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RESOLUTION AND NUMERICAL SIMULATION OF AN OPTIMAL CONTROL PROBLEM OF SURFACE WATER POLLUTION

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Abstract: We present in this paper the resolution and numerical simulation of an optimal control problem of surface water pollution. This resolution is based on vectorized implementation under Matlab of the $P^1 + bulle/P^1$ method for the resolution of the constraints which govern the transport and dissolution equations of the pollutants coupled with the Navier-Stokes equations in three dimension of space and the differentiation-discretization approach to analyze the optimization problem with constraints.

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1. Introduction

The aim of this article is the resolution and numerical simulation of an optimal control problem of surface water pollution with constraints which are

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modeled by a coupling of partial differential equations. The interest of this work is double, on the one hand we use nonlinear optimization to solve the problem because the state equations are nonlinear. This method consists in transforming the optimization problem with constraints into an optimization problem without constraints via Lagrange multipliers leading thus to the adjoint equations and the first-order optimality conditions. The optimal system thus obtained is consisted PDE which in general do not analytical solutions. It is then necessary to use numerical approaches for solving these equations. We chose the differentiation-discretization approach which consists in approaching the state equations and the cost functional calculus in continuous form to determine the adjoint equations of the problem and the optimalities conditions, equations which it remains to discretize to solve them.

On the other hand, we implement a vectorized implementation of the $P^1 + bubble/P^1$ method with Matlab because the classical operations of assembly are often less powerful and while taking up to 99% of the computing time CPU [7] for finite elements codes of linear elasticity.

The outline of this paper is as following: In the second part we present mathematical model which was the subject of our study in this paper. The third section is devoted the numerical resolution of the model by using the characteristics method and $P^1 + bulle/P^1$ method in three dimension of space. The fourth section is devoted to implementation of the optimization algorithm and the last part we present some numerical simulations and validation of our schema.

2. The Model Problem

Let Ω be a bounded domain of $\mathbb{R}^3$, with boundary Γ sufficiently regular. We denote by $\vec{x} = (x, y, z)$ an element of Ω.

We consider the following model:

$$\min J(v) = \frac{1}{2}\int_0^T \int_\Omega |c(v) - z_d|^2 d\vec{x}\, dt + \frac{N}{2}\int_0^T \int_\Omega |v|^2 d\vec{x}\, dt, \qquad (2.1)$$

subject to

$$\begin{cases} \frac{\partial c}{\partial t} + \sum_{i=1}^{3} \frac{\partial (u_i c)}{\partial x_i} - d\Delta c = g + v & \text{in } \Omega \times]0,T[\quad (2.a) \\ c = 0 & \text{on } \Gamma \times]0,T[\quad (2.b) \\ c(.,0) = c_0, & \text{in } \Omega \quad (2.c) \\ \frac{\partial u}{\partial t} + (u.\nabla)u - \nu\Delta u + \nabla p = f & \text{in } \Omega \times]0,T[\quad (2.d) \\ div\, u = 0 & \text{in } \Omega \times]0,T[\quad (2.e) \\ u = 0, & \text{on } \Gamma \times]0,T[\quad (2.f) \\ u(.,0) = u_0 & \text{in } \Omega \quad (2.g) \end{cases} \tag{2.2}$$

where:

- z_d is an observation function, D is a given linear continuous operator of observation, N a given positif real;
- c denotes the concentration of pollutants, g is a source term, d is a coefficient of diffusion, v represented the control which allows to act on the system;
- $u = (u_1, u_2, u_3)$ and $p = p(\vec{x}, t)$ denote respectively the velocity and the pressure of water, f external forces, ν the kinematic viscosity;
- Equations (2.a)-(2.c) modelling the transport and dissolution of pollutants;
- Systems (2.d)-(2.g) is Navier-Stokes equations.

We rewrite problems (2.1)-(2.2) in the following compact form:

$$\begin{cases} Find \quad u \in U_{ad} \quad \text{such that} \;: \\ J(u) = \min_{v \in U_{ad}} J(v) \end{cases} \tag{2.3}$$

where U_{ad} denotes set of admissible controls.

Existence and uniqueness of solution of the problem (2.4) has been the subject of several studies [5].

2.1. Resolution of Problem (2.1)-(2.2)

We write the transport and dissolution equations of the pollutants in the following conservative form:

$$\mathcal{L}_c(c) = \frac{\partial c}{\partial t} + \nabla(uc) - d\Delta c - g - v = 0, \tag{2.4}$$

where g is a source terme and v distributed control.

Equation (2.4) will be solved in the domain D defined by:

$$D = \{(\vec{x}, t) \in \Omega \times [0, T]\} \text{ where } \Omega = [0, 1]^3\},$$

and we will assume the existence of an initial condition given by:

$$c(\vec{x}, 0) = c_0(\vec{x}) \tag{2.5}$$

and boundary conditions

$$c(\vec{x}, t) = q \text{ with } \vec{x} \in \Gamma. \tag{2.6}$$

Let us introduce the Lagrangian associated with the problem (2.1)-(2.2) defined by:

$$L(c, v, c^*, q^*) = J(c, v) - \Big(\frac{\partial c}{\partial t} + \nabla(uc) - d\Delta c - g - v, c^*\Big)_D - (c(\vec{x}, t) - q, q^*)_t \tag{2.7}$$

where

$$(a, b)_D = \int_0^T \int_\Omega ab \, d\vec{x} \, dt$$

$$(a, b)_t = \int_0^T ab \, dt \text{ and } c^*, q^* \text{ denotes Lagrange multipliers .}$$

Using relation (2.1) we rewrite L in the form:

$$L(c, v, c^*, q^*) = \frac{1}{2} \int_0^T \int_\Omega |c(v) - z_d|^2 d\vec{x} \, dt + \frac{N}{2} \int_0^T \int_\Omega |v|^2 d\vec{x} \, dt \tag{2.8}$$

$$- \int_0^T \int_\Omega (\frac{\partial c}{\partial t} + \nabla(uc) - d\Delta c - g - v) c^* d\vec{x} \, dt - \int_0^T (c - q) q^* dt$$

We know that the function L admits an extremum if it is constant with respect to each of its arguments, so that we have the following relation:

$$\delta L = \frac{\partial L}{\partial c} \delta c + \frac{\partial L}{\partial v} \delta v + \frac{\partial L}{\partial c^*} \delta c^* + \frac{\partial L}{\partial q^*} \delta q^* = 0 \tag{2.9}$$

We assume that the arguments of L are independent of each other, the Fréchet derivative of L must be identically zero in all admissible directions so that

$$\frac{\partial L}{\partial c} \delta c = \frac{\partial L}{\partial v} \delta v = \frac{\partial L}{\partial c^*} \delta c^* = \frac{\partial L}{\partial q^*} \delta q^* = 0 \tag{2.10}$$

$$\frac{\partial L}{\partial c}\delta c = \int_0^T \int_\Omega (c(v) - z_d)\delta c \, d\vec{x} \, dt$$
$$- \Big(\int_0^T \int_\Omega \Big(\frac{\partial(\delta c)}{\partial t} + \nabla(u\delta c) - d\Delta(\delta c) \Big) c^* d\vec{x} \, dt$$
$$- \int_0^T (\delta c(\vec{x}, t)) q^* dt = 0. \quad (2.11)$$

$$- \int_0^T \int_\Omega \frac{\partial(\delta c)}{\partial t} c^* d\vec{x} \, dt = - \int_\Omega [\delta c \, c^*]_0^T dt + \int_0^T \int_\Omega \delta c \frac{\partial \, c^*}{\partial t} d\vec{x} \, dt$$

$$- \int_0^T \int_\Omega \nabla(u\delta c) c^* d\vec{x} \, dt = - \int_0^T \int_\Gamma u\delta c c^* d\vec{x} \, dt + \int_0^T \int_\Omega \delta c (u \nabla c^*) d\vec{x} \, dt$$

$$\int_0^T \int_\Omega d\Delta(\delta c) c^* d\vec{x} \, dt = d \int_0^T \int_\Gamma \nabla(\delta c) c^* d\vec{x} \, dt - d \int_0^T \int_\Omega \nabla(\delta c) \nabla c^* d\vec{x} \, dt =$$
$$d \int_0^T \int_\Gamma \nabla(\delta c) c^* d\vec{x} \, dt - d \int_0^T \int_\Gamma \delta c \nabla c^* d\vec{x} \, dt + d \int_0^T \int_\Omega \delta c \Delta c^* d\vec{x} \, dt.$$

Then we have:

$$\frac{\partial L}{\partial c}\delta c = \int_0^T \int_\Omega \Big(\frac{\partial c^*}{\partial t} + u\nabla c^* + d\Delta c^* + c - z_d \Big) \delta c d\vec{x} \, dt$$
$$- \int_\Omega \Big(\delta c(\vec{x}, T) c^*(\vec{x}, T) - \delta c(\vec{x}, 0) c^*(\vec{x}, 0) \Big) d\vec{x} \quad (2.12)$$

$$- \int_0^T \int_\Gamma u\delta c c^* d\vec{x} \, dt + d \int_0^T \int_\Gamma \nabla(\delta c) c^* d\vec{x} \, dt - d \int_0^T \int_\Gamma \delta c \nabla c^* d\vec{x} \, dt = 0$$

Problem (2.11) must be satisfied whatever the disturbance δc, the following cases may be considered successively:

- $\delta c \neq 0$ and all other variational factors are assumed to be zero

$$- \frac{\partial c^*}{\partial t} - u\nabla c^* - d\Delta c^* = c - z_d \quad (2.13)$$

  Problem (2.13) to be well posed, it will therefore be necessary to provide it with a terminal condition.

