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NUMERICAL ANALYSIS OF A SECOND-ORDER PURE LAGRANGE-GALERKIN METHOD FOR CONVECTION-DIFFUSION PROBLEMS. PART I: TIME DISCRETIZATION*

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Abstract. We propose and analyze a second order pure Lagrangian method for variable coefficient convection-(possibly degenerate) diffusion equations with mixed Dirichlet-Robin boundary conditions. First, the method is rigorously introduced for exact and approximate characteristics. Next, $l^\infty(H^1)$ stability is proved and $l^\infty(H^1)$ error estimates of order $O(\Delta t^2)$ are obtained. Moreover, $l^\infty(L^2)$ stability and $l^\infty(L^2)$ error estimates of order $O(\Delta t^2)$ with constants bounded in the hyperbolic limit are shown. For the particular case of Dirichlet boundary conditions, diffusion tensor $A = \epsilon I$ and right-hand side $f = 0$, the $l^\infty(H^1)$ stability estimate is independent of ϵ. Moreover, for incompressible flows the constants in the stability inequalities are independent of the final time. In a second part of this work, the pure Lagrangian scheme will be combined with Galerkin discretization using finite elements spaces and numerical examples will be presented.

Key words. convection-diffusion equation, pure Lagrangian method, characteristics method, stability, error estimates, second order schemes

AMS subject classifications. 65M12, 65M15, 65M25, 65M60

1. Introduction. The main goal of the present paper is to introduce and analyze a second order pure Lagrangian method for the numerical solution of convection-diffusion problems with possibly degenerate diffusion. Computing the solutions of these problems, especially in the convection dominated case, is an important and challenging problem that requires development of reliable and accurate numerical methods.

Linear convection-diffusion equations model a variety of important problems from different fields of engineering and applied sciences, such as thermodynamics, fluid mechanics, and finance (see for instance [21]). In many cases the diffusive term is much smaller than the convective one, giving rise to the so-called convection dominated problems (see [18]). Furthermore, in some cases the diffusive term becomes degenerate, as in some financial models (see, for instance, [27]).

This paper concerns the numerical solution of convection-diffusion problems with degenerate diffusion. For this kind of problems, methods of characteristics for time discretization are extensively used (see the review paper [18]). These methods are based on time discretization of the material time derivative and were introduced in the beginning of the eighties of the last century combined with finite-differences or finite elements for space discretization. When these methods are applied to the formulation of the problem in Lagrangian coordinates (respectively, Eulerian coordinates) they are called pure Lagrangian methods (respectively, semi-Lagrangian methods). The characteristics method has been mathematically analyzed and applied to different problems by several authors, primarily the semi-Lagrangian methods. In particular, the (classical) semi-Lagrangian method is first order accurate in time. It

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has been applied to time dependent convection-diffusion equations combined with finite elements ([17], [22]), finite differences ([17]), etc. Its adaptation to steady state convection-diffusion equations has been developed in [9] and, more recently, the combination of the classical first order scheme with discontinuous Galerkin methods has been used to solve first-order hyperbolic equations in [3], [2] and [4]. Higher order characteristics methods can be obtained by using higher order schemes for the discretization of the material time derivative. In [23] multistep Lagrange-Galerkin methods for convection-diffusion problems are analyzed. In [8] these kind of methods are applied to solve natural convection problems. In [12] and [13] multistep methods for approximating the material time derivative, combined with either mixed finite element or spectral methods, are studied to solve incompressible Navier-Stokes equations. Stability is proved and optimal error estimates for the fully discretized problem are obtained. In [26] a second order characteristics method for solving constant coefficient convection-diffusion equations with Dirichlet boundary conditions is studied. The Crank-Nicholson discretization has been used to approximate the material time derivative. For a divergence-free velocity field vanishing on the boundary and a smooth enough solution, stability and error estimates are stated (see also [10] and [11] for further analysis). In [16] semi-Lagrangian and pure Lagrangian methods are proposed and analyzed for convection-diffusion equation. 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 [14] and [15].
In the present paper, a pure Lagrangian formulation is used for a more general problem. Specifically, we consider 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 analyze a scheme with approximate characteristic curves.

The mathematical formalism of continuum mechanics (see for instance [19]) is used to introduce the schemes and to analyze the error. In most cases the exact characteristics curves cannot be determined analytically, so our analysis include, as a novelty with respect to [16], the case where the characteristics curves are approximated using a second order Runge-Kutta scheme. A proof of $l^\infty(L^2)$ stability inequality is developed which can be appropriately used to obtain $l^\infty(L^2)$ error estimates of order $O(\Delta t^2)$ between the solutions of the time semi-discretized problem and the continuous one; these estimates are uniform in the hyperbolic limit. Moreover, for the particular case of Dirichlet boundary conditions, diffusion tensor $A = \epsilon I$ and right-hand side $f = 0$, the $l^\infty(H^1)$ stability estimate is independent of ϵ (see Remark 4.6). Similar stability and error estimates of order $O(\Delta t^2)$ are proved in the $l^\infty(H^1)$ norm. In general, the constants involved in the stability inequalities depend on the size of the time interval. However, if the flow is incompressible we get constants that are independent of this size.

