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PURE LAGRANGIAN AND SEMI-LAGRANGIAN FINITE ELEMENT METHODS FOR THE NUMERICAL SOLUTION OF CONVECTION-DIFFUSION PROBLEMS

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This paper is dedicated to Professor Francisco J. Lisbona in his 65th birthday

Abstract. In this paper we propose a unified formulation to introduce and analyze (pure) Lagrangian and semi-Lagrangian methods for solving convection-diffusion partial differential equations. This formulation allows us to state classical and new numerical methods. Several examples are given. We combine them with finite element methods for spatial discretization. One of the pure Lagrangian methods we introduce has been analyzed in [4] and [5] where stability and error estimates for time semi-discretized and fully-discretized schemes have been proved. In this paper, we prove new stability estimates. More precisely, we obtain an $l^\infty(H^1)$ stability estimate independent of the diffusion coefficient and, if the underlying flow is incompressible, we get a stability inequality independent of the final time. Finally, the numerical solution of a test problem is presented that confirms the new stability results.

Key words. convection-diffusion equation, pure Lagrangian method, semi-Lagrangian method, Lagrange-Galergin method, characteristics method, second order schemes, finite element method.

1. Introduction

Convection-diffusion equations model a variety of important problems from different fields of engineering and applied sciences. In many cases the diffusive term is much smaller than the convective one and then upwinding has to be introduced in the numerical scheme. This can be done by using characteristics method which are based on time discretization of the material time derivative. These methods were introduced in the beginning of the 1980s combined with finite differences or finite elements for space discretization (see [11], [18]). In this context they are also called Lagrange-Galerkin methods. The classical methods of characteristics are written in Eulerian coordinates and they are related to semi-Lagrangian schemes (see [13]). Lagrange-Galerkin methods have been mathematically analyzed and applied to different problems by several authors. For example, in [23], [18] the classical first order characteristic method combined with finite elements applied to convection-diffusion equations is studied, and in [22], [6] and [7] second order Lagrange-Galerkin methods are analyzed. More precisely, if $\triangle t$ denotes the time step, h the mesh-size and k the degree of the finite elements space, estimates of the form $O(h^k)+O(\triangle t)$ in the $l^\infty(L^2(\mathbb{R}^d))$-norm are shown in [23] (d denotes the dimension of the spatial domain). In [18] error estimates of the form $O(h^k)+O(\triangle t)+O(h^{k+1}/\triangle t)$ in the $l^\infty(L^2(\Omega))$-norm are obtained under the assumption that the normal velocity vanishes on the boundary of Ω. In [22] a second order characteristics method for solving constant

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coefficient convection-diffusion equations with Dirichlet boundary conditions is studied. Stability and $O(\triangle t^2) + O(h^k)$ error estimates in the $l^\infty(L^2(\Omega))$-norm are stated (see also [6] and [7] for further analysis).

Recently, for linear convection diffusion problems, we have introduced the so-called *pure Lagrangian methods* combined with finite elements. They are obtained by discretizing the problem which has been first written in Lagrangian or material coordinates. In particular, in [4] and [5] $l^\infty(H^1(\Omega))$ stability and $l^\infty(H^1(\Omega))$ error estimates of order $O(\Delta t^2) + O(h^k)$ were proved for a second order pure Lagrange-Galerkin method. In [10], semi-Lagrangian and pure Lagrangian methods are proposed and analyzed for convection-diffusion equations. Error estimates for a Galerkin discretization of a pure Lagrangian formulation and for a discontinuous Galerkin discretization of a semi-Lagrangian formulation are obtained. The estimates are written in terms of the projections constructed in [8] and [9]. In [4] and [5] a pure Lagrangian formulation has been used for a more general problem. Specifically, we have considered a (possibly degenerate) variable coefficient diffusive term instead of the simpler Laplacian, general mixed Dirichlet-Robin boundary conditions, and a time dependent domain. Moreover, we have analyzed a scheme with approximate characteristic curves and presented numerical results for pure Lagrangian and semi-Lagrangian methods.

In the present paper, we introduce a unified formulation to state pure Lagrangian and semi-Lagrangian methods for solving linear convection-diffusion equations.

Our approach uses the formalism of continuum mechanics in which classical and new methods can be introduced in a natural way (see for instance [15]).

The paper is organized as follows. In Section 2 the linear convection-diffusion Cauchy problem is posed in a time dependent bounded domain and some hypotheses and notations concerning motions are stated. In Section 3, we introduce a quite general change of variable obtaining a new strong formulation of the linear convection-diffusion Cauchy problem. Moreover, the standard associated weak problem is obtained. In Section 4, pure Lagrangian and semi-Lagrangian schemes are proposed. All these methods arise from the formulation obtained in the previous section. In Section 5, a second order pure Lagrange-Galerkin scheme is proposed for second order approximate characteristics. We recall some properties verified by this method. Moreover, under suitable hypotheses on the data, two new stability results are proved for small enough time step. One of them is independent of the diffusion coefficient and the other one is independent of the final time. In Section 6, in order to check experimentally these stability results, we solve a linear convection-diffusion problem.

2. Statement of the linear convection diffusion problem. General assumptions and notations.

Let Ω be a bounded domain in $\mathbb{R}^d$ $(d = 2,3)$ with Lipschitz boundary Γ divided into two parts: $\Gamma = \Gamma^D \cup \Gamma^R$, with $\Gamma^D \cap \Gamma^R = \emptyset$. Let T be a positive constant and $X_e : \overline{\Omega} \times [0,T] \longrightarrow \mathbb{R}^d$ be a motion in the sense of Gurtin [15]. In particular, $X_e \in \mathbf{C}^3(\overline{\Omega} \times [0,T])$ and for each fixed $t \in [0,T]$, $X_e(\cdot,t)$ is a one-to-one function satisfying

$$\det F(p,t) > 0 \quad \forall p \in \overline{\Omega}, \tag{1}$$

being $F(\cdot,t)$ the Jacobian tensor of $X_e(\cdot,t)$. We call $\Omega_t = X_e(\Omega,t)$, $\Gamma_t = X_e(\Gamma,t)$, $\Gamma_t^D = X_e(\Gamma^D,t)$ y $\Gamma_t^R = X_e(\Gamma^R,t)$, for $t \in [0,T]$. We assume that $\Omega_0 = \Omega$. Let us introduce the *trajectory* of the motion

$$\mathcal{T} := \{(x,t) : x \in \overline{\Omega}_t,\ t \in [0,T]\},$$

and the set

$$\mathcal{O} := \bigcup_{t\in[0,T]} \overline{\Omega}_t. \tag{2}$$

For each t, $X_e(\cdot,t)$ is a one-to-one mapping from $\overline{\Omega}$ onto $\overline{\Omega}_t$; hence it has an inverse

$$P(\cdot,t) : \overline{\Omega}_t \longrightarrow \overline{\Omega}, \tag{3}$$

such that

$$X_e(P(x,t),t) = x, \qquad P(X_e(p,t),t) = p \quad \forall (x,t) \in \mathcal{T}\ \forall (p,t) \in \overline{\Omega} \times [0,T]. \tag{4}$$

Mapping $P : \mathcal{T} \longrightarrow \overline{\Omega}$, so defined is called the *reference map* of motion X_e and $P \in \mathbf{C}^3(\mathcal{T})$ (see [15] pp. $65-66$). Let us recall that the spatial description of the velocity $\mathbf{v} : \mathcal{T} \longrightarrow \mathbb{R}^d$ is defined by

$$\mathbf{v}(x,t) := \dot{X}_e(P(x,t),t) \quad \forall (x,t) \in \mathcal{T}. \tag{5}$$

We denote by L the gradient of $\mathbf{v}$ with respect to the space variables.

Let us consider the following initial-boundary value problem.