- $\delta c(\vec{x}, T) \neq 0$ and all other variational factors are assumed to be zero, we obtain the terminal condition of the adjoint problem:

$$c^*(\vec{x}, T) = 0 \quad (2.14)$$

- $\nabla(\delta c) \neq 0$ and all other variational factors are assumed to be zero, we obtain
$$c^*(\vec{x}, t) = 0 \quad \vec{x} \in \Gamma. \tag{2.15}$$

We deduce the adjoint equation given by:

$$-\frac{\partial c^*}{\partial t} - u\nabla c^* - d\Delta c^* = c - z_d \tag{2.16}$$
$$c^* = 0 \tag{2.17}$$
$$c^*(\vec{x}, T) = 0 \tag{2.18}$$

$$\frac{\partial L}{\partial v}\delta v = \int_0^T \int_\Omega \delta v(Nv + c^*) d\vec{x}\, dt = 0. \tag{2.19}$$

This condition must be verified whatever the perturbation δv, it must be so in the particular case where $\delta\, v \neq 0$, we have then:

$$Nv + c^* = 0 \tag{2.20}$$

This condition is verified exactly when the minimum of L is achieved, otherwise it can be considered that the gradient of the functional J with respect to the distributed control term v, then we obtain the optimal condition given by:

$$\nabla_v J = Nv + c^* \tag{2.21}$$

3. Numerical Resolution of the Problem (2.1)-(2.2)

Consider a triangulation of the domain by tetrahedrons $(T_k)_{k\geq 1}$. The coordinates of nodes and vertices of the tetrahedra are stored in two tables which are denoted by $pn(1 : np, 1 : 3)$ and $te(1 : nt, 1 : 4)$, where np is the number of nodes and nt the number of tetrahedra. The table te contains for each element the vertex numbers in the trigonometric direction. Denote by $(\hat{T}_k) = \{(0,0,0); (1,0,0); (0,1,0); (0,0,1)\}$ the reference tetrahedron. For a given integer $N_0 \geq 1$, we suppose a regular triangulation of Ω_h *i.e*

$$\Omega_h = \bigcup_{k=1}^{N_0} T_k$$

To discretize the system (2.2), it is necessary to choose a finite elements pair for the velocity and the pressure, this choice cannot be arbitrary but must satisfy the inf-sup condition [3, 4]. We choose in this work the $P_1 + bubble/P_1$ pair introduced by Arnold, Brezzi and Fortin [1] Since this element leads to a relatively small number of degrees of freedom with a relatively good approximate solution.

We define by P_1 the polynomials space with three variables of degree 1.

We define on the reference tetrahedron the basic functions by:

$$\begin{cases} \hat{\lambda}_1 = 1 - (\hat{x}_1 + \hat{x}_2 + \hat{x}_3) \\ \hat{\lambda}_2 = \hat{x}_1 \\ \hat{\lambda}_3 = \hat{x}_2 \\ \hat{\lambda}_4 = \hat{x}_3 \end{cases} \tag{3.1}$$

and the bubble function by:

$$\hat{\lambda}_b = 256\hat{\lambda}_1\hat{\lambda}_2\hat{\lambda}_3\hat{\lambda}_4. \tag{3.2}$$

We also defined a bijective transformation Π_{T_k} from the reference tetrahedron on a current one by $\Pi_{T_k}(\hat{T}_k) = T_k$, then we have for all $\hat{x} \in \hat{T}_k$, $\Pi_{T_k}(\hat{x}) = A_{T_k}\hat{x} + b_{T_k}$ where

$$A_{T_k} = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{pmatrix} \tag{3.3}$$

is the Jacobian of Π_{T_k} and

$$b_{T_k} = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} \tag{3.4}$$

is a vector. It's easy to verify that

$$|det\, A_{T_k}| = 6|T_k|, \tag{3.5}$$

where $|T_k|$ is the tetrahedron volume.

Given a current tetrahedron T_k of vertices $(a_i)_{i=1,\cdots,4}$, we approach the solutions u, p and c by the following formula:

$$u_h(\vec{x}, t) = \sum_{i=1}^{4} \lambda_i(\vec{x})u_i(t) + \lambda_b(\vec{x})u_b(t), \quad t \in [0, T], \quad \vec{x} \in T_k. \tag{3.6}$$

$$p_h(\vec{x}, t) = \sum_{i=1}^{4} \lambda_i(\vec{x})p_i(t), \quad t \in [0, T], \quad \vec{x} \in T_k \tag{3.7}$$

$$c_h(\vec{x},t)=\sum_{i=1}^{4}\lambda_i(\vec{x})c_i(t),\quad t\in[0,T],\quad \vec{x}\in T_k, \tag{3.8}$$

where $u_i(t)$, $p_i(t)$, $c_i(t)$ are the nodal values of u_h, p_h, c_h while $u_b(t)$ is the bubble value and $\{\lambda_i(\vec{x})\}$ are the basic functions on a current tetrahedron. Applying inverse transformation $\Pi_{T_k}^{-1}$ to relations (3.6)-(3.8), we can approach u, p and c in the reference tetrahedron by:

$$u_h(\vec{\hat{x}},t)=\sum_{i=1}^{4}\hat{\lambda}_i(\vec{\hat{x}})u_i(t)+\hat{\lambda}_b(\vec{\hat{x}})u_b(t),\quad t\in[0,T],\quad \vec{\hat{x}}\in\hat{T}_k \tag{3.9}$$

$$p_h(\vec{\hat{x}},t)=\sum_{i=1}^{4}\hat{\lambda}_i(\vec{\hat{x}})p_i(t),\quad t\in[0,T],\quad \vec{\hat{x}}\in\hat{T}_k \tag{3.10}$$

$$c_h(\vec{\hat{x}},t)=\sum_{i=1}^{4}\hat{\lambda}_i(\vec{\hat{x}})c_i(t),\quad t\in[0,T],\quad \vec{\hat{x}}\in\hat{T}_k \tag{3.11}$$

We set

$$\bar{u}_i=\begin{pmatrix}u_i(t)\\u_b(t)\end{pmatrix}\quad\text{and}\quad\bar{f}_i=\begin{pmatrix}f_i(t)\\f_b(t)\end{pmatrix} \tag{3.12}$$

3.1. Approximation of (2.2)

Let $S\in\mathbb{N}^*$ a given integer, we denote by $\Delta t=\frac{T}{S}$ the time discretization step, we subdivide $[0,T]$ into S subintervals $[t_n,t_{n+1}]$, $n\in[0,S]$ where $t_n=n\Delta t$, $n\geq 0$.

Rewriting the first and the forth equations of the problem (2.2) as

$$\frac{Dc}{Dt}-d\Delta c = g+v, \tag{3.13}$$

$$\frac{Du}{Dt}-\nu\Delta u = f, \tag{3.14}$$

where

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t}+(u.\nabla)c \tag{3.15}$$

$$\frac{Du}{Dt} = \frac{\partial u}{\partial t}+(u.\nabla)u, \tag{3.16}$$

and approaching $\frac{Dc}{Dt}$ and $\frac{Du}{Dt}$ by:

$$\frac{Dc}{Dt}(t_{n+1},\vec{x})=\frac{c(t_{n+1},\vec{x})-c(t_n,X^n(\vec{x}))}{\Delta t}+o(\Delta t), \tag{3.17}$$

$$\frac{Du}{Dt}(t_{n+1},\vec{x}) = \frac{u(t_{n+1},\vec{x}) - u(t_n, X^n(\vec{x}))}{\Delta t} + o(\Delta t), \tag{3.18}$$

where $X^n(\vec{x})$ represents the particule position at time t_n.
We obtain the following approximation of the model (2.2):

$$\begin{aligned}
\frac{c(t_{n+1},\vec{x}) - c(t_n, X^n(\vec{x}))}{\Delta t} - d\Delta c(t_{n+1},\vec{x}) &= g(t_{n+1},\vec{x}) + v(t_{n+1},\vec{x}), &(3.19)\\
c(t_{n+1},\vec{x}) &= c^\Gamma(t_{n+1},\vec{x}), \quad \vec{x}\in\Gamma &(3.20)\\
c(0,\vec{x}) &= c_0(\vec{x}), \quad \vec{x}\in\Omega &(3.21)\\
\frac{u(t_{n+1},\vec{x}) - u(t_n, X^n(\vec{x}))}{\Delta t} - \nu\Delta u(t_{n+1},\vec{x}) + \nabla p(t_{n+1},\vec{x}) &= f(t_{n+1},\vec{x}), \quad \vec{x}\in\Omega &(3.22)\\
div u(t_{n+1},\vec{x}) &= 0, \quad \vec{x}\in\Omega &(3.23)\\
u(t_{n+1},\vec{x}) &= u^\Gamma(t_{n+1},\vec{x}), \quad \vec{x}\in\Gamma &(3.24)\\
u(0,\vec{x}) &= u_0(\vec{x}), \quad \vec{x}\in\Omega &(3.25)
\end{aligned}$$

Let $c(t_n, X^n(\vec{x})) = c^n o X^n$ and $u(t_n, X^n(\vec{x})) = u^n o X^n$, then equations (3.19)-(3.25) become:

$$\begin{aligned}
\frac{1}{\Delta t}c^{n+1}(\vec{x}) - d\Delta c^{n+1}(\vec{x}) &= g^{n+1}(\vec{x} + v(t_{n+1},\vec{x})) + \frac{1}{\Delta t}c^n o X^n(\vec{x}), &(3.26)\\
c^{n+1}(\vec{x}) &= c^\Gamma(t_{n+1},\vec{x}), \quad \vec{x}\in\Gamma &(3.27)\\
c^0(\vec{x}) &= c_0(\vec{x}), \quad \vec{x}\in\Omega &(3.28)\\
\frac{1}{\Delta t}u^{n+1}(\vec{x}) - \nu\Delta u^{n+1}(\vec{x}) + \nabla p^{n+1}(\vec{x}) &= f^{n+1}(\vec{x}) + \frac{1}{\Delta t}u^n o X^n(\vec{x}), \quad \vec{x}\in\Omega &(3.29)\\
div u^{n+1} &= 0, \quad \vec{x}\in\Omega &(3.30)\\
u^{n+1}(\vec{x}) &= u^\Gamma(t_{n+1},\vec{x}), \quad \vec{x}\in\Gamma &(3.31)\\
u^0(\vec{x}) &= u_0(\vec{x}), \quad \vec{x}\in\Omega. &(3.32)
\end{aligned}$$

Using the following Taylor development of $X^n(\vec{x})$: $X^n(\vec{x}) = \vec{x} - \Delta t u^n(\vec{x}) + o(\Delta t^2)$ with u^n is known to step n, by meshed the second term; we can approximate $X^n(\vec{x})$ by $X^n(\vec{x}) \approx \vec{x} - \Delta t u^n(\vec{x})$.