The paper is organized as follows. In Section 2 the convection-diffusion Cauchy problem is stated in a time dependent bounded domain and some assumptions and notations concerning motions and functional spaces are introduced. In Section 3, the strong formulation of the convection-diffusion Cauchy problem is written in Lagrangian coordinates and the standard associated weak problem is obtained. In Section 4, a second order time discretization scheme is proposed for both exact and second order approximate characteristics. Next, under suitable hypotheses on the data, the $l^\infty(L^2)$ and $l^\infty(H^1)$ stability results are proved for small enough time step. Finally, assuming higher regularity on the data, $l^\infty(L^2)$ and $l^\infty(H^1)$ error estimates of order $O(\Delta t^2)$ for the solution of the time discretized problem are derived. In order to make reading the article easier, some technical results have been included in appendix and the main notations have been summarized in a table.

In a second part of this work (see [7]), a fully discretized pure Lagrange-Galerkin scheme by using finite elements in space will be analyzed and numerical results will be presented.

2. Statement of the 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 [19]. 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

$$\det F(p,t) > 0 \quad \forall p \in \overline{\Omega}, \tag{2.1}$$

being $F(\cdot,t)$ the Jacobian tensor of the deformation $X_e(\cdot,t)$. 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

$$\mathcal{T} := \{(x,t) : x \in \overline{\Omega}_t,\ t \in [0,T]\}, \tag{2.2}$$

and the set

$$\mathcal{O} := \bigcup_{t\in[0,T]} \overline{\Omega}_t. \tag{2.3}$$

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

$$P(\cdot,t) : \overline{\Omega}_t \longrightarrow \overline{\Omega}, \tag{2.4}$$

such that

$$X_e(P(x,t),t) = x, \qquad P(X_e(p,t),t) = p \quad \forall (x,t) \in \mathcal{T}\ \forall (p,t) \in \overline{\Omega} \times [0,T]. \tag{2.5}$$

The 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 [19] pp. 65 – 66). Let us recall that the spatial description of the velocity $\mathbf{v} : \mathcal{T} \longrightarrow \mathbb{R}^d$ is defined by

$$\mathbf{v}(x,t) := \dot{X}_e(P(x,t),t) \quad \forall (x,t) \in \mathcal{T}. \tag{2.6}$$

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

In expressions involving gradients and time derivatives we use the notations given in [19]. Moreover, fields defined in $\mathcal{T}$ are called spatial fields. If Ψ is a spatial field we define its material description Ψ_m by

$$\Psi_m(p,t) := \Psi(X_e(p,t),t). \tag{2.7}$$

Similar definition is used for functions, Ψ, defined in a subset of $\mathcal{T}$ or of $\mathcal{O}$.

The objective of this paper is the numerical solution of the following initial-boundary value problem.

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

$$\rho(x)\frac{\partial \phi}{\partial t}(x,t) + \rho(x)\mathbf{v}(x,t) \cdot \operatorname{grad} \phi(x,t) - \operatorname{div}(A(x) \operatorname{grad} \phi(x,t)) = f(x,t), \tag{2.8}$$

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

$$\phi(\cdot,t) = \phi_D(\cdot,t) \ \ on \ \Gamma_t^D, \tag{2.9}$$

$$\alpha\phi(\cdot,t) + A(\cdot)\,\mathrm{grad}\,\phi(\cdot,t)\cdot\mathbf{n}(\cdot,t) = g(\cdot,t) \ \ on \ \Gamma_t^R, \tag{2.10}$$

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

$$\phi(x,0) = \phi^0(x) \ \ in \ \Omega. \tag{2.11}$$

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.
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 $r = 1,2,\ldots,\infty$ 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

$$H^1_{\Gamma^D}(\mathcal{A}) := \left\{\varphi \in H^1(\mathcal{A}),\ \varphi|_{\Gamma^D} \equiv 0\right\}, \tag{2.12}$$

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

For a Banach function space X and an integer m, space $C^m([0,T],X)$ will be abbreviated as $C^m(X)$ and endowed with norm

$$||\varphi||_{C^m(X)} := \max_{t\in[0,T]}\left\{\max_{j=0,\ldots,m}||\varphi^{(j)}(t)||_X\right\}.$$

In the above definitions, $\varphi^{(j)}$ denotes the j-th derivative of φ with respect to time.
Finally, vector-valued function spaces will be distinguished by bold fonts, namely $\mathbf{L}^r(\mathcal{A})$, $\mathbf{W}^{m,r}(\mathcal{A})$ and $\mathbf{H}^m(\mathcal{A})$, and tensor-valued function spaces will be denoted by $\mathbb{L}^r(\mathcal{A})$, $\mathbb{W}^{m,r}(\mathcal{A})$ and $\mathbb{H}^m(\mathcal{A})$. For the particular case $m = 1$ and $r = \infty$, we consider the vector-valued space $\mathbf{W}^{1,\infty}(\mathcal{A})$ equipped with the following equivalent norm to the usual one

$$||\mathbf{w}||_{1,\infty,\mathcal{A}} := \max\left\{||\mathbf{w}||_{\infty,\mathcal{A}}, ||\,\mathrm{div}\,\mathbf{w}||_{\infty,\mathcal{A}}, ||\nabla\mathbf{w}||_{\infty,\mathcal{A}}\right\}, \tag{2.13}$$

being

$$||\nabla\mathbf{w}||_{\infty,\mathcal{A}} \ := \ \operatorname*{ess\,sup}_{x\in\mathcal{A}}||\nabla\mathbf{w}(x)||_2, \tag{2.14}$$

where $||\cdot||_2$ denotes the tensor norm subordinate to the Euclidean norm in $\mathbb{R}^d$.