(SP) **STRONG PROBLEM**. *Find a function $\phi : \mathcal{T} \longrightarrow \mathbb{R}$ such that*

$$\rho(x)\frac{\partial \phi}{\partial t}(x,t) + \rho(x)\mathbf{v}(x,t) \cdot \operatorname{grad}\phi(x,t) - \operatorname{div}(A(x)\operatorname{grad}\phi(x,t)) = f(x,t), \tag{6}$$

for $x \in \Omega_t$ and $t \in (0,T)$, subject to the boundary conditions

$$\begin{aligned} \phi(x,t) &= \phi_D(x,t) \text{ on } \Gamma_t^D, && (7)\\ \alpha\phi(x,t) + A(\cdot)\operatorname{grad}\phi(x,t)\cdot\mathbf{n}(x,t) &= g(x,t) \text{ on } \Gamma_t^R, && (8)\end{aligned}$$

for $t \in (0,T)$, and the initial condition

$$\phi(x,0) = \phi^0(x) \ \textit{in}\ \Omega. \tag{9}$$

In the above equations, $A : \mathcal{O} \longrightarrow Sym$ denotes the diffusion tensor field, where Sym is the space of symmetric tensors in the d-dimensional space, $\rho : \mathcal{O} \longrightarrow \mathbb{R}$, $f : \mathcal{T} \longrightarrow \mathbb{R}$, $\phi^0 : \Omega \longrightarrow \mathbb{R}$, $\phi_D(\cdot,t) : \Gamma_t^D \longrightarrow \mathbb{R}$ and $g(\cdot,t) : \Gamma_t^R \longrightarrow \mathbb{R}$, $t \in (0,T)$, are given scalar functions, and $\mathbf{n}(\cdot,t)$ is the outward unit normal vector to Γ_t.
For given $\tau \in [0,T]$, the motion X_e can also be defined relative to the configuration in time τ. It is the mapping

$$(X_e)_\tau : \quad \overline{\Omega}_\tau \times [0,T] \quad \longrightarrow \quad \mathbb{R}^d,$$

given by

$$(X_e)_\tau(y,t) := X_e(P(y,\tau),t) \quad \forall (y,t) \in \overline{\Omega}_\tau \times [0,T]. \tag{10}$$

Thus, the mapping $t \in (0,T) \to (X_e)_\tau(y,t)$ represents the trajectory described by a material point that is placed at position y at time τ. Moreover, we notice that $x = (X_e)_\tau(y,t)$ if and only if $y = (X_e)_t(x,\tau)$.

Remark 2.1. *For the sake of clarity in the notation, in expressions involving gradients and time derivatives we use the following notation (see, for instance,* [15]*):*

- *We denote by p the material points in $\overline{\Omega}$, by x the spatial points in $\overline{\Omega}_t$ with $t > 0$ and by y the points in $\overline{\Omega}_\tau$ with $\tau \geq 0$.*
- *A material field is a mapping with domain $\overline{\Omega} \times [0,T]$ and a spatial field is a mapping with domain $\mathcal{T}$.*

- *If φ is a smooth material field, we denote by $\nabla\varphi$ (respectively, by $\operatorname{Div}\varphi$) the gradient (respectively, the divergence) with respect to the first argument, and by $\dot{\varphi}$ the partial derivative with respect to the second argument (time).*
- *If ψ is a smooth spatial field, we denote by $\operatorname{grad}\psi$ (respectively, $\operatorname{div}\psi$) the gradient (respectively, the divergence) with respect to the first argument, and by ψ' the partial derivative with respect to the second argument (time). Moreover, $\dot{\psi}$ denotes the material time derivative with respect to time, that is*

$$\dot{\psi}(x,t) = \psi'(x,t) + \operatorname{grad}\psi(x,t)\cdot \mathbf{v}(x,t).$$

If Ψ is a spatial field, we introduce the field Ψ_τ, defined in $\overline{\Omega}_\tau \times [0,T]$ by

$$\Psi_\tau(y,t) := \Psi((X_e)_\tau(y,t),t) \quad \forall (y,t)\in \overline{\Omega}_\tau\times[0,T]. \tag{11}$$

Notice that, for $\tau = 0$, Ψ_0 is the material description of Ψ also denoted by Ψ_m. In the following $\mathcal{A}$ denotes a bounded domain in $\mathbb{R}^d$. Let us introduce the Lebesgue spaces $L^r(\mathcal{A})$ and the Sobolev spaces $W^{m,r}(\mathcal{A})$ with the usual norms $||\cdot||_{r,\mathcal{A}}$ and $||\cdot||_{m,r,\mathcal{A}}$, respectively, for $r = 1,2,\dots,\infty$ and m an integer. For the particular case $r = 2$, we endow space $L^2(\mathcal{A})$ with the usual inner product $\langle\cdot,\cdot\rangle_{\mathcal{A}}$, which induces a norm to be denoted by $||\cdot||_{\mathcal{A}}$ (see [1] for details).

Moreover, we denote by $H^1_{\Gamma^D}(\mathcal{A})$ the closed subspace of $H^1(\mathcal{A})$ defined by

$$H^1_{\Gamma^D}(\mathcal{A}) := \left\{\varphi\in H^1(\mathcal{A}),\ \varphi|_{\Gamma^D}\equiv 0\right\}, \tag{12}$$

where Γ_D is a part of the boundary of $\mathcal{A}$ of non-null measure.

Corresponding to the discretized scheme to be given below, we have to deal with sequences of functions $\widehat{\psi} = \{\psi^n\}_{n=0}^N$. More precisely, we will consider the spaces of sequences $l^\infty(L^2(\mathcal{A}))$ and $l^2(L^2(\mathcal{A}))$ equipped with their respective usual norms:

$$\left|\left|\widehat{\psi}\right|\right|_{l^\infty(L^2(\mathcal{A}))} := \max_{0\le n\le N} ||\psi^n||_{\mathcal{A}}, \quad \left|\left|\widehat{\psi}\right|\right|_{l^2(L^2(\mathcal{A}))} := \sqrt{\Delta t\sum_{n=0}^N ||\psi^n||^2_{\mathcal{A}}}.$$

Similar definitions are considered for functional spaces $l^\infty(L^2(\Gamma^R))$ and $l^2(L^2(\Gamma^R))$ associated with the Robin boundary condition and for vector-valued function spaces $l^\infty(\mathbf{L}^2(\mathcal{A}))$ and $l^2(\mathbf{L}^2(\mathcal{A}))$.

Moreover, let us introduce the notations

$$\widehat{\mathcal{S}[\psi]} := \{\psi^{n+1}+\psi^n\}_{n=0}^{N-1}, \quad \widehat{\mathcal{R}_{\Delta t}[\psi]} := \left\{\frac{\psi^{n+1}-\psi^n}{\Delta t}\right\}_{n=0}^{N-1}.$$

Throughout this paper, we assume that the diffusion tensor is symmetric and has the form $A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$, for some $n_1 \le d$ and Λ is a uniform lower bound for the eigenvalues of A_{n_1}. Moreover, we suppose that $\rho \ge \gamma > 0$ and the gradient of the velocity field, $L(x,t) := \operatorname{grad}\mathbf{v}(x,t)$ satisfies,

$$(I-B)L(x,t)B = 0 \quad \forall (x,t)\in\mathcal{T}, \tag{13}$$

where B denotes the $d\times d$ tensor,

$$B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}, \tag{14}$$

and I_{n_1} is the $n_1\times n_1$ identity matrix.