To approximate in space the equation (2.2), we consider the following spaces:

$$V_{0i}^D = \Big\{s \in H^1(\Omega) : s = u^D \text{ or } s = c^D \text{ in } \Gamma\Big\}, \qquad V_0^D = V_{01}^D \times V_{02}^D \times V_{03}^D,$$

$$V_{0i} = H_0^1(\Omega), \qquad V_0 = V_{01} \times V_{02} \times V_{03},$$

$$P = \Big\{r \in L^2(\Omega) : \int_\Omega r d\vec{x} = 0\Big\}.$$

We also introduce discrete spaces for the approximation of velocity, pressure and concentration.

The space associated the bubble function:

$$B_h = \{s_h \in \mathcal{C}^0(\overline{\Omega}), \forall T_k \in \Omega_h, s_h/T_k = \vec{x}b^{(T_k)}\}$$

$$V_{ih} = \{s_h \in \mathcal{C}^0(\overline{\Omega}), s_h/T_k \in P^1, \forall T_k \in \Omega_h, s_h/\Gamma = 0\}$$

$$V_{ih}^D = \{s_h \in \mathcal{C}^0(\overline{\Omega}), s_h/T_k \in P^1, \forall T_k \in \Omega_h, s_h/\Gamma = u_{ih}^D \text{ or } s_h/\Gamma = c_{ih}^D\}$$

$$P_h = \{r_h \in \mathcal{C}^0(\overline{\Omega}), r_h/T_k \in P^1, \forall T_k \in \Omega_h, \int_\Omega r_h/\Gamma = 0\},$$

and we have

$$X_{ih} = V_{ih} \oplus B_h, \qquad X_{ih}^D = V_{ih}^D \oplus B_h \tag{3.33}$$

$$X_h = X_{1h} \times X_{2h} \times X_{3h}, \qquad X_h^D = X_{1h}^D \times X_{2h}^D \times X_{3h}^D \tag{3.34}$$

In X_h^D Dirichlet condition must satisfy:

$$\int_\Omega u_h^D.\vec{n}d\vec{x} = 0,$$

$\vec{n}$ where n is the normal external vector of the domain Ω.

Multiply (3.26), (3.29) and (3.30) by tests functions $w \in [H_0^1(\Omega)]$, $y \in V_0^D$ and $r \in P$ respectively and integrate by parts, we obtain:

$$\frac{1}{\Delta t}\int_\Omega c^{n+1}w - d\int_\Omega \Delta c^{n+1}w = \int_\Omega (g^{n+1} + v^{n+1})w + \frac{1}{\Delta t}\int_\Omega c^n o X^n(\vec{x})w \tag{3.35}$$

$$\frac{1}{\Delta t}\int_\Omega \bar{u}^{n+1}y - \nu\int_\Omega \Delta\bar{u}^{n+1}y + \int_\Omega \nabla p^{n+1}y = \int_\Omega \bar{f}^{n+1}y + \frac{1}{\Delta t}\int_\Omega u^n o X^n(\vec{x})y \tag{3.36}$$

$$\int_\Omega r div\bar{u}^{n+1} = 0 \tag{3.37}$$

Appying Green's formula to relations (3.35) and (3.36), we obtain:

$$\frac{1}{\Delta t}\int_\Omega c^{n+1}w + d\int_\Omega \nabla c^{n+1}\nabla w = \int_\Omega (g^{n+1} + v^{n+1})w + \frac{1}{\Delta t}\int_\Omega c^n o X^n(\vec{x})w \tag{3.38}$$

$$\frac{1}{\Delta t}\int_\Omega \bar{u}^{n+1}y + \nu\int_\Omega \nabla\bar{u}^{n+1}\nabla y - \int_\Omega p^{n+1}\nabla y = \int_\Omega \bar{f}^{n+1}y + \frac{1}{\Delta t}\int_\Omega u^n o X^n(\vec{x})y \tag{3.39}$$

$$\int_\Omega r div\bar{u}^{n+1} = 0 \tag{3.40}$$

Let denote by $c_h \in V_{ih}^D$, $\bar{u}_h \in X_h^D$ and $r_h \in P_h$ approximation of c, u and p respectively in the basis $\{\lambda_j\}$ we obtain:

$$c_h(\vec{x}, t) = \sum_{j=1}^{V_{ih}^D} \lambda_j(\vec{x})c_j(t) \tag{3.41}$$

$$\bar{u}_{ih}(\vec{x}, t) = \sum_{j=1}^{X_h^D} \lambda_j(\vec{x})\bar{u}_{ij}(t) \quad i = 1, 2, 3 \tag{3.42}$$

$$p_h(\vec{x},t) = \sum_{j=1}^{P_h} \lambda_j(\vec{x}) p_j(t) \tag{3.43}$$

Injecting relation (3.41), (3.42) and (3.43) in (3.38)-(3.40) we obtain:

$$\frac{1}{\Delta t} \sum_{j=1}^{NV_{ih}^D} c_j^{n+1} \int_\Omega \lambda_j w_h + d \sum_{j=1}^{NV_{ih}^D} c_j^{n+1} \int_\Omega \nabla\lambda_j \nabla w_h \tag{3.44}$$

$$= \int_\Omega g^{n+1} w_h + \int_\Omega v^{n+1} w_h + \frac{1}{\Delta t} \int_\Omega (c^n o X^n) w_h \tag{3.45}$$

$$\frac{1}{\Delta t} \sum_{j=1}^{NX_h^D} \bar{u}_{ij}^{n+1} \int_\Omega \lambda_j y_h + d \sum_{j=1}^{NX_h^D} \bar{u}_{ij}^{n+1} \int_\Omega \nabla\lambda_j \nabla y_h - \sum_{l=1}^{NP_h} p_j^{n+1} \int_\Omega \nabla\lambda_j y_h \tag{3.46}$$

$$= \int_\Omega \bar{f}^{n+1} y_h + \frac{1}{\Delta t} \int_\Omega (u_i^n o X^n) y_h \tag{3.47}$$

$$\sum_{j=1}^{N_{X_h^D}} \bar{u}_{ij}^{n+1} \int_\Omega r_h div \lambda_j = 0 \tag{3.48}$$

Choosing $w_h = y_h = r_h = \lambda_k$, we obtain

$$\frac{1}{\Delta t} \sum_{j=1}^{NV_{ih}^D} c_j^{n+1} \int_\Omega \lambda_j \lambda_k + d \sum_{j=1}^{NV_{ih}^D} c_j^{n+1} \int_\Omega \nabla\lambda_j \nabla \lambda_k \tag{3.49}$$

$$= \int_\Omega g^{n+1} \lambda_k + \int_\Omega v^{n+1} \lambda_k + \frac{1}{\Delta t} \int_\Omega (c^n o X^n) \lambda_k \tag{3.50}$$

$$\frac{1}{\Delta t} \sum_{j=1}^{NX_h^D} \bar{u}_{ij}^{n+1} \int_\Omega \lambda_j \lambda_k + d \sum_{j=1}^{NX_h^D} \bar{u}_{ij}^{n+1} \int_\Omega \nabla\lambda_j \nabla \lambda_k - \sum_{l=1}^{NP_h} p_j^{n+1} \int_\Omega \nabla\lambda_j \lambda_k \tag{3.51}$$

$$= \int_\Omega \bar{f}^{n+1} \lambda_k + \frac{1}{\Delta t} \int_\Omega (u_i^n o X^n) \lambda_k \tag{3.52}$$

$$\sum_{j=1}^{N_{X_h^D}} \bar{u}_{ij}^{n+1} \int_\Omega \lambda_k div \lambda_j = 0 \tag{3.53}$$

System (3.50)-(3.53) can be rewritten in the following algebraic form:

$$\begin{pmatrix} A_0 & 0 & 0 & 0 & 0 \\ 0 & \bar{A} & 0 & 0 & -\bar{B}_1^t \\ 0 & 0 & \bar{A} & 0 & -\bar{B}_2^t \\ 0 & 0 & 0 & \bar{A} & -\bar{B}_3^t \\ 0 & -\bar{B}_1 & -\bar{B}_2 & -\bar{B}_3 & 0 \end{pmatrix} \begin{pmatrix} c^{n+1} \\ \bar{u}_1^{n+1} \\ \bar{u}_2^{n+1} \\ \bar{u}_3^{n+1} \\ p^{n+1} \end{pmatrix}$$
$$= \begin{pmatrix} G^{n+1} + V^{n+1} \\ \bar{F}_1^{n+1} \\ \bar{F}_2^{n+1} \\ \bar{F}_3^{n+1} \\ 0 \end{pmatrix} + \begin{pmatrix} b_0^n \\ b_1^n \\ b_2^n \\ b_3^n \\ 0 \end{pmatrix}, \quad (3.54)$$

where $A_0 = M + dK$, $\bar{A} = \bar{M} + \nu\bar{K}$ with $\bar{M}$ and M mass matrices with and without bubble respectively, $\bar{K}$ and K stiffness matrices with and without bubble respectively and $\bar{B}_i$ the divergence matrix defined by:

$$\bar{M}_{jk} = \int_{\Omega_h} \frac{1}{\Delta t}\lambda_j(\vec{x})\lambda_k(\vec{x}) \quad (3.55)$$

$$\bar{K}_{jk} = \int_{\Omega_h} \nabla\lambda_j(\vec{x})\nabla\lambda_k(\vec{x}) \quad (3.56)$$

$$\bar{B}_{jk} = \int_{\Omega_h} \partial_1\lambda_j(\vec{x})\lambda_k(\vec{x}) + \partial_2\lambda_j(\vec{x})\lambda_k(\vec{x}) + \partial_3\lambda_j(\vec{x})\lambda_k(\vec{x}) \quad (3.57)$$

$$G_j = \int_{\Omega_h} g^{n+1}(\vec{x})\lambda_j(\vec{x}). \quad (3.58)$$

$$V_j = \int_{\Omega_h} v^{n+1}(\vec{x})\lambda_j(\vec{x}). \quad (3.59)$$

$$\bar{F}_{ij} = \int_{\Omega_h} \overline{f}_i^{n+1}(\vec{x})\lambda_j(\vec{x}) \quad i = 1,2,3 \quad (3.60)$$