Corresponding to the semidiscretized scheme, we have to deal with sequences of functions $\widehat{\psi} = \{\psi^n\}_{n=0}^N$. Thus, 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:

$$\left|\left|\widehat{\psi}\right|\right|_{l^\infty(L^2(\mathcal{A}))} := \max_{0\le n\le N}||\psi^n||_{\mathcal{A}}, \quad \left|\left|\widehat{\psi}\right|\right|_{l^2(L^2(\mathcal{A}))} := \sqrt{\Delta t\sum_{n=0}^N||\psi^n||^2_{\mathcal{A}}}. \tag{2.15}$$

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 article some of the following assumptions will be made on the data of the problem:

Hypothesis 1. There exists a parameter $\delta > 0$, such that the velocity field $\mathbf{v}$ is defined in $\mathcal{T}^\delta$ and $\mathbf{v} \in \mathbf{C}^1(\mathcal{T}^\delta)$, where

$$\mathcal{T}^\delta := \bigcup_{t\in[0,T]} \overline{\Omega}_t^\delta \times \{t\}, \ \textit{being } \Omega_t^\delta := \bigcup_{x\in\overline{\Omega}_t} B(x,\delta). \tag{2.16}$$

Moreover, some properties can be improved if we consider a motion satisfying the following assumption (see, for instance, Appendix A):

Hypothesis 2. The motion X_e satisfies

$$\overline{\Omega}_t = \overline{\Omega} \quad X_e(p,t) = p \quad \forall p \in \Gamma \ \forall t \in [0,T].$$

In order to introduce approximations to the characteristic curves and gradient tensors some additional assumptions are required.

Firstly, we introduce the following set

$$\mathcal{O}^\delta := \bigcup_{t\in[0,T]} \overline{\Omega}_t^\delta. \tag{2.17}$$

Moreover, we define

$$\mathcal{T}^\delta_{\Gamma^R} := \bigcup_{t\in[0,T]} \overline{G}_t^\delta \times \{t\}, \text{ being } G_t^\delta = \bigcup_{x\in\Gamma_t^R} B(x,\delta). \tag{2.18}$$

Hypothesis 3. Function ρ is defined in $\mathcal{O}^\delta$ and belongs to $W^{1,\infty}(\mathcal{O}^\delta)$, being $\mathcal{O}^\delta$ the set defined in (2.17). Moreover,
$0 < \gamma \le \rho(x)$ a.e. $x \in \mathcal{O}^\delta$.

Let us denote $\rho_{1,\infty} = ||\rho||_{1,\infty,\mathcal{O}^\delta}$.

Hypothesis 4. The diffusion tensor, A, is defined in $\mathcal{O}^\delta$ and belongs to $\mathbb{W}^{1,\infty}(\mathcal{O}^\delta)$. Moreover, A is symmetric and has the following form:

$$A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}, \tag{2.19}$$

with A_{n_1} being a positive definite symmetric $n_1 \times n_1$ tensor ($n_1 \ge 1$) and Θ an appropriate zero tensor. Besides, there exists a strictly positive constant, Λ, which is a uniform lower bound for the eigenvalues of A_{n_1}.

Remark 2.1. 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 satisfies Hypothesis 4.

Hypothesis 5. Function f is defined in $\mathcal{T}^\delta$ and it is continuous with respect to the time variable, in space L^2.

Hypothesis 6. Function g is defined in $\mathcal{T}^{\delta}_{\Gamma^R}$ and it is continuous with respect to the time variable, in space H^1. Besides, coefficient α in boundary condition (2.10) is strictly positive.

Let us denote by B the $d \times d$ tensor,

$$B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}, \tag{2.20}$$

where I_{n_1} is the $n_1 \times n_1$ identity matrix. Clearly, under Hypothesis 4 we have

$$\Lambda ||B\mathbf{w}||^2_{\Omega} \leq \langle A\mathbf{w}, \mathbf{w} \rangle_{\Omega} \quad \forall \mathbf{w} \in \mathbb{R}^d. \tag{2.21}$$

As far as the velocity field is defined in $\mathcal{T}^{\delta}$ (see Hypothesis 1), we can introduce the following assumption:

Hypothesis 7. The velocity field satisfies,

$$(I - B)L(x,t)B = 0 \quad \forall (x,t) \in \mathcal{T}^{\delta}. \tag{2.22}$$

Remark 2.2. Hypothesis 7 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. For any $d \times d$ tensor E of the form given in (2.19) it is easy to check that

$$\langle EH^T\mathbf{w}_1, \mathbf{w}_2 \rangle = \langle EH^T B\mathbf{w}_1, B\mathbf{w}_2 \rangle,$$

for any $d \times d$ tensor H satisfying $(I - B)HB = 0$, and vectors $\mathbf{w}_1$, $\mathbf{w}_2 \in \mathbb{R}^d$. This equality will be used below without explicitly stated.

