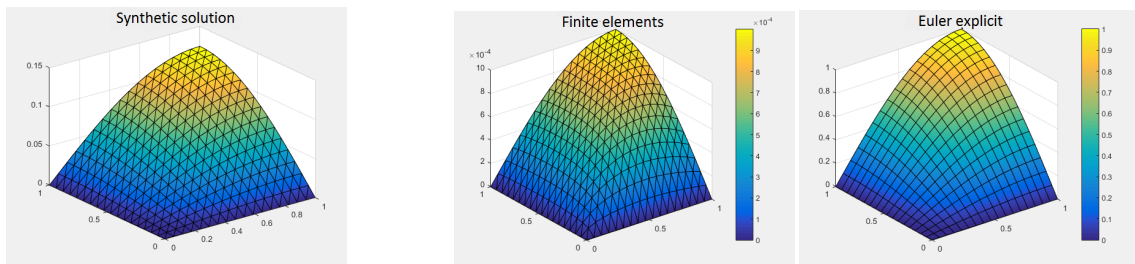
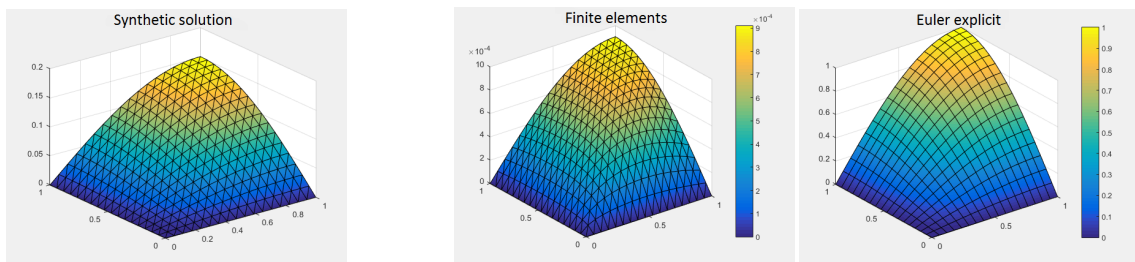
Table 12. Table of error estimates for $N = 400$

M^2	225	400	625	900	1225	1600
$L^2\mathbf{E}$	1.3578e-04	1.1221e-04	9.0025e-05	6.9988e-05	5.2668e-05	1.5579e-05
$L^\infty\mathbf{E}$	0.0029	0.0014	0.0012	0.0010	8.4198e-04	3.5127e-04

4.2. Simulations

4.2.1. If the CFL is satisfied

With $\alpha_1 = 5$, $\alpha_2 = 10$, $\mu = 0.5$ et $\sigma = 1$

**Fig. 1.** solutions for $M^2 = 324$, $N = 650$ **Fig. 2.** solutions for $M^2 = 324$, $N = 700$ **Fig. 3.** solutions for $M^2 = 324$, $N = 800$

4.2.2. The CFL condition is not satisfied

1. After analysis of the results recorded in tables (1) - (4) for finite differences and tables (5) - (8) for finite elements, it appears that if the CFL condition (66) is respected, the finite element method gives us very satisfactory results with very low errors, when the time and space steps increase. The finite difference method converges by varying the number of nodes with a fixed time step. However, it should be noted that the error values obtained by the finite element method are smaller than those obtained by the finite difference method when we compare the tables for a given time step value.

Moreover, by reading the tables in columns (which implies that we fix the time step by varying the space steps), we can see that the errors in finite differences vary in a very slight way but still increase, while they decrease with the second method.

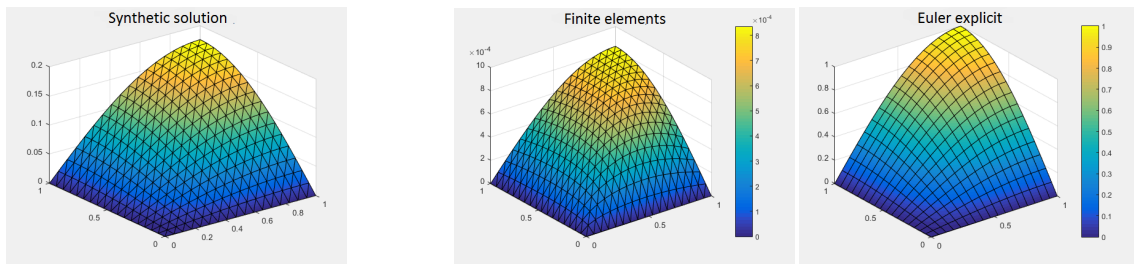


Fig. 4. solutions for $M^2 = 324, N = 900$

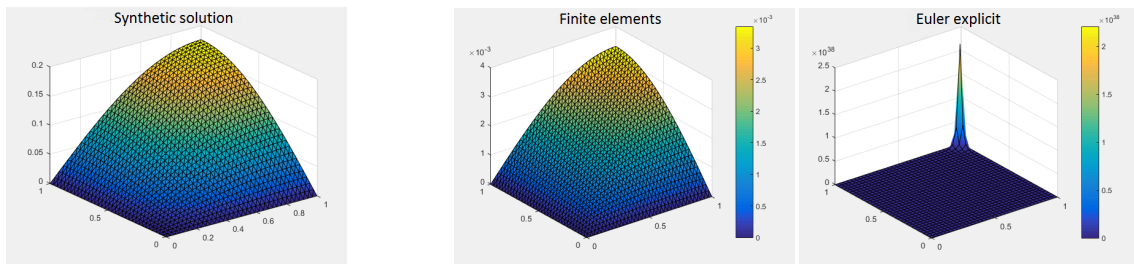


Fig. 5. solutions for $M^2 = 1225, N = 300$

Moreover, by analyzing tables (9) and (10), we can say that the errors decrease as long as the CFL condition is respected. However, if we leave the framework of this condition, we can observe a rapid increase of the errors found: the solution blows up.

With the finite element method, by observing tables (11) and (12), the situation does not change whether the CFL condition is respected or not. The errors decrease and have very low values compared to those observed for the first method.

We could add that given the very low values of the errors found, the finite element method reveals an efficiency for the resolution of such problems.

2. The graphs below allow us to observe the approximate solutions obtained using the finite element and finite difference methods and to compare them to the synthetic solution.

We have first fixed the space step to 324 and varied N . Thus in each case, the synthetic solution obtained after implementation in Matlab environment is represented on the left and on the right the solutions obtained by the finite element method and the finite difference method (in order).

Figures (1) - (4) show that the solutions obtained by both methods converge to the synthetic solution. However, we can notice that the finite element method is more accurate than the finite difference method. The observation is not the same on figure (5) where we can see that the solution explodes in finite differences when the CFL condition is not respected.

5. Conclusion

In this paper the resolution and the numerical simulation of a pollution model in a bounded domain of the atmosphere in dimension two of space using the variational formulation has been done, after the study of the existence and uniqueness of the solution. Two numerical methods were used: the finite difference method and the finite element method.

At the end of this study, it was found that the finite element method is more suitable and more efficient for the numerical solution of our problem.

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