$$b_{0j} = \int_{\Omega_h} (c^n o X^n)\lambda_j \quad (3.61)$$

$$b_{ij} = \int_{\Omega_h} (u_i^n o X^n)\lambda_j \quad i = 1,2,3 \quad (3.62)$$

Expressing the coefficients of mass matrices, stiffness, divergence and the second member on a current tetrahedron we obtain:

$$\bar{M}_{jk}^{T_k} = \int_{T_k} \frac{1}{\Delta t}\lambda_j(\vec{x})\lambda_k(\vec{x}) \quad (3.63)$$

$$\bar{K}_{jk}^{T_k} = \int_{T_k} \nabla\lambda_j(\vec{x})\nabla\lambda_k(\vec{x}) \tag{3.64}$$

$$\bar{B}_{jk}^{T_k} = \int_{T_k} \partial_1\lambda_j(\vec{x})\lambda_k(\vec{x}) + \partial_2\lambda_j(\vec{x})\lambda_k(\vec{x}) + \partial_3\lambda_j(\vec{x})\lambda_k(\vec{x}) \tag{3.65}$$

$$G_j^{T_k} = \int_{T_k} g^{n+1}(\vec{x})\lambda_j(\vec{x}) \tag{3.66}$$

$$V_j^{T_k} = \int_{T_k} v^{n+1}(\vec{x})\lambda_j(\vec{x}). \tag{3.67}$$

$$\bar{F}_{ij}^{T_k} = \int_{T_k} \overline{f}_i^{n+1}(\vec{x})\lambda_j(\vec{x}) \quad i = 1, 2, 3 \tag{3.68}$$

$$b_{0j}^{T_k} = \int_{T_k} (c^n o X^n)\lambda_j \tag{3.69}$$

$$b_{ij}^{T_k} = \int_{T_k} (u_i^n o X^n)\lambda_j \quad i = 1, 2, 3 \tag{3.70}$$

then

$$\bar{M}_{jk} = \sum_{T_k \in \Omega_h} \overline{M}_{jk}^{T_k}$$

$$\bar{K}_{jk} = \sum_{T_k \in \Omega_h} \overline{K}_{jk}^{T_k}$$

$$\bar{B}_{jk} = \sum_{T_k \in \Omega_h} \overline{B}_{jk}^{T_k}$$

$$G_j = \sum_{T_k \in \Omega_h} G_j^{T_k}$$

$$V_j = \sum_{T_k \in \Omega_h} V_j^{T_k}$$

$$\overline{F}_{ij} = \sum_{T_k \in \Omega_h} \overline{F}_{ij}^{T_k} \quad i = 1, 2, 3$$

$$b_{0j} = \sum_{T_k \in \Omega_h} b_{0j}^{T_k}$$

$$b_{ij} = \sum_{T_k \in \Omega_h} b_{ij}^{T_k} \quad i = 1, 2, 3$$

Applying the same technical in the previous section to the system (2.16)-(2.18), we obtain the matrix system:

$$(M - dK)c^{*^{n+1}} = -M_* c^{n+1} + ZD^{n+1} + b_4^n, \tag{3.71}$$

where

$$\begin{aligned} M_* &= \Delta t \, M \\ c^{*^n} &= \left(c_1^{*^n}, \cdots, c_{N_{V_{ih}^D}}^{*^n}\right)^t \\ ZD_j^{n+1} &= \int_{\Omega_h} zd^{n+1}\lambda_j \\ b_{4j}^n &= \int_{\Omega_h} \frac{1}{\Delta t}(c^{*^n} oX^n)\lambda_j. \end{aligned}$$

It is also ZD and b_4 over a current tetrahedron by:

$$ZD_j^{(n+1)T_k} = \int_{T_k} zd^{n+1}\lambda_j \tag{3.72}$$

$$b_{4j}^{(n)T_k} = \int_{T_k} \frac{1}{\Delta t}(c^{*^n} oX^n)\lambda_j, \tag{3.73}$$

then

$$ZD_j^{n+1} = \sum_{T_k \in \Omega_h} ZD_j^{(n+1)T_k} \tag{3.74}$$

$$b_{4j}^n = \sum_{T_k \in \Omega_h} b_{4i}^{(n)T_k}. \tag{3.75}$$

3.2. Assembling Matrices and Second Members

3.2.1. Assembling the Stiffness Matrix

For a current tetrahedron T_k of vertices $\{(x_i, y_i, z_i)\}_{i=1,2,3,4}$ and basis function $\{\lambda_i\}_{i=1,2,3,4}$, the gradients of λ_i are given by:

$$\begin{pmatrix} \nabla\lambda_1^t \\ \nabla\lambda_2^t \\ \nabla\lambda_3^t \\ \nabla\lambda_4^t \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ z_1 & z_2 & z_3 & z_4 \end{pmatrix}^{-1} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3.76}$$

$$= \frac{1}{6|T_k|}\begin{pmatrix} (y_4-y_2)(z_3-z_2)-(y_3-y_2)(z_4-z_2) & (x_3-x_2)(z_4-z_2)-(x_4-x_2)(z_3-z_2) \\ (y_3-y_1)(z_4-z_1)-(y_4-y_1)(z_3-z_1) & (x_4-x_1)(z_3-z_1)-(x_3-x_1)(z_4-z_1) \\ (y_4-y_1)(z_2-z_1)-(y_2-y_1)(z_4-z_1) & (x_2-x_1)(z_4-z_1)-(x_4-x_1)(z_2-z_1) \\ (y_2-y_1)(z_3-z_1)-(y_3-y_1)(z_4-z_1) & (x_3-x_1)(z_2-z_1)-(x_2-x_1)(z_3-z_1) \end{pmatrix.$$

$$\begin{matrix} (x_4-x_2)(y_3-y_2)-(x_3-x_2)(y_4-y_2) \\ (x_3-x_1)(y_4-y_1)-(x_4-x_1)(y_3-y_1) \\ (x_4-x_1)(y_2-y_1)-(x_2-x_1)(y_4-y_1) \\ (x_2-x_1)(y_3-y_1)-(x_3-x_1)(y_2-y_1) \end{pmatrix}, \quad (3.77)$$

where $|T_k|$ is tetrahedron volume given by:

$$6|T_k| = \det \begin{pmatrix} x_2-x_1 & x_3-x_1 & x_4-x_1 \\ y_2-y_1 & y_3-y_1 & y_4-y_1 \\ z_2-z_1 & z_3-z_1 & z_4-z_1 \end{pmatrix} \quad (3.78)$$

$$= (x_2-x_1)(y_3-y_1)(z_4-z_1)+(y_2-y_1)(z_3-z_1)(x_4-x_1)+(z_2-z_1)(x_3-x_1)(y_4-y_1) \quad (3.79)$$
$$-(z_2-z_1)(y_3-y_1)(z_4-z_1)-(x_2-x_1)(z_3-z_1)(y_4-y_1)-(y_2-y_1)(x_3-x_1)(z_4-z_1).$$

Let us introduce the following notations:

$$x_{ij} = x_i - x_j, \quad y_{ij} = y_i - y_j, \quad z_{ij} = z_i - z_j \quad i = 1,2,3,4 \quad (3.80)$$

and

$$x_a^{T_k} = \begin{pmatrix} x_{32} \\ x_{41} \\ x_{21} \\ x_{31} \end{pmatrix} \quad x_b^{T_k} = \begin{pmatrix} x_{42} \\ x_{31} \\ x_{41} \\ x_{21} \end{pmatrix} \quad (3.81)$$

$$y_a^{T_k} = \begin{pmatrix} y_{32} \\ y_{41} \\ y_{21} \\ y_{31} \end{pmatrix} \quad y_b^{T_k} = \begin{pmatrix} y_{42} \\ y_{31} \\ y_{41} \\ y_{21} \end{pmatrix} \quad (3.82)$$

$$z_a^{T_k} = \begin{pmatrix} z_{32} \\ z_{41} \\ z_{21} \\ z_{31} \end{pmatrix} \quad z_b^{T_k} = \begin{pmatrix} z_{42} \\ z_{31} \\ z_{41} \\ z_{21} \end{pmatrix} \quad (3.83)$$

By using (3.81)-(3.83), we can write (3.77) in the form:

$$(\partial_x \lambda_i) = \frac{1}{6|T_k|}\left(y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k} \right) \quad (3.84)$$

$$(\partial_y \lambda_i) = \frac{1}{6|T_k|}\left(x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k} \right) \quad (3.85)$$

$$(\partial_z \lambda_i) = \frac{1}{6|T_k|}\Big(x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k}\Big), \tag{3.86}$$

$$|T_k| = \Big(x_{a3}^{T_k} y_{a4}^{T_k} z_{a2}^{T_k} + y_{a3}^{T_k} z_{a4}^{T_k} x_{a2}^{T_k} + z_{a3}^{T_k} x_{a4}^{T_k} y_{a3}^{T_k} - z_{a3}^{T_k} y_{a4}^{T_k} x_{a2}^{T_k} - x_{a3}^{T_k} z_{a4}^{T_k} y_{a2}^{T_k} - y_{a3}^{T_k} x_{a4}^{T_k} z_{a3}^{T_k}\Big)/6. \tag{3.87}$$

The elementary stiffness matrix $\bar{K}$, for $1 \leq j, k \leq 4$ is given by:

$$\begin{aligned} \bar{K}_{jk} = \frac{1}{6|T_k|}\Big[&(y_{bj}^{T_k} z_{aj}^{T_k} - y_{aj}^{T_k} z_{aj}^{T_k})(y_{bk}^{T_k} z_{ak}^{T_k} - y_{ak}^{T_k} z_{ak}^{T_k})^t \\ &+ (x_{aj}^{T_k} z_{bj}^{T_k} - x_{bj}^{T_k} z_{aj}^{T_k})(x_{ak}^{T_k} z_{bk}^{T_k} - x_{bk}^{T_k} z_{ak}^{T_k})^t \\ &+ (x_{bj}^{T_k} y_{aj}^{T_k} - x_{aj}^{T_k} y_{bj}^{T_k})(x_{bk}^{T_k} y_{ak}^{T_k} - x_{ak}^{T_k} y_{bk}^{T_k})^t\Big]. \end{aligned} \tag{3.88}$$

If we pose $K = (\overline{K}_{jk})_{j,k=1,\cdots,4}$, the nonbubble part of $\overline{K}_{jk}$, we obtain:

$$\begin{aligned} K = \frac{1}{6|T_k|}\Big[&(y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})(y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})^t \\ &+ (x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})(x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})^t \\ &+ (x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})(x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})^t\Big]. \end{aligned} \tag{3.89}$$

$\bar{K}$ being symmetric, It remains to calculate the bubble part $\bar{K}_{bj}$ for $j = 1, \cdots, 4$.