3. Weak formulation. We are going to develop some formal computations in order to write a weak formulation of the above problem (SP) in Lagrangian coordinates p. First, by using the chain rule, we have

$$\dot{\phi}_m(p,t) = \phi'(X_e(p,t),t) + \operatorname{grad}\phi(X_e(p,t),t) \cdot \mathbf{v}(X_e(p,t),t). \tag{3.1}$$

Next, by evaluating equation (2.8) at point $x = X_e(p,t)$ and then using (3.1), we obtain

$$\rho_m(p,t)\dot{\phi}_m(p,t) - \left[\operatorname{div}(A \operatorname{grad}\phi)\right]_m(p,t) = f_m(p,t), \tag{3.2}$$

for $(p,t) \in \Omega \times (0,T)$. Note that in (3.2) there are derivatives with respect to the Eulerian variable x. In order to obtain a strong formulation of problem (SP) in Lagrangian coordinates we introduce the change of variable $x = X_e(p,t)$. By using the chain rule we get (see [6])

$$\left[\operatorname{div}(A \operatorname{grad}\phi)\right]_m = \operatorname{Div}\left[F^{-1}A_m F^{-T}\nabla\phi_m \det F\right]\frac{1}{\det F}.$$

Then, ϕ_m satisfies

$$\rho_m\dot{\phi}_m \det F - \operatorname{Div}\left[F^{-1}A_m F^{-T}\nabla\phi_m \det F\right] = f_m \det F. \tag{3.3}$$

Throughout this article, we use the notation

$$\widetilde{A}_m(p,t) := F^{-1}(p,t)A_m(p,t)F^{-T}(p,t)\det F(p,t) \quad \forall (p,t) \in \overline{\Omega} \times [0,T],$$
$$\widetilde{m}(p,t) := |F^{-T}(p,t)\mathbf{m}(p)| \det F(p,t) \quad \forall (p,t) \in \Gamma \times [0,T],$$

where $\mathbf{m}$ is the outward unit normal vector to Γ. By using the chain rule and noting that

$$\mathbf{n}(X_e(p,t),t) = \frac{F^{-T}(p,t)\mathbf{m}(p)}{|F^{-T}(p,t)\mathbf{m}(p)|} \quad (p,t) \in \Gamma \times (0,T),$$

we get

$$A(x)\,\mathrm{grad}\,\phi(x,t)\cdot\mathbf{n}(x,t) = F^{-1}(p,t)A_m(p,t)F^{-T}(p,t)\nabla\phi_m(p,t)\cdot\frac{\mathbf{m}(p)}{|F^{-T}(p,t)\mathbf{m}(p)|},$$

for $(p,t)\in\Gamma\times(0,T)$ and $x = X_e(p,t)$. Thus, from (2.9)-(2.11) and (3.3), we deduce the following pure Lagrangian formulation of the initial-boundary value problem (SP):

(LSP) **LAGRANGIAN STRONG PROBLEM**. *Find a function* $\phi_m : \overline{\Omega}\times[0,T] \longrightarrow \mathbb{R}$ *such that*

$$\rho_m(p,t)\dot{\phi}_m(p,t)\det F(p,t) - \mathrm{Div}\left[\widetilde{A}_m(p,t)\nabla\phi_m(p,t)\right] = f_m(p,t)\det F(p,t), \tag{3.4}$$

for $(p,t)\in\Omega\times(0,T)$, subject to the boundary conditions

$$\phi_m(p,t) = \phi_D(X_e(p,t),t) \ \text{ on } \Gamma^D\times(0,T), \tag{3.5}$$

$$\alpha\widetilde{m}(p,t)\phi_m(p,t) + \widetilde{A}_m(p,t)\nabla\phi_m(p,t)\cdot\mathbf{m}(p) = \widetilde{m}(p,t)g(X_e(p,t),t) \ \text{ on } \Gamma^R\times(0,T), \tag{3.6}$$

and the initial condition

$$\phi_m(p,0) = \phi^0(p) \ \text{ in } \Omega. \tag{3.7}$$

We consider the standard weak formulation associated with this pure Lagrangian strong problem:

$$\begin{aligned}
&\int_\Omega \rho_m(p,t)\dot{\phi}_m(p,t)\psi(p)\det F(p,t)\,dp + \int_\Omega \widetilde{A}_m(p,t)\nabla\phi_m(p,t)\cdot\nabla\psi(p)\,dp \\
&\quad +\alpha\int_{\Gamma^R}\widetilde{m}(p,t)\phi_m(p,t)\psi(p)\,dA_p = \int_\Omega f_m(p,t)\psi(p)\det F(p,t)\,dp \\
&\quad\quad + \int_{\Gamma^R}\widetilde{m}(p,t)g_m(p,t)\psi(p)\,dA_p,
\end{aligned} \tag{3.8}$$

$\forall\psi\in H^1_{\Gamma^D}(\Omega)$ and $t\in(0,T)$. These are formal computations, i.e., we have assumed appropriate regularity on the involved data and solution.

4. Time discretization. In this section we introduce a second order scheme for time semi-discretization of (3.8). We consider the general case where the diffusion tensor depends on the space variable and can degenerate, and the velocity field is not divergence-free. Moreover, mixed Dirichlet-Robin boundary conditions are also allowed instead of merely Dirichlet ones.

In the first part, we propose a time semi-discretization of (3.8) assuming that the characteristic curves are exactly computed. Next, we propose a second-order Runge-Kutta scheme to approximate them. Finally, stability and error estimates are rigorously stated.