Remark 2.2. *Equality (13) is equivalent to having a velocity field $\mathbf{v}$ whose $d-n_1$ last components depend only on the last $d-n_1$ variables.*

Remark 2.3. *Notice that the diffusion tensor can be degenerate in some applications. This is the case, for instance, in some financial models where, nevertheless, the diffusion tensor has the form of A. In* [14] *and* [17] *existence and uniqueness results are proved for convection-(possibly degenerate) diffusion equations, but these issues are beyond the scope of this paper.*

3. Weak formulation.

We are going to develop some formal computations in order to write a weak formulation of the above problem (SP) in configuration Ω_τ, where $\tau \in [0,T]$. First, from the definition of the material derivative and by using the chain rule, we have

$$\dot{\phi}(x,t) = \phi'(x,t) + \operatorname{grad}_x \phi(x,t) \cdot \mathbf{v}(x,t) = \frac{\partial}{\partial t}\phi_\tau(y,t)_{|y=(X_e)_t(x,\tau)} \ \forall (x,t) \in \mathcal{T}. \tag{15}$$

Next, by evaluating equation (6) at point $x = (X_e)_\tau(y,t)$ and then using (15), we obtain

$$\begin{aligned} \rho((X_e)_\tau(y,t))\frac{\partial}{\partial t}\phi_\tau(y,t) - \operatorname{div}_x(A((X_e)_\tau(y,t)) \operatorname{grad}_x \phi((X_e)_\tau(y,t),t)) \\ = f((X_e)_\tau(y,t),t), \end{aligned} \tag{16}$$

for $(y,t) \in \Omega_\tau \times (0,T)$. Note that in (16) there are derivatives with respect to the Eulerian variable x. In order to obtain a strong formulation of problem (SP) in coordinates $(y,t) \in \Omega_\tau \times (0,T)$ we use the divergence theorem, the change of variable $x = (X_e)_\tau(y,t)$ and the localization theorem, obtaining (see [2] for further details)

$$\begin{aligned} &\operatorname{div}_x(A((X_e)_\tau(y,t)) \operatorname{grad}_x \phi((X_e)_\tau(y,t),t)) \\ &= \operatorname{div}_y \left[F_\tau^{-1}(y,t) A_\tau(y,t) F_\tau^{-T}(y,t) \operatorname{grad}_y \phi_\tau(y,t) \det F_\tau(y,t)\right] \frac{1}{\det F_\tau(y,t)}, \end{aligned}$$

for $(y,t) \in \Omega_\tau \times (0,T)$ and where F_τ is the Jacobian matrix of the transformation $(X_e)_\tau$. Then, ϕ_τ satisfies

$$\begin{aligned} &\rho_\tau(y,t)\frac{\partial}{\partial t}\phi_\tau(y,t) \\ &- \operatorname{div}_y \left[F_\tau^{-1}(y,t) A_\tau(y,t) F_\tau^{-T}(y,t) \operatorname{grad}_y \phi_\tau(y,t) \det F_\tau(y,t)\right] \frac{1}{\det F_\tau(y,t)} = f_\tau(y,t), \end{aligned}$$

for $(y,t) \in \Omega_\tau \times (0,T)$. Moreover, from (7), (8) and (9), we obtain the following initial and boundary conditions for ϕ_τ:

$$\begin{aligned} \phi_\tau(y,t) &= (\phi_D)_\tau(y,t) \text{ in } \Gamma_\tau^D \times (0,T), \\ |F_\tau^{-T}(y,t)\mathbf{m}(y)|\alpha\phi_\tau(y,t) &+ A_\tau(y,t)F_\tau^{-T}(y,t) \operatorname{grad}_y \phi_\tau(y,t) \cdot F_\tau^{-T}(y,t)\mathbf{m}(y) \\ &= |F_\tau^{-T}(y,t)\mathbf{m}(y)| g_\tau(y,t) \text{ on } \Gamma_\tau^R \times (0,T), \\ \phi_\tau(y,0) &= \phi^0(P(y,\tau)) \text{ in } \overline{\Omega}_\tau, \end{aligned}$$

where $\mathbf{m}$ is the outward unit normal vector to $\partial\Omega_\tau$. The second condition has been obtained by using the chain rule and noting that

$$\mathbf{n}((X_e)_\tau(y,t),t) = \frac{F_\tau^{-T}(y,t)\mathbf{m}(y)}{\left|F_\tau^{-T}(y,t)\mathbf{m}(y)\right|} \quad (y,t) \in \Gamma_\tau \times (0,T).$$

Thus, we have the following formulation in $\Omega_\tau \times (0,T)$ of the initial-boundary value problem (SP):

(SP)$_\tau$ **STRONG PROBLEM IN** $\Omega_\tau \times (0,T)$. *Find a function* $\phi_\tau : \overline{\Omega}_\tau \times [0,T] \longrightarrow \mathbb{R}$ *such that*

$$\rho_\tau(y,t)\frac{\partial}{\partial t}\phi_\tau(y,t) - \operatorname{div}_y \left[F_\tau^{-1}(y,t)A_\tau(y,t)F_\tau^{-T}(y,t)\operatorname{grad}_y\phi_\tau(y,t)\det F_\tau(y,t)\right]\frac{1}{\det F_\tau(y,t)} = f_\tau(y,t), \tag{17}$$

for $(y,t) \in \Omega_\tau \times (0,T)$*, subject to the boundary conditions*

$$\phi_\tau(y,t) = (\phi_D)_\tau(y,t) \text{ on } \Gamma_\tau^D \times (0,T), \tag{18}$$

$$|F_\tau^{-T}(y,t)\mathbf{m}(y)|\alpha\phi_\tau(y,t) + A_\tau(y,t)F_\tau^{-T}(y,t)\operatorname{grad}_y\phi_\tau(y,t)\cdot F_\tau^{-T}(y,t)\mathbf{m}(y) = |F_\tau^{-T}(y,t)\mathbf{m}(y)|g_\tau(y,t) \text{ on } \Gamma_\tau^R \times (0,T), \tag{19}$$

and the initial condition

$$\phi_\tau(y,0) = \phi^0(P(y,\tau)) \text{ in } \overline{\Omega}_\tau. \tag{20}$$

Remark 3.1. *From (13) it is easy to check that* F_τ *verifies*

$$(I-B)F_\tau(y,t)B = 0 \quad \forall (y,t) \in \overline{\Omega}_\tau \times (0,T),$$

and then we can easy deduce that the diffusion tensor in (17) has the same form as A.

Depending of the choice of τ, we can obtain different Lagrangian and semi-Lagrangian methods. More precisely, the pure Lagrangian methods (respectively, the semi-Lagrangian methods) are obtained when $\tau = 0$ (respectively, when $\tau \neq 0$). Now, in order to write a weak formulation of (SP)$_\tau$, let us multiply (17) by $\det F_\tau$ and by a test function $\psi \in H^1_{\Gamma_\tau^D}(\Omega_\tau)$, integrate in Ω_τ and apply the usual Green's formula and (19). We get

$$\begin{aligned} &\int_{\Omega_\tau} \rho_\tau(y,t)\frac{\partial}{\partial t}\phi_\tau(y,t)\psi(y)\det F_\tau(y,t)\,dy \\ &+ \int_{\Omega_\tau} F_\tau^{-1}(y,t)A_\tau(y,t)F_\tau^{-T}(y,t)\operatorname{grad}_y\phi_\tau(y,t)\cdot\operatorname{grad}_y\psi(y)\det F_\tau(y,t)\,dy \\ &+ \int_{\Gamma_\tau^R} |F_\tau^{-T}(y,t)\mathbf{m}(y)|\alpha\phi_\tau(y,t)\psi(y)\det F_\tau(y,t)\,dA_y \\ &= \int_{\Omega_\tau} f_\tau(y,t)\psi(y)\det F_\tau(y,t)\,dy + \int_{\Gamma_\tau^R} |F_\tau^{-T}(y,t)\mathbf{m}(y)|g_\tau(y,t)\psi(y)\det F_\tau(y,t)\,dA_y, \end{aligned} \tag{21}$$

for $t \in (0,T)$. These are formal computations, i.e., we have assumed appropriate regularity of the involved data and solution.