A direct calculation gives us:

$$\bar{K}_{bj} = \frac{256}{120}|T_k| \sum_{i=1}^{4} \nabla\lambda_i \quad i = 1, 2, 3, 4$$

$$\bar{K}_{bj} = \frac{32}{15}|T_k| \sum_{i=1}^{4} \nabla\lambda_i \quad i = 1, 2, 3, 4. \tag{3.90}$$

For the diagonal input corresponding to the bubble (i.e $i = j = b$), we have:

$$\bar{K}_{bb} = (256)^2 \int_{T_k} \nabla(\lambda_1\lambda_2\lambda_3\lambda_4).\nabla(\lambda_1\lambda_2\lambda_3\lambda_4)$$

$$\begin{aligned} = \frac{8192}{945}|T_k|\Big(&|\nabla\lambda_1|^2 + |\nabla\lambda_2|^2 + |\nabla\lambda_3|^2 + |\nabla\lambda_4|^2 + \nabla\lambda_1\nabla\lambda_2 + \nabla\lambda_1\nabla\lambda_3 + \nabla\lambda_1\nabla\lambda_4 \\ &+ \nabla\lambda_2\nabla\lambda_3 + \nabla\lambda_2\nabla\lambda_4 + \nabla\lambda_3\nabla\lambda_4\Big] \end{aligned}$$

$$\bar{K}_{bb} = \frac{8192}{945}|T_k|\Big(|\nabla\lambda_1|^2+|\nabla\lambda_2|^2+|\nabla\lambda_3|^2+\nabla\lambda_1\nabla\lambda_2+\nabla\lambda_1\nabla\lambda_3+\nabla\lambda_2\nabla\lambda_3\Big) =: w_K. \quad (3.91)$$

With the above results, the elementary stiffness matrix is given by:

$$\bar{K} = \begin{pmatrix} K & 0 \\ 0 & w_K \end{pmatrix} \quad (3.92)$$

3.2.2. Assembling the Mass Matrix

Let denote by $M = (\bar{M}_{jk})_{j,k=1,\cdots,4}$ the non-bubble part of the elementary mass matrix. Un calcul direct nous donne:

$$M_{jk} = \begin{cases} \frac{|T_k|}{10\Delta t} \text{ si } & j = k \\ \frac{|T_k|}{20\Delta t} \text{ si } & j \neq k. \end{cases} \quad (3.93)$$

The bubble part of the mass matrix is given by:

$$\bar{M}_{bj} = \frac{4}{105\Delta t}|T_k| \quad (3.94)$$

$$\bar{M}_{bb} = \frac{512}{51975\Delta t}|T_k| =: w_M. \quad (3.95)$$

The elementary mass matrix is given by:

$$\bar{M} = \begin{pmatrix} M & z \\ z^t & w_M \end{pmatrix}, \quad (3.96)$$

where $z^t = \frac{4}{105\Delta t}|T_k| \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$.

Finally, the elementary rigidity/mass matrix $\bar{A}$ is:

$$\bar{A} = \begin{pmatrix} A & z \\ z^t & w \end{pmatrix}, \quad (3.97)$$

where we posed $A = M + \nu K$ and $w = w_K + w_M$.

By using (3.36), (3.39), (3.40), (3.41), (3.54) and (3.57) we have:

$$w = \frac{8192}{34020}|T_k|\Big[(y_{b1}^{T_k} z_{a1}^{T_k} - y_{a1}^{T_k} z_{b1}^{T_k})^2 + (x_{a1}^{T_k} z_{b1}^{T_k} - x_{b1}^{T_k} z_{a1}^{T_k})^2$$
$$+ (x_{b1}^{T_k} y_{a1}^{T_k} - x_{a1}^{T_k} y_{b1}^{T_k})^2 + (y_{b2}^{T_k} z_{a2}^{T_k} - y_{a2}^{T_k} z_{b2}^{T_k})^2 + (x_{a2}^{T_k} z_{b2}^{T_k} - x_{b2}^{T_k} z_{a2}^{T_k})^2$$

$$
\begin{aligned}
&+ (x_{a2}^{T_k} z_{b2}^{T_k} - x_{b2}^{T_k} z_{a2}^{T_k})^2 + (x_{a2}^{T_k} z_{b2}^{T_k} - x_{b2}^{T_k} z_{a2}^{T_k})^2 + (x_{b2}^{T_k} y_{a2}^{T_k} - x_{a2}^{T_k} y_{b2}^{T_k})^2 \\
&+ (y_{b3}^{T_k} z_{a3}^{T_k} - y_{a3}^{T_k} z_{b3}^{T_k})^2 + (x_{a3}^{T_k} z_{b3}^{T_k} - x_{b3}^{T_k} z_{a3}^{T_k})^2 + (x_{b3}^{T_k} y_{a3}^{T_k} - x_{a3}^{T_k} y_{b3}^{T_k})^2 \\
&\quad + (y_{b1}^{T_k} z_{a1}^{T_k} - y_{a1}^{T_k} z_{b1}^{T_k})(y_{b2}^{T_k} z_{a2}^{T_k} - y_{a2}^{T_k} z_{b2}^{T_k}) + (x_{a1}^{T_k} z_{b1}^{T_k} - x_{b1}^{T_k} z_{a1}^{T_k}) \\
&\quad (x_{a2}^{T_k} z_{b2}^{T_k} - x_{b2}^{T_k} z_{a2}^{T_k}) + (x_{b1}^{T_k} y_{a1}^{T_k} - x_{a1}^{T_k} y_{b1}^{T_k})(x_{b2}^{T_k} y_{a2}^{T_k} - x_{a2}^{T_k} y_{b2}^{T_k}) \\
&\quad + (y_{b1}^{T_k} z_{a1}^{T_k} - y_{a1}^{T_k} z_{b1}^{T_k})(y_{b3}^{T_k} z_{a3}^{T_k} - y_{a3}^{T_k} z_{b3}^{T_k}) + (x_{a1}^{T_k} z_{b1}^{T_k} - x_{b1}^{T_k} z_{a1}^{T_k}) \\
&\quad (x_{a3}^{T_k} z_{b3}^{T_k} - x_{b3}^{T_k} z_{a3}^{T_k}) + (x_{b1}^{T_k} y_{a1}^{T_k} - x_{a1}^{T_k} y_{b1}^{T_k})(x_{b3}^{T_k} y_{a3}^{T_k} - x_{a3}^{T_k} y_{b3}^{T_k}) \\
&\quad + (y_{b2}^{T_k} z_{a2}^{T_k} - y_{a2}^{T_k} z_{b2}^{T_k})(y_{b3}^{T_k} z_{a3}^{T_k} - y_{a3}^{T_k} z_{b3}^{T_k}) + (x_{a2}^{T_k} z_{b2}^{T_k} - x_{b2}^{T_k} z_{a2}^{T_k}) \\
&\quad (x_{a3}^{T_k} z_{b3}^{T_k} - x_{b3}^{T_k} z_{a3}^{T_k}) + (x_{b2}^{T_k} y_{a2}^{T_k} - x_{a2}^{T_k} y_{b2}^{T_k})(x_{b3}^{T_k} y_{a3}^{T_k} - x_{a3}^{T_k} y_{b3}^{T_k})\Big] \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + \frac{512}{51975\Delta t}|T_k|.
\end{aligned}
$$

3.2.3. Assembling the Divergence Matrix

By performing a direct integration, the elementary divergence matrix gives:

$$
\begin{aligned}
-\bar{B} &= [-\bar{B}_1 \ -\bar{B}_2 \ -\bar{B}_3] \\
&= |T_k| \begin{pmatrix} -s\nabla\lambda_1 & -s\nabla\lambda_2 & -s\nabla\lambda_3 & -s\nabla\lambda_4 & -t\nabla\lambda_1 \\ -s\nabla\lambda_1 & -s\nabla\lambda_2 & -s\nabla\lambda_3 & -s\nabla\lambda_4 & -t\nabla\lambda_2 \\ -s\nabla\lambda_1 & -s\nabla\lambda_2 & -s\nabla\lambda_3 & -s\nabla\lambda_4 & -t\nabla\lambda_3 \\ -s\nabla\lambda_1 & -s\nabla\lambda_2 & -s\nabla\lambda_3 & -s\nabla\lambda_4 & -t\nabla\lambda_4 \end{pmatrix}, \qquad (3.98)
\end{aligned}
$$

where $s = \frac{1}{4}$ and $t = \frac{16}{315}$.