4.1. Second order semidiscretized scheme with exact characteristic curves. We introduce the number of time steps, N, the time step $\Delta t = T/N$, and the mesh-points $t_n = n\Delta t$ for $n = 0, 1/2, 1, \dots, N$. Throughout this work, we use the notation $\psi^n(y) := \psi(y, t_n)$ for a function $\psi(y,t)$.
The semi-discretization scheme we are going to study is a Crank-Nicholson-like scheme:

$$\begin{aligned}
&\frac{1}{2}\int_\Omega \left(\rho_m^{n+1}(p)\det F^{n+1}(p) + \rho_m^n(p)\det F^n(p)\right)\frac{\phi_{m,\triangle t}^{n+1}(p) - \phi_{m,\triangle t}^n(p)}{\Delta t}\,\psi(p)\,dp\\
&+\frac{1}{4}\int_\Omega \left(\widetilde{A}_m^{n+1}(p) + \widetilde{A}_m^n(p)\right)\left(\nabla\phi_{m,\triangle t}^{n+1}(p) + \nabla\phi_{m,\triangle t}^n(p)\right)\cdot\nabla\psi(p)\,dp\\
&+\frac{\alpha}{4}\int_{\Gamma^R}\left(\widetilde{m}^{n+1}(p) + \widetilde{m}^n(p)\right)\left(\phi_{m,\triangle t}^{n+1}(p) + \phi_{m,\triangle t}^n(p)\right)\,\psi(p)\,dA_p\\
&= \frac{1}{2}\int_\Omega \left(\det F^{n+1}(p) f_m^{n+1}(p) + \det F^n(p) f_m^n(p)\right)\,\psi(p)\,dp\\
&+\frac{1}{2}\int_{\Gamma^R}\left(\widetilde{m}^{n+1}(p) g_m^{n+1}(p) + \widetilde{m}^n(p) g_m^n(p)\right)\,\psi(p)\,dA_p.
\end{aligned} \tag{4.1}$$

Remark 4.1. In Section 4.4 we will prove that the approximations involved in scheme (4.1) are $O(\Delta t^2)$ at point $(p, t_{n+\frac{1}{2}})$. Moreover, this order does not change if we replace the exact characteristic curves and gradients F by accurate enough approximations.

4.2. Second order semidiscretized scheme with approximate characteristic curves. In most cases, the analytical expression for motion X_e is unknown; instead, we know the velocity field $\mathbf{v}$. Let us assume that $X_e(p, 0) = p \ \forall p \in \overline{\Omega}$. Then, the motion X_e, assuming it exists, is the solution to the initial-value problem

$$\dot{X}_e(p,t) = \mathbf{v}_m(p,t) \quad X_e(p,0) = p. \tag{4.2}$$

Since the characteristics $X_e(p, t_n)$ cannot be exactly tracked in general, we propose the following second order Runge-Kutta scheme to approximate X_e^n, $n \in \{0, \dots, N\}$. For $n = 0$:

$$X_{RK}^0(p) := p \quad \forall p \in \overline{\Omega}, \tag{4.3}$$

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

$$X_{RK}^{n+1}(p) := X_{RK}^n(p) + \triangle t\mathbf{v}^{n+\frac{1}{2}}(Y^n(p)) \quad \forall p \in \overline{\Omega}, \tag{4.4}$$

being

$$Y^n(p) := X_{RK}^n(p) + \frac{\triangle t}{2}\mathbf{v}^n(X_{RK}^n(p)). \tag{4.5}$$

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

$$F_{RK}^0(p) = I, \tag{4.6}$$

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

$$F_{RK}^{n+1}(p) = F_{RK}^n(p) + \Delta t L^{n+\frac{1}{2}}(Y^n(p))\left(I + \frac{\Delta t}{2}L^n(X_{RK}^n(p))\right)F_{RK}^n(p). \tag{4.7}$$

In appendix, we state some lemmas concerning properties of the approximate characteristics X^n_{RK}.

Let us define the following sequences of functions of p.

$$\widetilde{A}^n_{RK} := (F^n_{RK})^{-1} A \circ X^n_{RK} (F^n_{RK})^{-T} \det F^n_{RK},\ \widetilde{m}^n_{RK} = |(F^n_{RK})^{-T}\mathbf{m}| \det F^n_{RK},$$

for $0 \leq n \leq N$. Since usually the characteristic curves cannot be exactly computed, we replace in (4.1) the exact characteristic curves and gradient tensors by accurate enough approximations,

$$\begin{aligned}
&\frac{1}{2}\int_\Omega \left(\rho\circ X^{n+1}_{RK} \det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK}\right) \frac{\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}}{\Delta t}\,\psi\, dp\\
&+\frac{1}{4}\int_\Omega \left(\widetilde{A}^{n+1}_{RK} + \widetilde{A}^n_{RK}\right)\left(\nabla\phi^{n+1}_{m,\Delta t} + \nabla\phi^n_{m,\Delta t}\right)\cdot\nabla\psi\, dp\\
&+\frac{\alpha}{4}\int_{\Gamma^R} \left(\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}\right)\left(\phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right)\psi\, dA_p\\
&=\frac{1}{2}\int_\Omega \left(\det F^{n+1}_{RK} f^{n+1}\circ X^{n+1}_{RK} + \det F^n_{RK} f^n\circ X^n_{RK}\right)\psi\, dp\\
&+\frac{1}{2}\int_{\Gamma^R} \left(\widetilde{m}^{n+1}_{RK} g^{n+1}\circ X^{n+1}_{RK} + \widetilde{m}^n_{RK} g^n\circ X^n_{RK}\right)\psi\, dA_p.
\end{aligned}\tag{4.8}$$