4. Time discretization: characteristics methods

In this section, we present pure Lagrangian and semi-Lagrangian methods. They are obtained by introducing different time semi-discretizations of problem (SP)$_\tau$. For simplicity, we assume that the characteristic curves, i.e., the trajectories of the motion are exactly computed. The more usual case where they have to be approximated will be considered below.

Let us introduce the number of time steps, N, the time step $\Delta t = T/N$, and the mesh-points $t_n = n\Delta t$ for $n = 0, 1/2, 1, \ldots, N$. Throughout this work, we use the notation $\psi^n(y) := \psi(y, t_n)$ for a function $\psi(y,t)$. Two different formulas are considered to approximate the time derivative $\dfrac{\partial}{\partial t}\phi_\tau(y,t)$, namely,

- Two-point second order centered formula:

$$\frac{\phi_\tau(y, t + \frac{\Delta t}{2}) - \phi_\tau(y, t - \frac{\Delta t}{2})}{\Delta t}. \tag{22}$$

- Three point second order backward formula:

$$\frac{1}{2\Delta t}(3\phi_\tau(y,t) - 4\phi_\tau(y, t - \Delta t) + \phi_\tau(y, t - 2\Delta t)). \tag{23}$$

According to the values of τ and of t, and of the numerical formula used to approximate the different terms we can obtain different characterictics methods. We use the following notation to present them

$$\psi_j^l(x) = \psi_{t_j}(x, t_l) \quad 0 \le j, l \le N. \tag{24}$$

We notice that $\psi_l^l = \psi^l$ and $F_l^l = I$ for $0 \le l \le N$.

- <u>*One-step semi-Lagrangian schemes*</u>: This one-parameter family of methods arises from fixing $\tau = t_{n+1}$ and $t = t_{n+\theta}$ in (17), and using a convex linear combination involving the values $t = t_n$ and $t = t_{n+1}$ to approximate the rest of the terms at time $t_{n+\theta}$. More precisely:

$$\begin{aligned}
&\left(\theta\rho + (1-\theta)\rho_{n+1}^n\right) \frac{\phi^{n+1} - \phi_{n+1}^n}{\Delta t} - \theta \operatorname{div}\left[A \operatorname{grad}\phi^{n+1}\right] \\
&-(1-\theta)\operatorname{div}\left[(F_{n+1}^n)^{-1} A_{n+1}^n (F_{n+1}^n)^{-T} \operatorname{grad}\phi_{n+1}^n \det F_{n+1}^n\right] \frac{1}{\det F_{n+1}^n} \\
&= \theta f^{n+1} + (1-\theta) f_{n+1}^n \quad \text{ in } \Omega_{t_{n+1}},
\end{aligned} \tag{25}$$

  where $0 \le n \le N-1$.

  We notice that $\rho^{n+1} = \rho$ and $A^{n+1} = A$ because ρ and A are time independent,

  Particular cases:

  (1) When $\theta = 1$, we obtain the classical first order semi-Lagrangian scheme.
  (2) When $\theta = 1/2$, we obtain the second order semi-Lagrangian scheme proposed and analyzed in [21].

- <u>*One-step second order semi-Lagrangian scheme*</u>: This method can be obtained by multiplying (17) by $\det F_\tau$, taking $\tau = t_n$ and $t = t_{n+\frac{1}{2}}$, and using a convex linear combination involving the values at $t = t_n$ and $t = t_{n+1}$ to approximate the rest of the terms. More precisely,

$$\begin{aligned}
&\frac{\rho_n^{n+1}\det F_n^{n+1} + \rho}{2} \frac{\phi_n^{n+1} - \phi^n}{\Delta t} \\
&-\frac{1}{4}\operatorname{div}\left[\left((F_n^{n+1})^{-1} A_n^{n+1} (F_n^{n+1})^{-T} \det F_n^{n+1} + A\right) \operatorname{grad}\phi_n^{n+1}\right] \\
&-\frac{1}{4}\operatorname{div}\left[\left((F_n^{n+1})^{-1} A_n^{n+1} (F_n^{n+1})^{-T} \det F_n^{n+1} + A\right) \operatorname{grad}\phi^n\right] \\
&= \frac{\det F_n^{n+1} f_n^{n+1} + f^n}{2} \quad \text{ in } \Omega_{t_n},
\end{aligned} \tag{26}$$

  where $0 \le n \le N-1$.

- One-step pure Lagrangian schemes: By multiplying (17) by $\det F_\tau$, taking $\tau = t_0$ and $t = t_{n+\theta}$, and using a convex linear combination involving the values at $t = t_n$ and $t = t_{n+1}$ to approximate the rest of the terms, we obtain

$$
\begin{aligned}
&\left(\theta\rho_m^{n+1}(p)\det F^{n+1}(p) + (1-\theta)\rho_m^n(p)\det F^n(p)\right)\frac{\phi_m^{n+1}(p)-\phi_m^n(p)}{\Delta t}\\
&-\theta^2 \operatorname{Div}\left[(F^{n+1})^{-1}(p)A_m^{n+1}(p)(F^{n+1})^{-T}(p)\nabla\phi_m^{n+1}(p)\det F^{n+1}(p)\right]\\
&-\theta(1-\theta)\operatorname{Div}\left[(F^n)^{-1}(p)A_m^n(p)(F^n)^{-T}(p)\nabla\phi_m^{n+1}(p)\det F^n(p)\right]\\
&-\theta(1-\theta)\operatorname{Div}\left[(F^{n+1})^{-1}(p)A_m^{n+1}(p)(F^{n+1})^{-T}(p)\nabla\phi_m^n(p)\det F^{n+1}(p)\right]\\
&-(1-\theta)^2\operatorname{Div}\left[(F^n)^{-1}(p)A_m^n(p)(F^n)^{-T}(p)\nabla\phi_m^n(p)\det F^n(p)\right]\\
&= \theta\det F^{n+1}(p)f_m^{n+1}(p) + (1-\theta)\det F^n(p)f_m^n(p), \quad p\in\Omega,
\end{aligned}
\tag{27}
$$

  for $0 \le n \le N-1$, where we have used that $\psi_0^l = \psi_m^l$ and $F_0^l = F^l$. When $\theta = 1$ it is a first order pure Lagrangian method and when $\theta = 1/2$ we obtain the Crank-Nicholson pure Lagrangian scheme analyzed in [4] and [5].

- Two-steps second order semi-Lagrangian scheme: This method has been proposed in [12]. It can be introduced in our framework by taking $\tau = t_{n+1}$, $t = t_{n+1}$, and using the second order backward formula (23).

$$
\begin{aligned}
&\rho(x)\frac{3\phi^{n+1}(x) - 4\phi_{n+1}^n(x) + \phi_{n+1}^{n-1}(x)}{2\Delta t}\\
&-\operatorname{div}_y\left[A(x)\operatorname{grad}\phi^{n+1}(x)\right] = f^{n+1}(x),\ x\in\Omega_{t_{n+1}},
\end{aligned}
\tag{28}
$$

  where $1 \le n \le N-1$.

In practice, the characteristics $X_e(p,t_n)$ cannot be exactly tracked, therefore, in the above schemes, they will be approximated by using numerical formulas.