We denote by

$$
B_i = \frac{|T_k|}{4} \begin{pmatrix} \partial_i\lambda_1 & \partial_i\lambda_2 & \partial_i\lambda_3 & \partial_i\lambda_4 \\ \partial_i\lambda_1 & \partial_i\lambda_2 & \partial_i\lambda_3 & \partial_i\lambda_4 \\ \partial_i\lambda_1 & \partial_i\lambda_2 & \partial_i\lambda_3 & \partial_i\lambda_4 \\ \partial_i\lambda_1 & \partial_i\lambda_2 & \partial_i\lambda_3 & \partial_i\lambda_4 \end{pmatrix} \quad i = 1, 2, 3, \qquad (3.99)
$$

and

$$
B_{ib} = \frac{16|T_k|}{315} \begin{pmatrix} \partial_i\lambda_1 \\ \partial_i\lambda_2 \\ \partial_i\lambda_3 \\ \partial_i\lambda_4 \end{pmatrix} \quad i = 1, 2, 3, \qquad (3.100)
$$

so that

$$
\bar{B}_i = [B_i \ \ B_{ib}] \quad i = 1, 2, 3. \qquad (3.101)
$$

From (3.99), The elements of the sub-matrix B_i are given by:

$$B_{ijk} = \frac{|T_k|}{4}\partial_k \lambda_j \quad j,k = 1,2,3,4 \quad i = 1,2,3. \tag{3.102}$$

By using (3.81)-(3.86), we obtain

$$B_1 = \frac{1}{24}\begin{pmatrix} (y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})^t \\ (y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})^t \\ (y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})^t \\ (y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})^t \end{pmatrix} \tag{3.103}$$

$$B_2 = \frac{1}{24}\begin{pmatrix} (x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})^t \\ (x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})^t \\ (x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})^t \\ (x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})^t \end{pmatrix} \tag{3.104}$$

$$B_3 = \frac{1}{24}\begin{pmatrix} (x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})^t \\ (x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})^t \\ (x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})^t \\ (x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})^t \end{pmatrix}. \tag{3.105}$$

A similar calculation gives us the bubble divergence matrix

$$\begin{aligned} B_{1b} =& \frac{8}{945}(y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k}), \\ B_{2b} =& \frac{8}{945}(x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k}), \\ B_{3b} =& \frac{8}{945}(x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k}). \end{aligned} \tag{3.106}$$

3.2.4. Assembling the Second Member Vectors

The second member vectors are defined by:

$$G_j^{n+1} = \int_{T_k} g^{n+1}\lambda_j(\vec{x})d\vec{x}, \quad V_j^{n+1} = \int_{T_k} v^{n+1}\lambda_j(\vec{x})d\vec{x},$$

$$\bar{F}_{ij}^{n+1} = \int_{T_k} \bar{f}_i^{n+1}\lambda_j(\vec{x})d\vec{x} \text{ and } \quad ZD_j^{n+1} = \int_{T_k} zd^{n+1}\lambda_j(\vec{x})d\vec{x}.$$

We decompose $g^{n+1}(\vec{x})$, $v^{n+1}(\vec{x})$, $\bar{f}^{n+1}(\vec{x})$ and $zd^{n+1}(\vec{x})$ into the product of two vectors i.e.:

$$g^{n+1}(\vec{x}) = g_c^{n+1} g_d(\vec{x}), \quad v^{n+1}(\vec{x}) = v_c^{n+1} v_d(\vec{x}),$$

$$zd^{n+1}(\vec{x}) = zd_c^{n+1} zd_c(\vec{x}) \text{ and } \quad \bar{f}_i^{n+1}(\vec{x}) = \bar{f}_{ic}^{n+1} \bar{f}_{id}(\vec{x}).$$

Assuming the values of g_d, v_d and zd_d are known on all vertices of the mesh, vectors G_j, V_j and ZD_j are given by:

$$G^{n+1} = \frac{g_c^{n+1}|T_k|}{4} g_d \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \tag{3.107}$$

$$V^{n+1} = \frac{v_c^{n+1}|T_k|}{} v_d \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \tag{3.108}$$

$$ZD^{n+1} = \frac{zd_c^{n+1}|T_k|}{4} zd_d \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \tag{3.109}$$

where

$$g_d(\vec{x}) = \begin{cases} g_d, & \text{if } g_d \text{ is constant} \\ (g_d(\vec{x}_1) + g_d(\vec{x}_2) + g_d(\vec{x}_3) + g_d(\vec{x}))/4 & \text{otherwise ,} \end{cases} \tag{3.110}$$

$$v_d(\vec{x}) = \begin{cases} v_d, & \text{if } v_d \text{ is constant} \\ (v_d(\vec{x}_1) + v_d(\vec{x}_2) + v_d(\vec{x}_3) + v_d(\vec{x}))/4 & \text{otherwise ,} \end{cases} \tag{3.111}$$

$$zd_d(\vec{x}) = \begin{cases} zd_d, & \text{if } zd_d \text{ is constant} \\ (zd_d(\vec{x}_1) + zd_d(\vec{x}_2) + zd_d(\vec{x}_3) + zd_d(\vec{x}))/4 & \text{otherwise .} \end{cases} \tag{3.112}$$

The Contribution of the source term F_{ij} non-bubble is given by

$$F_i^{n+1} = \frac{f_{ic}^{n+1}|T_k|}{4} f_{id} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \tag{3.113}$$

where

$$f_{id}(\vec{x}) = \begin{cases} f_{id} & \text{if } f_{id} \text{ is constant} \\ (f_{id}(\vec{x}_1) + f_{id}(\vec{x}_2) + f_{id}(\vec{x}_3) + f_{id}(\vec{x}))/4 & \text{otherwise .} \end{cases} \tag{3.114}$$

The second member with the term bubble F_{ib} is given by:

$$F_{ib} = \frac{16 f_{ic}^{n+1}|T_k|}{4} f_{id} \quad i = 1, \cdots, 3. \tag{3.115}$$

3.3. Evaluation of b_{0j}, $b_{ij}, i = 1, \cdots, 3$ and b_{4j}

$$b_{0j}^n = \frac{1}{\Delta t}\int_{T_k}(c^n o X^n)\lambda_j, \quad b_{ij}^n = \frac{1}{\Delta t}\int_{T_k}(u_i^n o X^n)\lambda_j \quad b_{4j}^n = \frac{1}{\Delta t}\int_{T_k}(c^{*^n} o X^n)\lambda_j.$$

We approximate X^n by an explicit scheme of 1^{er} order:

$$X^n(\vec{x}) \approx \vec{x} - \Delta t u^n, \tag{3.116}$$

where u^n Is the velocity resulting from the resolution of the Navier-Stokes equations at time t_n, then b_{0j}, b_{ij} and b_{4j} are given by:

$$b_{0j} \approx \sum_{k=1}^{4} \Pi_k c_h^n(X_h^n(\xi_k))\lambda_j(\xi_k) \tag{3.117}$$

$$b_{ij} \approx \sum_{k=1}^{4} \Pi_i u_{ih}^n(X_h^n(\xi_k))\lambda_j(\xi_k) \quad i = 1, 2, 3 \tag{3.118}$$

$$b_{4j} \approx \sum_{i=1}^{4} \Pi_i c^{*^n}(X_h^n(\xi_i))\lambda_j(\xi_k), \tag{3.119}$$

where ξ_i are the points of Gauss and Π_i their associated weights.

3.4. Elimination of the Bubble Unknowns

With the elementary matrices and vectors computed previously the system corresponding to (3.54) coupled to the adjoint problem gives:

$$\begin{pmatrix} A_1 & M_* & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A & z & 0 & 0 & 0 & 0 & -B_1^t \\ 0 & 0 & z^t & w & 0 & 0 & 0 & 0 & B_{1b}^t \\ 0 & 0 & 0 & 0 & A & z & 0 & 0 & -B_2^t \\ 0 & 0 & 0 & 0 & z^t & w & 0 & 0 & B_{1b}^t \\ 0 & 0 & 0 & 0 & 0 & 0 & A & z & -B_3^t \\ 0 & 0 & 0 & 0 & 0 & 0 & z^t & w & B_{1b}^t \\ 0 & 0 & -B_1 & B_{1b} & -B_2 & B_{2b} & -B_3 & B_{3b} & 0 \end{pmatrix} \begin{pmatrix} c^{*^{n+1}} \\ c^{n+1} \\ u_1^{n+1} \\ u_{1b}^{n+1} \\ u_2^{n+1} \\ u_{2b}^{n+1} \\ u_3^{n+1} \\ u_{3b}^{n+1} \\ P^{n+1} \end{pmatrix}$$

$$= \begin{pmatrix} ZD^{n+1} \\ G^{n+1} + V^{n+1} \\ F_1^{n+1} \\ F_{1b}^{n+1} \\ F_1^{n+1} \\ F_{2b}^{n+1} \\ F_1^{n+1} \\ F_{3b}^{n+1} \\ 0 \end{pmatrix} + \begin{pmatrix} b_4^n \\ b_0^n \\ b_1^n \\ 0 \\ b_2^n \\ 0 \\ b_3^n \\ 0 \\ 0 \end{pmatrix}, \quad (3.120)$$

where $A_1 = M - dK$.

To show the diagonal blocks (3.120) can be rearranged as follows:

$$\begin{pmatrix} A_1 & M_* & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A & 0 & 0 & z & 0 & 0 & -B_1^t \\ 0 & 0 & 0 & A & 0 & 0 & z & 0 & -B_2^t \\ 0 & 0 & 0 & 0 & A & 0 & 0 & z & -B_3^t \\ 0 & 0 & z^t & 0 & 0 & w & 0 & 0 & B_{1b}^t \\ 0 & 0 & 0 & z^t & 0 & 0 & w & 0 & B_{2b}^t \\ 0 & 0 & 0 & 0 & z^t & 0 & 0 & w & B_{3b}^t \\ 0 & 0 & -B_1 & -B_2 & -B_3 & B_{1b} & B_{2b} & B_{3b} & 0 \end{pmatrix} \begin{pmatrix} {c^*}^{n+1} \\ c^{n+1} \\ u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ u_{1b}^{n+1} \\ u_{2b}^{n+1} \\ u_{3b}^{n+1} \\ P^{n+1} \end{pmatrix}$$

$$= \begin{pmatrix} ZD^{n+1} \\ G^{n+1} + V^{n+1} \\ F_1^{n+1} \\ F_{1b}^{n+1} \\ F_1^{n+1} \\ F_{2b}^{n+1} \\ F_1^{n+1} \\ F_{3b}^{n+1} \\ 0 \end{pmatrix} + \begin{pmatrix} b_4^n \\ b_0^n \\ b_1^n \\ b_2^n \\ b_3^n \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (3.121)$$