For these computations we have made the assumptions of Lemma A.3, and Hypothesis 3, 4, 5 and 6.
Notice that we have used a lowest order characteristics approximation formula preserving second order in time accuracy.
Let us introduce $\mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\phi] \in (H^1(\Omega))'$ and $\mathcal{F}^{n+\frac{1}{2}}_{\Delta t} \in (H^1(\Omega))'$ defined by

$$\begin{aligned}
\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\phi], \psi\right\rangle &:= \left\langle \frac{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK}\right)}{2}\frac{\phi^{n+1}-\phi^n}{\Delta t}, \psi\right\rangle_\Omega\\
&+\left\langle \frac{\left(\widetilde{A}^{n+1}_{RK} + \widetilde{A}^n_{RK}\right)}{2}\frac{\left(\nabla\phi^{n+1} + \nabla\phi^n\right)}{2}, \nabla\psi\right\rangle_\Omega\\
&+\alpha\left\langle \frac{\left(\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}\right)}{2}\frac{\left(\phi^{n+1}+\phi^n\right)}{2}, \psi\right\rangle_{\Gamma^R},\\
\left\langle \mathcal{F}^{n+\frac{1}{2}}_{\Delta t}, \psi\right\rangle &:= \left\langle \frac{\det F^{n+1}_{RK} f^{n+1}\circ X^{n+1}_{RK} + \det F^n_{RK} f^n\circ X^n_{RK}}{2}, \psi\right\rangle_\Omega\\
&+\left\langle \frac{\widetilde{m}^{n+1}_{RK} g^{n+1}\circ X^{n+1}_{RK} + \widetilde{m}^n_{RK} g^n\circ X^n_{RK}}{2}, \psi\right\rangle_{\Gamma^R},
\end{aligned}$$

for $\phi \in C^0(H^1(\Omega))$ and $\psi \in H^1(\Omega)$.

Remark 4.2. Regarding the definitions of $\mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\phi]$ and $\mathcal{F}^{n+\frac{1}{2}}_{\Delta t}$, only the values of function ϕ at discrete time steps $\{t_n\}_{n=0}^N$ are required. Thus, the above definitions can also be stated for a sequence of functions $\widehat{\phi} = \{\phi^n\}_{n=0}^N \in [H^1(\Omega)]^{N+1}$.
Then the semidiscretized time scheme can be written as follows:

$$\left\{\begin{array}{l}
\text{Given } \phi^0_{m,\Delta t},\ \text{find } \widehat{\phi_{m,\Delta t}} = \{\phi^n_{m,\Delta t}\}_{n=1}^N \in \left[H^1_{\Gamma^D}(\Omega)\right]^N \text{ such that}\\
\quad\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \psi\right\rangle = \left\langle \mathcal{F}^{n+\frac{1}{2}}_{\Delta t}, \psi\right\rangle \quad \forall\, \psi \in H^1_{\Gamma^D}(\Omega) \text{ for } n = 0, \dots, N-1.
\end{array}\right.\tag{4.9}$$

Remark 4.3. The stability and convergence properties to be studied in the next sections still remain valid if we replace the approximation of characteristics appearing in scheme (4.9) by higher order ones or by the exact value.

4.3. Stability of the semidiscretized scheme. Firstly, we notice that, as a consequence of Hypothesis 4, there exists a unique positive definite symmetric $n_1 \times n_1$ tensor field, C_{n_1}, such that $A_{n_1} = (C_{n_1})^2$. Let us denote by C the symmetric and positive semidefinite $d \times d$ tensor defined by

$$C = \begin{pmatrix} C_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}. \tag{4.10}$$

Notice that $A = C^2$ and $C \in \mathbb{W}^{1,\infty}(\mathcal{O}^\delta)$. Let us denote by G the matrix with coefficients $G_{ij} = |\operatorname{grad} C_{ij}|$, $1 \le i, j \le d$. At this point, let us introduce the constant

$$c_A = \max\{||G||^2_{\infty,\mathcal{O}^\delta}, ||C||^2_{\infty,\mathcal{O}^\delta}\}, \tag{4.11}$$

and the sequence of tensor fields

$$\widetilde{C}^n_{RK} := C \circ X^n_{RK} (F^n_{RK})^{-T} \sqrt{\det F^n_{RK}} \quad \forall n \in \{0, \dots, N\}.$$

Let us introduce the sequence of tensor fields

$$\widetilde{B}^n_{RK} := B (F^n_{RK})^{-T} \sqrt{\det F^n_{RK}} \quad \forall n \in \{0, \dots, N\},$$

where tensor B has been defined in (2.20).

Now, it is convenient to notice that Hypothesis 4 also covers the nondegenerate case. This hypothesis is usual in ultraparabolic equations (see, for instance, [25]), which represent a wide class of degenerate diffusion equations arising from many applications (see, for instance, [5]). Furthermore, as stated in [20], ultraparabolic problems either have C^∞ solutions or can be reduced to nondegenerate problems posed in a lower spatial dimension. This is an important point, as the stability and error estimates will be obtained under regularity assumptions on the solution.