5. Second order pure Lagrangian scheme with approximate characteristic curves

In this section we show some results concerning the numerical analysis of the pure Lagrangian scheme proposed in [4] and [5]. In most practical cases, the analytical expression for motion X_e is unknown; instead, we know the velocity field $\mathbf{v}$. Let us assume that $X_e(p,t_0) = p\ \forall p \in \overline{\Omega}$. In order to approximate X_e^n, $n \in \{0,\dots,N\}$ we propose the following second order Runge-Kutta scheme:

For $n = 0$,

$$X_{RK}^0(p) := p \quad \forall p\in\overline{\Omega}, \tag{29}$$

and for $0 \le n \le N-1$ we define by recurrence,

$$X_{RK}^{n+1}(p) := X_{RK}^n(p) + \triangle t\mathbf{v}^{n+\frac{1}{2}}(Y^n(p)) \quad \forall p\in\overline{\Omega}, \tag{30}$$

being

$$Y^n(p) := X_{RK}^n(p) + \frac{\triangle t}{2}\mathbf{v}^n(X_{RK}^n(p)). \tag{31}$$

A similar notation to the one in Section 2 is used for the Jacobian tensor of X_{RK}^n, namely, F_{RK}^n. We have

$$F_{RK}^0(p) = I, \tag{32}$$

and for $0 \leq n \leq N-1$,

$$F_{RK}^{n+1}(p) = F_{RK}^{n}(p) + \Delta t L^{n+\frac{1}{2}}(Y^n(p)) \left(I + \frac{\Delta t}{2} L^n(X_{RK}^n(p)) \right) F_{RK}^n(p). \tag{33}$$

Let us define the following sequences of functions of p: for $0 \leq n \leq N$,

$$\widetilde{A}_{RK}^n := (F_{RK}^n)^{-1} A \circ X_{RK}^n (F_{RK}^n)^{-T} \det F_{RK}^n, \ \widetilde{m}_{RK}^n = |(F_{RK}^n)^{-T}\mathbf{m}| \det F_{RK}^n,$$
$$\widetilde{C}_{RK}^n := C \circ X_{RK}^n (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n}, \ \widetilde{B}_{RK}^n := B (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n},$$

where tensor C is the square root of A. Notice that if $\Delta t < C(\mathbf{v})$, where $C(\mathbf{v})$ is a constant depending on $\mathbf{v}$, it is easy to prove that $\det F_{RK}^n > c(\mathbf{v}, T)$, and F_{RK}^n and $(F_{RK}^n)^{-1}$ are bounded by constants depending only on $\mathbf{v}$ and T, for $0 \leq n \leq N$ (see [2] for details). It will be used below without explicitly stated. Let us choose $\theta = 1/2$ in (27) and replace X_e with X_{RK} and F with F_{RK}. The weak formulation of the resulting problem reads as follows:

$$\begin{aligned}
&\frac{1}{2} \int_\Omega \left(\rho \circ X_{RK}^{n+1} \det F_{RK}^{n+1} + \rho \circ X_{RK}^n \det F_{RK}^n \right) \frac{\phi_{m,\Delta t}^{n+1} - \phi_{m,\Delta t}^n}{\Delta t} \psi \, dp \\
&+ \frac{1}{4} \int_\Omega \left(\widetilde{A}_{RK}^{n+1} + \widetilde{A}_{RK}^n \right) \left(\nabla \phi_{m,\Delta t}^{n+1} + \nabla \phi_{m,\Delta t}^n \right) \cdot \nabla \psi \, dp \\
&+ \frac{\alpha}{4} \int_{\Gamma^R} \left(\widetilde{m}_{RK}^{n+1} + \widetilde{m}_{RK}^n \right) \left(\phi_{m,\Delta t}^{n+1} + \phi_{m,\Delta t}^n \right) \psi \, dA_p \\
&= \frac{1}{2} \int_\Omega \left(\det F_{RK}^{n+1} f^{n+1} \circ X_{RK}^{n+1} + \det F_{RK}^n f^n \circ X_{RK}^n \right) \psi \, dp \\
&+ \frac{1}{2} \int_{\Gamma^R} \left(\widetilde{m}_{RK}^{n+1} g^{n+1} \circ X_{RK}^{n+1} + \widetilde{m}_{RK}^n g^n \circ X_{RK}^n \right) \psi \, dA_p.
\end{aligned} \tag{34}$$

We notice that the approximate characteristics can go out of the domain. Therefore, for simplicity, in this paper we assume that ρ, A, $\mathbf{v}$, f and g can be extended to a wider domain preserving smoothness. This time semi-discretized problem has been analyzed in [4]. Stability and error estimates of order $O(\Delta t^2)$ have been proved. More precisely, the following stability estimates have been obtained:

$$\begin{aligned}
&\sqrt{\gamma} \left|\left| \widehat{\phi_{m,\Delta t}} \right|\right|_{l^\infty(L^2(\Omega))} + \sqrt{\frac{\Lambda}{4}} \left|\left| \widetilde{B}_{RK} \widehat{\mathcal{S}[\nabla \phi_{m,\Delta t}]} \right|\right|_{l^2(\mathbf{L}^2(\Omega))} \\
&\qquad + \sqrt{\frac{\alpha}{8}} \left|\left| \mathcal{S}[\widehat{\phi_{m,\Delta t}}] \right|\right|_{l^2(L^2(\Gamma^R))} \\
&\leq J_1 \left(||\phi_{m,\Delta t}^0||_\Omega + \left|\left| \widehat{f \circ X_{RK}} \right|\right|_{l^2(L^2(\Omega))} + \left|\left| \widehat{g \circ X_{RK}} \right|\right|_{l^2(L^2(\Gamma^R))} \right),
\end{aligned} \tag{35}$$

for $\Delta t < J_2$ and

$$\begin{aligned}
&\sqrt{\frac{\gamma}{4}} \left|\left| \mathcal{R}_{\Delta t}[\widehat{\phi_{m,\Delta t}}] \right|\right|_{l^2(L^2(\Omega))} + \sqrt{\frac{\Lambda}{2}} \left|\left| \widetilde{B}_{RK} \widehat{\nabla \phi_{m,\Delta t}} \right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \\
&+ \sqrt{\frac{\alpha}{4}} \left|\left| \widehat{\phi_{m,\Delta t}} \right|\right|_{l^\infty(L^2(\Gamma^R))} \leq J_3 \left(\sqrt{\frac{\Lambda}{2}} ||B \nabla \phi_{m,\Delta t}^0||_\Omega + \sqrt{\frac{\alpha}{4}} ||\phi_{m,\Delta t}^0||_{\Gamma^R} \right. \\
&\left. + \left|\left| \widehat{f \circ X_{RK}} \right|\right|_{l^2(L^2(\Omega))} + \left|\left| \widehat{g \circ X_{RK}} \right|\right|_{l^\infty(L^2(\Gamma^R))} + \left|\left| \mathcal{R}_{\Delta t}[\widehat{g \circ X_{RK}}] \right|\right|_{l^2(L^2(\Gamma^R))} \right),
\end{aligned} \tag{36}$$

for $\Delta t < J_4$. In the above inequalities, $\widehat{X_{RK}} = \{X_{RK}^n\}_{n=0}^N$ is a second order Runge-Kutta approximation of X_e. Here, constants J_1 and J_2 do not depend on the diffusion tensor but J_3 and J_4 do. However for the particular case of a diffusion tensor of the form $A = \epsilon B$, J_3 does not depend on it and J_4 is bounded below away from zero in the hyperbolic limit, i.e., as $\epsilon \to 0$. To prove these estimates we have assumed that the exact solution and data of the problem are smooth. In [4], error estimates of order $O(\Delta t^2)$ has been also proved.

We propose a space discretization of the time semi-discretized problem (34) by using finite elements spaces V_h^k, where h denotes the mesh-size and the positive integer k is the "approximation degree" in the following sense:

Hypothesis 1. *There exists an interpolation operator* $\pi_h : C^0(\overline{\Omega}) \longrightarrow V_h^k$ *satisfying*

$$||\pi_h \psi - \psi||_{s,2,\Omega} \leq Q h^{r-s} ||\psi||_{r,2,\Omega} \quad \forall \psi \in C^0(\overline{\Omega}) \cap H^r(\Omega) \quad 0 \leq r \leq k+1, \ s = 0, 1,$$

for a positive constant Q *independent of* h.