We can eliminate the unknown bubbles u_{1b}^{n+1}, u_{2b}^{n+1} and u_{3b}^{n+1} because they correspond to the diagonal blocks $(3.121)_6$, $(3.121)_7$ and $(3.121)_8$, we have:

$$z^t u_1^{n+1} + w u_{1b}^{n+1} + B_{1b}^t P^{n+1} = F_{1b}^{n+1} \quad (3.122)$$

$$z^t u_2^{n+1} + w u_{2b}^{n+1} + B_{2b}^t P^{n+1} = F_{2b}^{n+1} \quad (3.123)$$

$$z^t u_3^{n+1} + w u_{3b}^{n+1} + B_{3b}^t P^{n+1} = F_{3b}^{n+1}. \quad (3.124)$$

We obtain so:

$$\begin{aligned} u_{1b}^{n+1} &= (F_{1b}^{n+1} - B_{1b}^t P^{n+1} - z^t u_1^{n+1})/w && (3.125)\\ u_{2b}^{n+1} &= (F_{2b}^{n+1} - B_{2b}^t P^{n+1} - z^t u_2^{n+1})/w && (3.126)\\ u_{3b}^{n+1} &= (F_{3b}^{n+1} - B_{3b}^t P^{n+1} - z^t u_3^{n+1})/w. && (3.127)\end{aligned}$$

By substituting (3.125)-(3.126) in $(3.121)_3$, $(3.121)_4$, $(3.121)_5$ and $(3.121)_9$, The system is obtained by $({c^*}^{n+1}, c^{n+1}, u_1^{n+1}, u_2^{n+1}, u_3^{n+1}, P^{n+1})^t$ whose the global matrix is defined by:

$$\left(\begin{array}{cccccc} A_1 & M_* & 0 & 0 & 0 & 0\\ 0 & A_0 & 0 & 0 & 0 & 0\\ 0 & 0 & A - w^{-1}zz^t & 0 & 0 & -B_1^t - w^{-1}zB_{1b}^t\\ 0 & 0 & 0 & A - w^{-1}zz^t & 0 & -B_2^t - w^{-1}zB_{2b}^t\\ 0 & 0 & 0 & 0 & A - w^{-1}zz^t & -B_3^t - w^{-1}zB_{3b}^t\\ 0 & 0 & -B_1 - w^{-1}B_{1b}z^t & -B_2 - w^{-1}B_{2b}z^t & -B_3 - w^{-1}B_{3b}z^t & -w^{-1}(B_{1b}B_{1b}^t + B_{2b}B_{2b}^t + B_{3b}B_{3b}^t \end{array}\right) \quad (3.128)$$

And the second members are given by:

$$\begin{pmatrix} ZD^{n+1}\\ G^{n+1} + V^{n+1}\\ F_1^{n+1} - w^{-1}zF_{1b}^{n+1}\\ F_2^{n+1} - w^{-1}zF_{2b}^{n+1}\\ F_3^{n+1} - w^{-1}zF_{3b}^{n+1}\\ -w^{-1}\Big(B_{1b}F_{1b}^{n+1} + B_{2b}F_{2b}^{n+1} + B_{3b}F_{3b}^{n+1}\Big) \end{pmatrix} \text{ and } \begin{pmatrix} b_4^n\\ b_0^n\\ b_1^n\\ b_2^n\\ b_3^n\\ 0 \end{pmatrix}. \quad (3.129)$$

The matrices and vectors from the system (3.128)-(3.129) are computed using x_k^T, y_k^T et z_k^T with $k = a, b$.

Pose

$$E = -w^{-1}(B_{1b}B_{1b}^t + B_{2b}B_{2b}^t + B_{3b}B_{3b}^t). \quad (3.130)$$

By using (3.81)-(3.83) and (3.106), the elementary pressure matrix is given by:

$$E = -\frac{64}{893025w}\Big((y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})(y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k})^t + (x_a^{T_k} z_b^{T_k}$$

$$- x_b^{T_k} z_a^{T_k})(x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k})^t \quad (3.131)$$

$$+(x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})(x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k})^t\Big).$$

In the same way, we pose:

$$\tilde{B}_1 = B_1 + w^{-1} B_{1b} z^t, \quad \tilde{B}_2 = B_1 + w^{-1} B_{2b} z^t, \quad \tilde{B}_3 = B_1 + w^{-1} B_{3b} z^t, \quad (3.132)$$

then by using (3.81)-(3.83) et (3.103)-(3.105), we obtain:

$$\tilde{B}_1 = \frac{1}{24}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} + \frac{8}{945w}(y_b^{T_k} z_a^{T_k} - y_a^{T_k} z_b^{T_k}) z^t, \quad (3.133)$$

$$\tilde{B}_2 = \frac{1}{24}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} + \frac{8}{945w}(x_a^{T_k} z_b^{T_k} - x_b^{T_k} z_a^{T_k}) z^t, \quad (3.134)$$

$$\tilde{B}_3 = \frac{1}{24}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} + \frac{8}{945w}(x_b^{T_k} y_a^{T_k} - x_a^{T_k} y_b^{T_k}) z^t \quad (3.135)$$

4. Implementation of the Optimization Algorithm

Then we use the conjugate gradient algorithm of **Hesteness-Stiefel** coupled with linear Search for **Armijo Crouching**.
It is fixed v_0, then calculating $J_0 = J(v_0)$ and $\nabla J_0 = \nabla J(v_0)$, The algorithm is initialized by a simple gradient step. We have $\eta_0 = \nabla J_0$.

As long as a convergence criterion is not verified:$\|\nabla_v J\| < 10^{-5}$

1. Determination of a step α_k by the method of **Hesteness-Stiefel**:

Initialization: Choice of a step α_k^1 and a parameter $\tau \in]0,1[$, $i = 1$.

a. Test: The step α_k^i is accepted if it satisfies the condition of **Armijo**:

$$J(v_k + \alpha_k^i) \leq J(v_k) + e_1 \alpha_k^i (\nabla J(v_k), \eta_k), \quad e_1 \in]0,1[$$

otherwise

b. We choose $\alpha_k^{i+1} \in [\tau \alpha_k^i, (1-\tau)\alpha_k^i]$.

c. We pose $i = i + 1$ and $\alpha_k = \alpha_k^i$, and then returns to step a.
Calculation of a new iterated: $v_{k+1} = v_k + \alpha_k \eta_k$
2. Evaluation of a new gradient $\nabla J_{k+1} = \nabla J(v_{k+1})$.
3. Calculation of the β_{k+1} parameter by the **Hesteness-Stiefel** method

$$\beta_{k+1} = \frac{\nabla J_{k+1}^t (\nabla J_{k+1} - \nabla J_k)}{(\nabla J_{k+1} - \nabla J_k)^t \eta_k}$$

4. Construction of a new descent direction:

$$\eta_{k+1} = -\nabla J_{k+1} + \beta_{k+1} \eta_k$$

5. Incrementation $k = k + 1$

5. Numerical Simulation

In this section, concentration, velocity vector $u = (u_1, u_2, u_3)$ and pressure p are approximated. The computational domain is a cube of side $L = 1$ equipped with boundary conditions. These calculations have been performed on homogeneous meshes compounds of 8 to 1000 dots along the three directions in space. The reference number Reynolds using in this simulation is $Re = 1000$. The simulations are conducted in time $T = 1$ and the successful test case is the Green-Taylor vortex corresponding to an analytical solution of the equations of the three-dimensional Navier-Stokes. Analytical fields, concentration, velocity and pressure are given by the following:

$$c(x, y, z, t) = (\cos(2\pi x)\sin(2\pi y)\cos(2\pi z) - \sin(2\pi x)\cos(2\pi y)\cos(2\pi z))\exp(-\nu t)$$

$$u_1(x, y, z, t) = \sin(2\pi x)\cos(2\pi y)\cos(2\pi z)\exp(-\nu t)$$

$$u_2(x, y, z, t) = -\cos(2\pi x)\sin(2\pi y)\cos(2\pi z)\exp(-\nu t), \qquad u_3(x, y, z, t) = 0$$

and

$$p(x, y, z, t) = ((\cos(4\pi z) + 2\cos(4\pi x) + 2\cos(4\pi y) - 2)\exp(-2\nu t))/16.$$

5.1. Error Estimates

Different errors estimations are reported in the followings tables.

Table 1. Table of error estimates for 8 points

S	20	50	100	200	300
Err. L^2u	4.4717e-020	2.8282e-020	1.9998e-020	1.4141e-020	1.1546e-020
Err. H^1u	4.7953e-020	3.8504e-020	2.0296e-020	1.4247e-020	1.1604e-020
Err. L^2p	8.3848e-005	5.3032e-005	3.7500e-005	2.6516e-005	2.1651e-005

Table 2. Table of error estimates for 64 points

S	20	50	100	200	300
Err. L^2u	5.9946e-005	3.7914e-005	2.6809e-005	1.8957e-005	1.5478e-005
Err. H^1u	2.3284e-004	9.7659e-005	5.2381e-005	2.9421e-005	2.1554e-005
Err. L^2p	6.9874e-005	4.4193e-005	3.1250e-005	2.2097e-005	1.8042e-005

Table 3. Table of error estimates for 216 points

S	20	50	100	200	300
Err. L^2u	8.0213e-005	5.0732e-005	3.5873e-005	2.5366e-005	2.0711e-005
Err. H^1u	2.6685e-004	1.1375e-04	6.2274e-005	3.5934e-005	2.6774e-005
Err. L^2p	6.7233e-005	4.2523e-05	3.0069e-005	2.1262e-005	1.7360e-005

Table 4. Table of error estimates for 512 points

S	20	50	100	200	300
Err. L^2u	9.2803e-005	5.8695e-005	4.1504e-005	2.9348e-005	2.3962e-005
Err. H^1u	2.7891e-004	1.2048e-004	6.7007e-005	3.9410e-005	2.9693e-005
Err. L^2p	7.2163e-005	4.5641e-005	3.2273e-005	2.2821e-005	1.8633e-005

Table 5. Table of error estimates for 1000 points

S	20	50	100	200	300
Err. L^2u	9.9505e-005	6.2933e-005	4.4501e-005	3.1467e-005	2.5693e-005
Err. H^1u	2.8454e-004	1.2382e-004	6.9447e-005	4.1241e-005	3.1240e-005
Err. L^2p	7.5311e-05	4.7632e-005	3.3681e-005	2.3816e-005	1.9446e-005

5.2. Discussion

The results in Tables 1-5 give us the error evolution according to the time discretization parameters and the number of mesh nodes.