In what follows, c_v denotes the positive constant

$$c_v := \max_{t \in [0,T]} ||\mathbf{v}(\cdot, t)||_{1,\infty,\Omega^\delta_t}, \tag{4.12}$$

where $||\cdot||_{1,\infty,\Omega^\delta_t}$ is the norm given in (2.13). Moreover, C_v (respectively, J and D) will denote a generic positive constant, related to the norm of the velocity field $\mathbf{v}$ (respectively, to the rest of the data of the problem), not necessarily the same at each occurrence.

LEMMA 4.1. *Let us assume Hypotheses 1, 3 and 4. Let $\{\phi^n_{m,\Delta t}\}_{n=1}^N$ be the solution of (4.9) . Then, there exist a positive constant $c(\mathbf{v}, T, \delta)$ such that, for $\Delta t < c$, we have*

$$\begin{aligned}
&\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t} \right\rangle \\
&\ge \frac{1}{\Delta t} \left|\left| \sqrt{\rho \circ X^{n+1}_{RK} \det F^{n+1}_{RK}}\, \phi^{n+1}_{m,\Delta t} \right|\right|^2_\Omega - \frac{1}{\Delta t} \left|\left| \sqrt{\rho \circ X^n_{RK} \det F^n_{RK}}\, \phi^n_{m,\Delta t} \right|\right|^2_\Omega \\
&+ \frac{1}{4} \left|\left| \widetilde{C}^{n+1}_{RK} \left(\nabla \phi^{n+1}_{m,\Delta t} + \nabla \phi^n_{m,\Delta t} \right) \right|\right|^2_\Omega + \frac{1}{4} \left|\left| \widetilde{C}^n_{RK} \left(\nabla \phi^{n+1}_{m,\Delta t} + \nabla \phi^n_{m,\Delta t} \right) \right|\right|^2_\Omega
\end{aligned} \tag{4.13}$$

$$
\begin{aligned}
&+\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}+\widetilde{m}_{RK}^{n}}\left(\phi_{m,\Delta t}^{n+1}+\phi_{m,\Delta t}^{n}\right)\right|\right|_{\Gamma^R}^2\\
&-\widehat{c}\gamma\left(\left|\left|\sqrt{\det F_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^2+\left|\left|\sqrt{\det F_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^2\right),
\end{aligned}
$$

where $\widehat{c}=\rho_{1,\infty}(c_v+C_v\Delta t)/\gamma$ *and* $n\in\{0,\dots,N-1\}$.

Proof. First, we decompose $\left\langle\mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}],\phi_{m,\Delta t}^{n+1}+\phi_{m,\Delta t}^{n}\right\rangle=I_1+I_2+I_3$, with

$$
\begin{aligned}
I_1&=\left\langle\frac{\left(\rho\circ X_{RK}^{n+1}\det F_{RK}^{n+1}+\rho\circ X_{RK}^{n}\det F_{RK}^{n}\right)}{2}\frac{\phi_{m,\Delta t}^{n+1}-\phi_{m,\Delta t}^{n}}{\Delta t},\phi_{m,\Delta t}^{n+1}+\phi_{m,\Delta t}^{n}\right\rangle_{\Omega},\\
I_2&=\frac{1}{4}\left\langle\left(\widetilde{A}_{RK}^{n+1}+\widetilde{A}_{RK}^{n}\right)\left(\nabla\phi_{m,\Delta t}^{n+1}+\nabla\phi_{m,\Delta t}^{n}\right),\nabla\phi_{m,\Delta t}^{n+1}+\nabla\phi_{m,\Delta t}^{n}\right\rangle_{\Omega},\\
I_3&=\frac{\alpha}{4}\left\langle\left(\widetilde{m}_{RK}^{n+1}+\widetilde{m}_{RK}^{n}\right)\left(\phi_{m,\Delta t}^{n+1}+\phi_{m,\Delta t}^{n}\right),\phi_{m,\Delta t}^{n+1}+\phi_{m,\Delta t}^{n}\right\rangle_{\Gamma^R}.
\end{aligned}
$$

Let K be the constant appearing in Corollary A.4. If $\Delta t<K$, we first have

$$
\begin{aligned}
I_1&=\left\langle\frac{\left(\rho\circ X_{RK}^{n+1}\det F_{RK}^{n+1}+\rho\circ X_{RK}^{n}\det F_{RK}^{n}\right)}{2}\frac{\phi_{m,\Delta t}^{n+1}-\phi_{m,\Delta t}^{n}}{\Delta t},\phi_{m,\Delta t}^{n+1}+\phi_{m,\Delta t}^{n}\right\rangle_{\Omega}\\
&=\frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X_{RK}^{n+1}\det F_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^2-\frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X_{RK}^{n}\det F_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^2\\
&+\frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X_{RK}^{n}\det F_{RK}^{n}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^2-\frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X_{RK}^{n+1}\det F_{RK}^{n+1}}\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^2,
\end{aligned}
\tag{4.14}
$$