In order to obtain fully discrete schemes of the time semi-discretizated problem (34), we replace the function space $H^1_{\Gamma^D}(\Omega)$ with V_h^k:

Given $\phi^0_{m,\Delta t,h} \in V_h^k$, *find* $\widehat{\phi_{m,\Delta t,h}} = \{\phi^n_{m,\Delta t,h}\}_{n=1}^N \in \left[V_h^k\right]^N$ *such that*

$$\begin{aligned}
&\frac{1}{2} \int_\Omega \left(\rho \circ X_{RK}^{n+1} \det F_{RK}^{n+1} + \rho \circ X_{RK}^n \det F_{RK}^n\right) \frac{\phi^{n+1}_{m,\Delta t,h} - \phi^n_{m,\Delta t,h}}{\Delta t} \psi_h \, dp \\
&+ \frac{1}{4} \int_\Omega \left(\widetilde{A}_{RK}^{n+1} + \widetilde{A}_{RK}^n\right) \left(\nabla \phi^{n+1}_{m,\Delta t,h} + \nabla \phi^n_{m,\Delta t,h}\right) \cdot \nabla \psi_h \, dp \\
&+ \frac{\alpha}{4} \int_{\Gamma^R} \left(\widetilde{m}_{RK}^{n+1} + \widetilde{m}_{RK}^n\right) \left(\phi^{n+1}_{m,\Delta t,h} + \phi^n_{m,\Delta t,h}\right) \psi_h \, dA_p \\
&= \frac{1}{2} \int_\Omega \left(\det F_{RK}^{n+1} f^{n+1} \circ X_{RK}^{n+1} + \det F_{RK}^n f^n \circ X_{RK}^n\right) \psi_h \, dp \\
&+ \frac{1}{2} \int_{\Gamma^R} \left(\widetilde{m}_{RK}^{n+1} g^{n+1} \circ X_{RK}^{n+1} + \widetilde{m}_{RK}^n g^n \circ X_{RK}^n\right) \psi_h \, dA_p, \quad \forall \psi_h \in V_h^k,
\end{aligned} \tag{37}$$

for $n = 0, \ldots, N-1$.

Remark 5.1. *In* [5], *error estimates of order* $O(\Delta t^2 + h^k)$ *for norms similar to those involved in (35) and (36) have been proved. Moreover, some test problems have been solved in order to verify rates of convergence for this second order pure Lagrangian method and compared the numerical results obtained with semi-Lagrangian and pure Lagrangian methods. These results allow us to conclude that the advantages of the pure Lagrangian methods over semi-Lagrangian ones are that the computational domain is time-independent, they are accurate in zones of strong gradients or discontinuities of the solution and terms of the form* $O(h^\alpha/\Delta t)$ *are not observed in the error as it is typical of semi-Lagrangian methods.*

Remark 5.2. *Notice that, the error estimates (35) and (36) depend on diffusion tensor and on the final time. However, in some particular cases, we can get stability inequalities with constants independent of diffusion tensor or independent of* T *as the theorems below show.*

Theorem 5.1. *Let us assume Dirichlet boundary conditions (i.e.* $\Gamma^D \equiv \Gamma$*), the diffusion tensor of the form* $A \equiv \epsilon B$ *and* $f \equiv 0$. *Let* $\widehat{\phi_{m,\Delta t,h}}$ *be the solution of (37) subject to the initial value* $\phi^0_{m,\Delta t,h} \in V_h^k$. *Then there exist positive constants* J *and* $C(\mathbf{v})$, *independent of the diffusion tensor, such that for* $\Delta t < C(\mathbf{v})$, *we have*

$$\left|\left| \widetilde{B}_{RK} \widehat{\nabla \phi_{m,\Delta t,h}} \right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \leq J \left|\left| B \nabla \phi^0_{m,\Delta t,h} \right|\right|_\Omega, \tag{38}$$

and

(39)
$$\sqrt{\frac{\gamma}{2}}\left|\left|\sqrt{\mathcal{S}[\widehat{\det F_{RK}]}\mathcal{R}_{\Delta t}[\phi_{m,\Delta t,h}]}\right|\right|_{l^2(L^2(\Omega))} \leq J\sqrt{\epsilon}\,||B\nabla\phi^0_{m,\Delta t,h}||_\Omega \quad \forall\epsilon \geq 0.$$

Proof. First, for the mass term, we have

$$\left\langle \frac{(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK})}{2}\frac{\phi^{n+1}_{m,\Delta t,h}-\phi^n_{m,\Delta t,h}}{\Delta t}, \phi^{n+1}_{m,\Delta t,h}-\phi^n_{m,\Delta t,h}\right\rangle_\Omega$$
$$= \frac{1}{2\Delta t}\left|\left|\sqrt{(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK})}\left(\phi^{n+1}_{m,\Delta t,h}-\phi^n_{m,\Delta t,h}\right)\right|\right|^2_\Omega.$$

For the diffusion term, we have

$$\begin{aligned}
&\frac{1}{4}\left\langle\left(\widetilde{A}^{n+1}_{RK}+\widetilde{A}^n_{RK}\right)\left(\nabla\phi^{n+1}_{m,\Delta t,h}+\nabla\phi^n_{m,\Delta t,h}\right), \nabla\phi^{n+1}_{m,\Delta t,h}-\nabla\phi^n_{m,\Delta t,h}\right\rangle_\Omega\\
&= \frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega - \frac{1}{4}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega + \frac{1}{4}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega\\
&\qquad -\frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega.
\end{aligned}$$

Then, by using (33), (13) and that $A = \epsilon B$, we get

$$\frac{1}{4}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega \geq \frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega - \epsilon C_v\Delta t\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega, \tag{40}$$

and

$$-\frac{1}{4}||\widetilde{C}^{n+1}_{RK}\nabla\phi^n_{m,\Delta t,h}||^2_\Omega \geq -\frac{1}{4}||\widetilde{C}^n_{RK}\nabla\phi^n_{m,\Delta t,h}||^2_\Omega - \epsilon C_v\Delta t||\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t,h}||^2_\Omega, \tag{41}$$

for some constant C_v depending only on $\mathbf{v}$ and T. Thus, from (40) and (41) we obtain the following inequality:

$$\begin{aligned}
&\frac{1}{4}\left\langle\left(\widetilde{A}^{n+1}_{RK}+\widetilde{A}^n_{RK}\right)\left(\nabla\phi^{n+1}_{m,\Delta t,h}+\nabla\phi^n_{m,\Delta t,h}\right), \nabla\phi^{n+1}_{m,\Delta t,h}-\nabla\phi^n_{m,\Delta t,h}\right\rangle_\Omega\\
&\qquad \geq \frac{1}{2}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega - \frac{1}{2}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega\\
&\qquad -\epsilon C_v\Delta t\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega - \epsilon C_v\Delta t\left|\left|\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega.
\end{aligned}\tag{42}$$

We use equality (37) for $\psi_h = \phi^{n+1}_{m,\Delta t,h}-\phi^n_{m,\Delta t,h} \in V^k_h$ and the above inequalities to obtain,

$$\begin{aligned}
&\frac{1}{2\Delta t}\left|\left|\sqrt{(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK})}\left(\phi^{n+1}_{m,\Delta t,h}-\phi^n_{m,\Delta t,h}\right)\right|\right|^2_\Omega\\
&\qquad +\frac{1}{2}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega - \frac{1}{2}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega\\
&\qquad \leq C_v\Delta t\epsilon\left(\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega + \left|\left|\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega\right).
\end{aligned}\tag{43}$$