While conducting a horizontal reading of the results, we note that the error decreases according to the time discretization when the number of mesh nodes is stationary. However, a vertical reading of the tables shows that the error of the velocity slightly increases with the number of nodes, with the exception of the Table 1 where one notices a great difference. On the order hand, the pressure error decreases globally in the two senses. In a general manner, the velocity error and the pressure are the order 10^{-5}. It is evident from this analysis that our numeric approach a good numeric stability.

In this validation study, the cost of control is not a priority in the optimization process. Nevertheless, for the problem to be well posed, one considered the regulation parameter $N \neq 0$. More precisely, we took $N = 10^{-4}$ in all the simulations.

At the level of the various figures are shown respectively the profiles of the setpoint z_d, the uncontrolled C solution ($v = 0$), the solution C_{opt} of the optimal control problem and the distributed control V_{opt} in space-time coordinates when the time discretization step and the number of nodes increases. It is observed that the profile of the optimal solution is very near to the profile z_d, thus enabling numerical validation of the whole approach.

Qualitatively, the spatio-temporal evolution of the control is in good agreement with the profiles of the setpoint and the uncontrolled solution. Also the amplitude of this control increases fairly strongly when the time $t = 1$ is approached. This result is explained by the fact that the objective is double at $t = 1$.

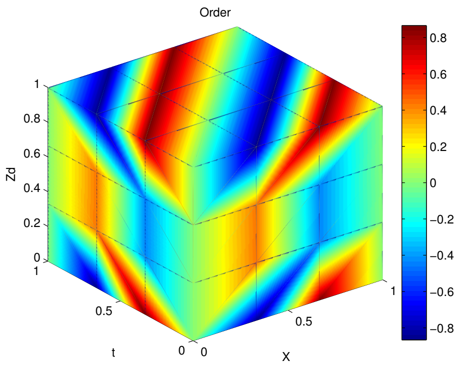

Figure 1: Representation in coordinates Space-time profile of the set-point for $S = 50$ and 64 points

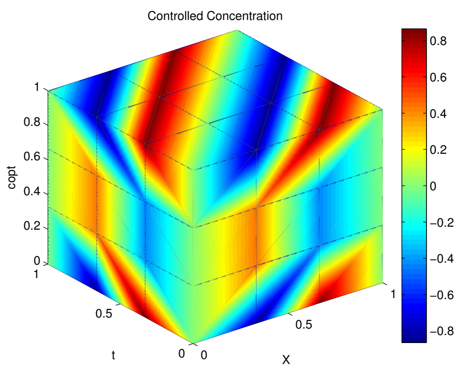

Figure 2: Representation in coordinates Space-time optimal profile for $S = 50$ and 64 points

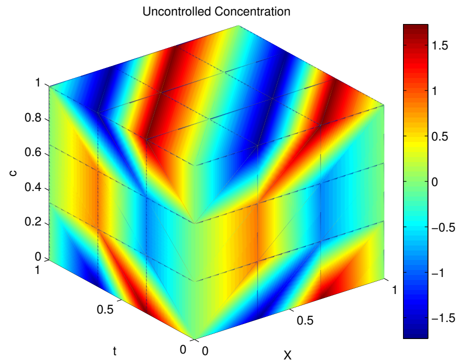

Figure 3: Representation in coordinates Space-time of the uncontrolled profile for $S = 50$ and 64 points

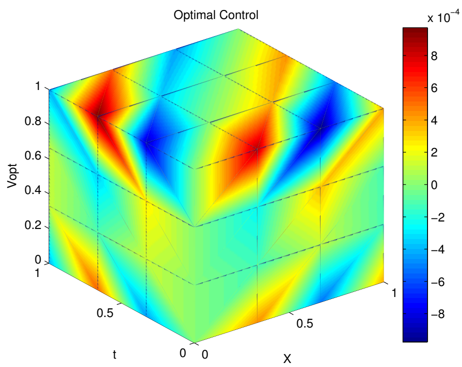

Figure 4: Representation in coordinates Space-time of optimal distributed control for $S = 50$ and 64 points

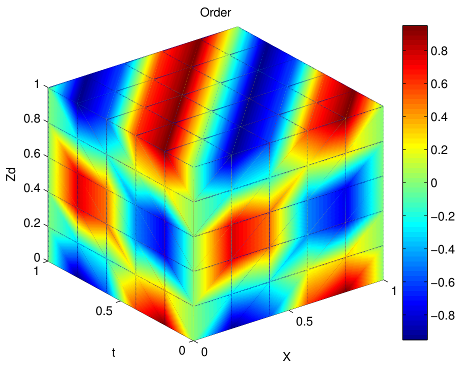

Figure 5: Representation in coordinates Space-time profile of the set-point for $S = 100$ and 216 points

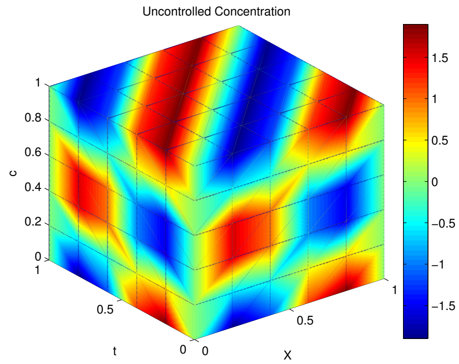

Figure 7: Representation in coordinates Space-time of the uncontrolled profile for $S = 100$ and 216 points

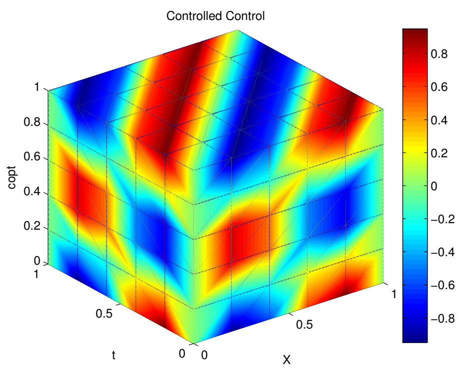

Figure 6: Representation in coordinates Space-time optimal profile for $S = 100$ and 216 points

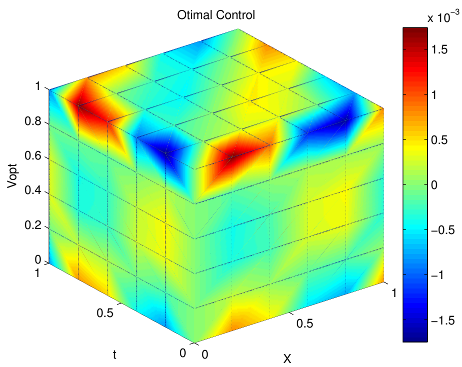

Figure 8: Representation in coordinates Space-time of optimal distributed control for $S = 100$ and 216 points

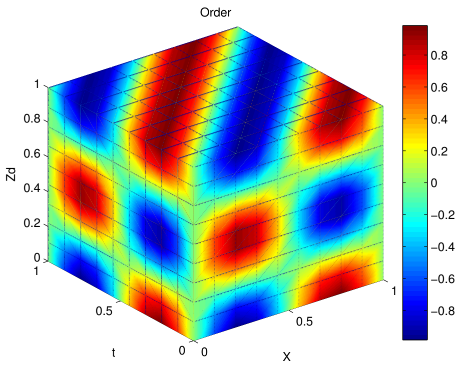

Figure 9: Representation in coordinates Space-time profile of the set-point for $S = 300$ and 1000 points

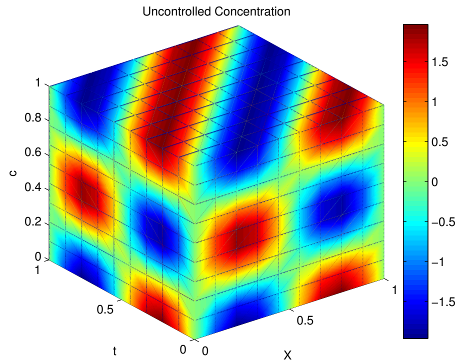

Figure 11: Representation in coordinates Space-time of the uncontrolled profile for $S = 300$ and 1000 points

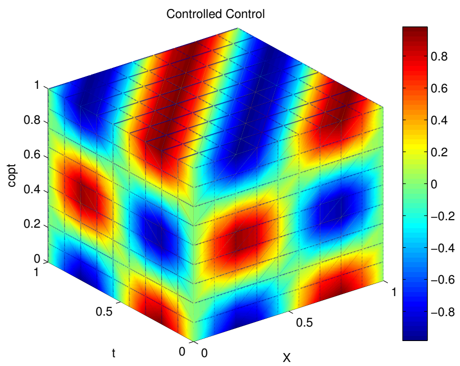

Figure 10: Representation in coordinates Space-time optimal profile for $S = 300$ and 1000 points

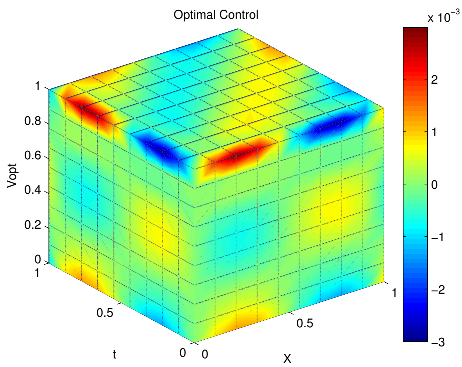

Figure 12: Representation in coordinates Space-time of optimal distributed control for $S = 300$ and 1000 points

6. Conclusion

The objective of this article was to solve and numerical simulation of an optimal control problem of surface water pollution by reducing the problem to an optimization problem without constraint using Lagrange multipliers and the differentiation-discretisation approach in which we have opted for a vectorization of the $P^1 + bubble/P^1$ method. We have demonstrated that the vectorized code is much more efficient than a standard implementation with a loop on the tetrahedrons [2, 6] in the assembly of the different matrices and this allowed us to save a huge computational time. The different profiles of the solutions presented allowed us to validate numerically the whole approach.

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