Let us introduce the notation

$$\theta_n^1 := \frac{\gamma}{2\Delta t}\sum_{s=0}^{n-1}\left|\left|\sqrt{\det F_{RK}^{s+1} + \det F_{RK}^{s}}\left(\phi_{m,\Delta t,h}^{s+1} - \phi_{m,\Delta t,h}^{s}\right)\right|\right|_{\Omega}^2,$$

$$\theta_n^2 := \frac{1}{2}\left|\left|\widetilde{B}_{RK}^n \nabla \phi_{m,\Delta t,h}^n\right|\right|_{\Omega}^2.$$

Now, for a fixed integer $q \geq 1$, let us sum (43) from $n = 0$ to $n = q-1$. Then, with the above notation we have

$$\theta_q^1 + (1 - 2C_v\Delta t)\epsilon\theta_q^2 \leq 4C_v\Delta t\epsilon\sum_{n=0}^{q-1}\theta_n^2 + \epsilon\theta_0^2. \tag{44}$$

From this inequality, we get

$$(1 - 2C_v\Delta t)\theta_q^2 \leq 4C_v\Delta t\sum_{n=0}^{q-1}\theta_n^2 + \theta_0^2, \tag{45}$$

$$\theta_q^1 \leq 4C_v\Delta t\epsilon\sum_{n=0}^{q-1}\theta_n^2 + \epsilon\theta_0^2. \tag{46}$$

For Δt small enough, we can apply in (45) the discrete Gronwall inequality (see, for instance, [20]) and take the maximun in $q \in \{1, \ldots, N\}$, obtaining

$$\frac{1}{2}\left|\left|\widetilde{B}_{RK}\widehat{\nabla\phi_{m,\Delta t,h}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))}^2 \leq C(\mathbf{v}, T)\frac{1}{2}\left|\left|B\nabla\phi_{m,\Delta t,h}^0\right|\right|_{\Omega}^2.$$

By using this inequality and (46), we get the result. □

In the particular case of incompressible flows, we can obtain a stability inequality with constant independent of T for the semi-discretized scheme (37) replacing $\det F_{RK}$ with 1. We notice that this replacement is plausible because for incompressible motion $\det F = 1$.

Theorem 5.2. *Let us suppose $f \equiv 0$, $\operatorname{div}\mathbf{v} = 0$, $\rho \equiv 1$. Let $\widehat{\phi_{m,\Delta t,h}}$ be the solution of (37) subject to the initial value $\phi_{m,\Delta t,h}^0 \in V_h^k$. Then there exists a positive constant J, which is independent of T, such that for $\Delta t < C(\mathbf{v})$, we have*

$$\begin{aligned}&\left|\left|\widehat{\phi_{m,\Delta t,h}}\right|\right|_{l^\infty(L^2(\Omega))} + \sqrt{\frac{\Lambda}{4}}\left|\left|\widetilde{B}_{RK}\widehat{\mathcal{S}[\nabla\phi_{m,\Delta t,h}]}\right|\right|_{l^2(\mathbf{L}^2(\Omega))}\\ &+\sqrt{\frac{\alpha}{8}}\left|\left|\sqrt{\mathcal{S}\,[\widetilde{m}_{RK}]}\widehat{\mathcal{S}[\phi_{m,\Delta t,h}]}\right|\right|_{l^2(L^2(\Gamma^R))} \leq J\left(||\phi_{m,\Delta t,h}^0||_\Omega\right.\\ &\left.+\left|\left|\widehat{\sqrt{\widetilde{m}_{RK}}g\circ X_{RK}}\right|\right|_{l^2(L^2(\Gamma^R))}\right).\end{aligned} \tag{47}$$

Proof. First, by applying (37) for $\psi_h = \phi^{n+1}_{m,\Delta t,h} + \phi^n_{m,\Delta t,h} \in V^k_h$, and replacing $\det F_{RK}$ with 1, we obtain

$$
\begin{aligned}
&\frac{1}{\Delta t}\left|\left|\phi^{n+1}_{m,\Delta t,h}\right|\right|^2_\Omega - \frac{1}{\Delta t}\left|\left|\phi^n_{m,\Delta t,h}\right|\right|^2_\Omega \\
&+\frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t,h} + \nabla\phi^n_{m,\Delta t,h}\right)\right|\right|^2_\Omega + \frac{1}{4}\left|\left|\widetilde{C}^n_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t,h} + \nabla\phi^n_{m,\Delta t,h}\right)\right|\right|^2_\Omega \\
&+\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}}\left(\phi^{n+1}_{m,\Delta t,h} + \phi^n_{m,\Delta t,h}\right)\right|\right|^2_{\Gamma^R} \\
&= \left\langle \frac{\widetilde{m}^{n+1}_{RK} g^{n+1}\circ X^{n+1}_{RK} + \widetilde{m}^n_{RK} g^n \circ X^n_{RK}}{2}, \phi^{n+1}_{m,\Delta t,h} + \phi^n_{m,\Delta t,h}\right\rangle_{\Gamma^R}.
\end{aligned}
\tag{48}
$$

By applying the Cauchy-Schwarz and Young inequalities, we get

$$
\begin{aligned}
&\left\langle \frac{\widetilde{m}^{n+1}_{RK} g^{n+1}\circ X^{n+1}_{RK} + \widetilde{m}^n_{RK} g^n \circ X^n_{RK}}{2}, \phi^{n+1}_{m,\Delta t,h} + \phi^n_{m,\Delta t,h}\right\rangle_{\Gamma^R} \\
&\leq \frac{1}{2\alpha}||\sqrt{\widetilde{m}^n_{RK}} g^n \circ X^n_{RK}||^2_{\Gamma^R} + \frac{\alpha}{8}||\sqrt{\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}}\{\phi^{n+1}_{m,\Delta t,h} + \phi^n_{m,\Delta t,h}\}||^2_{\Gamma^R} \\
&\quad + \frac{1}{2\alpha}||\sqrt{\widetilde{m}^{n+1}_{RK}} g^{n+1} \circ X^{n+1}_{RK}||^2_{\Gamma^R}.
\end{aligned}
\tag{49}
$$

Now, for a fixed integer $q \geq 1$, let us sum (48) multiplied by Δt from $n = 0$ to $n = q - 1$, use (49) and take the maximun in $q \in \{1, \ldots, N\}$. Then, the result follows. □

6. Numerical results

In order to assess the performance of the above numerical method and to check the obtained theoretical results, we solve a test problem in two space dimensions. The reference domain is $\Omega = (-1, 1) \times (-1, 1)$ and the final time is of the form $T = m\pi$ with m an integer. The diffusion tensor is of the form $A = aI$ with $a \geq 0$. Moreover, $\mathbf{v} = (-x_2, x_1)$, $\rho = 1$ and the right-hand side $f = 0$. We also impose appropriate Dirichlet boundary and initial conditions such that the solution of the problem is

$$
\phi(x_1, x_2, t) = \frac{b}{b + 4at}\exp\left\{-\frac{(\overline{x}(t) - x_c)^2 + (\overline{y}(t) - y_c)^2}{b + 4at}\right\},
\tag{50}
$$

where

$$
\overline{x}(t) = x_1\cos t + x_2 \sin t,\ \overline{y}(t) = -x_1 \sin t + x_2\cos t,
$$
$$
(x_c, y_c) = (0.25, 0),\ b = 0.01.
$$

We solve this problem by using the second order pure Lagrangian method given in (37). We have chosen for space discretization piecewise quadratic finite elements, that is $k = 2$. In order to obtain an approximate solution of ϕ^n in Eulerian coordinates, we compute the spatial description of material field $\phi^n_{m,\Delta t,h}$ by

$$
\phi^n_{\Delta t,h}(x) := \phi^n_{m,\Delta t,h}(P(x, t_n)) \quad \forall x \in \overline{\Omega}_{t_n},\ 0 \leq n \leq N.
\tag{51}
$$

Notice that, for this example, the exact characteristics can be easily determined and then they can be used to obtain $\phi^n_{\Delta t,h}$. Otherwise, we could use accurate enough approximations of P preserving the error order of the method. Then $\widehat{\phi_{\Delta t,h}}$ is an approximation of $\widehat{\phi}$. In practice, in order to obtain more efficient schemes we can consider $\phi^n_{\Delta t,h}$ as a piecewise quadratic function on Ω_{t_n}. The value of $\phi^n_{\Delta t,h}$ at a node can be obtained by using (51).

In practice the inner products in the Galerkin formulation are calculated using numerical quadrature. In fact, the H^1 and L^2 norms of both the error and the approximate solution are calculated by using a quadrature formula exact for polynomials of degree 5. Similarly, the integrals appearing in (37) are approximated by using a quadrature formula exact for polynomials of degree 2. It is well-known (see, for instance, [16], [19], [24], [7], [3]) that the numerical quadrature may add terms to the final error of the form $O(h^\alpha/\Delta t)$ and, in some cases, it produces the loss of unconditional stability. For this particular example, neither these errors nor an unstable behaviour are observed (see Figure 2).

As predicted by Theorem 5.1, we obtain numerical results showing that the scheme (37) is stable with stability constants independent of the diffusion coefficient. The results are shown in Table 1 and in Figure 1. In Table 1 we show the values of

$$\left|\left|\nabla\widehat{\phi_{m,\Delta t,h}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} / \left|\left|\nabla\phi^0_{m,\Delta t,h}\right|\right|_\Omega , \quad \left|\left|\mathcal{R}_{\Delta t}\widehat{[\phi_{m,\Delta t,h}]}\right|\right|_{l^2(L^2(\Omega))} / \left|\left|\nabla\phi^0_{m,\Delta t,h}\right|\right|_\Omega ,$$

for different diffusion coefficients and $T = 2\pi$. The first value will be called briefly by $norm_1^a$ and the second one by $norm_2^a$. In Figure 1 we have fixed the final time, namely $T = 2\pi$, and shown the value of $norm_2^a$ versus a. As predicted by Theorem 5.1, the numerical results show that: (1) the $l^\infty(L^2(\Omega))$-norm of the gradient of the approximated solution is bounded by a constant independent of the diffusion coefficient; (2) the $l^2(L^2(\Omega))$-norm of the discrete time derivative of the approximate solution tends to zero in the limit when the diffusion tensor vanishes. Moreover, for this example, it is easy to prove that $||\dot{\phi}_m||_{L^\infty(L^2(\Omega))} = O(a)$. Notice that, as we can observe in Figure 1, the approximate solution verifies also this property.

TABLE 1. Norms of the computed solution for pure Lagrangian scheme (37) with $h = 1/132$ and $\Delta t = \pi/50$.

Diffusion coefficient (a)	$norm_1^a$	$norm_2^a$
1000	0.99968	5.34900
100	0.99686	4.31910
10	0.97092	2.16313
1	0.79036	0.70708
0.1	0.34492	0.22360
0.01	0.79748	0.070658
0.001	0.97548	0.02143
0.0001	0.99749	0.00425
0.00001	0.99975	0.00049
0	1	$6.46656E-014$

In Figure 2 we have shown, for different diffusion coefficient, the $l^\infty(H^1(\Omega_{t_n}))$ error between discrete solution $\widehat{\phi_{\Delta t,h}}$, given in (51), and exact solution $\widehat{\phi}$, namely

$$\left|\left|\widehat{\phi_{\Delta t,h}} - \widehat{\phi}\right|\right|_{l^\infty(H^1(\Omega_{t_n}))} := \max_{0\le n\le N} \left|\left|\phi^n_{\Delta t,h} - \phi^n\right|\right|_{1,2,\Omega_{t_n}} .$$

More precisely, on the left, we represent the computed $l^\infty(H^1(\Omega_{t_n}))$ error versus the number of time steps for a uniform spatial mesh of 521×521 vertices. On the right we have fixed a small time step, namely $\Delta t = \pi/500$, and shown $l^\infty(H^1(\Omega_{t_n}))$ error

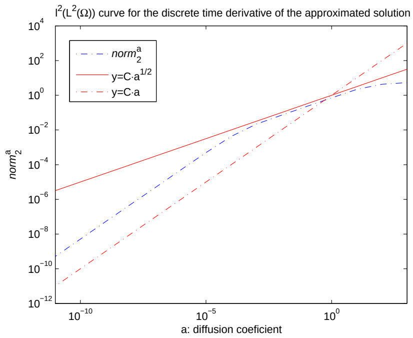

FIGURE 1. Computed $l^2(L^2(\Omega))$ norm of the discrete time derivative of approximated solution over $L^2(\Omega)$ norm of the gradient of approximated solution at initial time.

versus $1/h$. We can observe that the $l^\infty(H^1(\Omega_{t_n}))$ error is of the form $O(\Delta t^2) + O(h^2)$, with constants bounded in the hyperbolic limit.

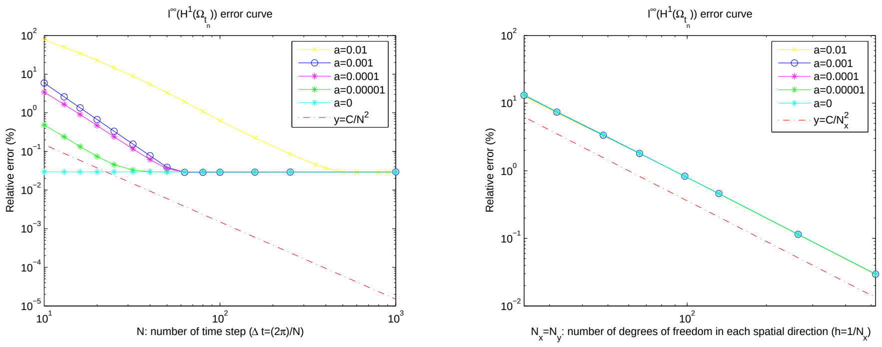

FIGURE 2. Computed $l^\infty(H^1(\Omega_{t_n}))$ errors for pure Lagrangian scheme (37), in log-log scale. On the left errors versus the number of time steps, for a fixed spatial mesh of 521×521 vertices. On the right errors versus $1/h$, for $\Delta t = \pi/500$.

In Table 2 we show the values of

$$\left|\left|\widehat{\phi_{m,\Delta t,h}}\right|\right|_{l^\infty(L^2(\Omega))} / ||\phi^0_{m,\Delta t,h}||_\Omega, \quad \left|\left|\widetilde{B}_{RK}\mathcal{S}[\widehat{\nabla\phi_{m,\Delta t,h}}]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} / ||\phi^0_{m,\Delta t,h}||_\Omega,$$

for different final time and having $a = 0.001$. The first value will be denoted by $norm_1^T$ and the second one by $norm_2^T$. These results show that, as predicted by Theorem 5.2, the $l^\infty(L^2(\Omega))$ norm of the approximate solution and the $l^2(L^2(\Omega))$ norm for the semi-sum of the gradient of the approximate solution at two consecutive time steps are bounded by a constant independent of the final time.

TABLE 2. Norms of the computed solution for pure Lagrangian scheme (37) with $h = 1/32$ and $\Delta t = \pi/50$.

Final time (T)	$norm_1^T$	$norm_2^T$
2π	0.98756	37.78052
4π	0.98756	40.80408
8π	0.98756	42.61668
16π	0.98756	43.61765
32π	0.98756	44.13624
64π	0.98756	44.37476
128π	0.98756	44.46069
256π	0.98756	44.48311
512π	0.98756	44.48750
1024π	0.98756	44.48820

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