where we have used Hypothesis 3. Next, we introduce the function $Y_{RK}^n(p,\cdot):[t_n,t_{n+1}]\longrightarrow\Omega_{t_n}^{\delta}$, defined by $Y_{RK}^n(p,s):=X_{RK}^n(p)-(t_n-s)\mathbf{v}^{n+\frac{1}{2}}(Y^n(p))$, which satisfies $Y_{RK}^n(p,t_n)=X_{RK}^n(p)$ and $Y_{RK}^n(p,t_{n+1})=X_{RK}^{n+1}(p)$. If Δt is small enough, it is easy to prove that $Y_{RK}^n(p,\cdot)\subset\Omega_{t_n}^{\delta}$. By hypothesis, ρ is a differentiable function, then by Barrow's rule and the chain rule, the following identity holds:

$$
\rho(X_{RK}^n(p))=\rho(X_{RK}^{n+1}(p))-\zeta^n(p)\quad\text{for a.e. } p\in\Omega,
\tag{4.15}
$$

where

$$
\zeta^n(p):=\int_{t_n}^{t_{n+1}}\operatorname{grad}\rho(Y_{RK}^n(p,s))\cdot\mathbf{v}^{n+\frac{1}{2}}(Y^n(p))\,ds\quad\text{for a.e. } p\in\Omega,
\tag{4.16}
$$

verifies $|\zeta^n(p)|\le\rho_{1,\infty}c_v\Delta t$. Then, by using (A.6), (A.7) and (4.15) in (4.14), we get

$$
\begin{aligned}
I_1&\ge\frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X_{RK}^{n+1}\det F_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^2-\frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X_{RK}^{n}\det F_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^2\\
&-\rho_{1,\infty}\left(c_v+C_v\Delta t\right)\left\{\left|\left|\sqrt{\det F_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^2+\left|\left|\sqrt{\det F_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^2\right\}.
\end{aligned}
\tag{4.17}
$$

For I_2 we use the fact that $A=C^2$ being C a symmetric tensor field. We obtain,

$$
\begin{aligned}
I_2&:=\frac{1}{4}\left\langle\left(\widetilde{A}_{RK}^{n+1}+\widetilde{A}_{RK}^{n}\right)\left(\nabla\phi_{m,\Delta t}^{n+1}+\nabla\phi_{m,\Delta t}^{n}\right),\nabla\phi_{m,\Delta t}^{n+1}+\nabla\phi_{m,\Delta t}^{n}\right\rangle_{\Omega}\\
&=\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n+1}\left(\nabla\phi_{m,\Delta t}^{n+1}+\nabla\phi_{m,\Delta t}^{n}\right)\right|\right|_{\Omega}^2+\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n}\left(\nabla\phi_{m,\Delta t}^{n}+\nabla\phi_{m,\Delta t}^{n}\right)\right|\right|_{\Omega}^2.
\end{aligned}
\tag{4.18}
$$

For I_3 we have

$$I_3 = \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}+\widetilde{m}^{n}_{RK}}\left(\phi^{n+1}_{m,\Delta t}+\phi^{n}_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R}. \tag{4.19}$$

Then, by summing up (4.17), (4.18) and (4.19) we get inequality (4.13). □

LEMMA 4.2. *Let us assume Hypotheses 1, 3, 4 and 7. Let $\{\phi^n_{m,\Delta t}\}_{n=1}^N$ be the solution of (4.9) and $\alpha>0$ be the constant appearing in the Robin boundary condition (2.10). Then, there exist a positive constant $c(\mathbf{v},T,\delta)$ such that, for $\Delta t<c$, we have*

$$\begin{aligned}
&\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t}-\phi^n_{m,\Delta t}\right\rangle\\
&\geq \frac{1}{2\Delta t}\left|\left|\sqrt{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}+\rho\circ X^{n}_{RK}\det F^{n}_{RK}\right)}\left(\phi^{n+1}_{m,\Delta t}-\phi^n_{m,\Delta t}\right)\right|\right|^2_{\Omega}\\
&+\frac{1}{2}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Omega}-\frac{1}{2}\left|\left|\widetilde{C}^{n}_{RK}\nabla\phi^{n}_{m,\Delta t}\right|\right|^2_{\Omega}+\frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R}\\
&-\frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_{\Gamma^R}-\widehat{c}\Delta t\Lambda\left(\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Omega}+\left|\left|\widetilde{B}^{n}_{RK}\nabla\phi^{n}_{m,\Delta t}\right|\right|^2_{\Omega}\right)\\
&-\widehat{c}\Delta t\alpha\left(\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R}+\left|\left|\sqrt{\widetilde{m}^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_{\Gamma^R}\right),
\end{aligned}\tag{4.20}$$

where $\widehat{c}=\max\{c_AC_v/\Lambda, C_v\}$ and $n\in\{0,\dots,N-1\}$.

Proof. First, we decompose $\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t}-\phi^n_{m,\Delta t}\right\rangle = I_1+I_2+I_3$, with

$$\begin{aligned}
I_1 &= \left\langle \frac{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}+\rho\circ X^{n}_{RK}\det F^{n}_{RK}\right)}{2}\frac{\phi^{n+1}_{m,\Delta t}-\phi^n_{m,\Delta t}}{\Delta t}, \phi^{n+1}_{m,\Delta t}-\phi^n_{m,\Delta t}\right\rangle_{\Omega},\\
I_2 &= \frac{1}{4}\left\langle\left(\widetilde{A}^{n+1}_{RK}+\widetilde{A}^{n}_{RK}\right)\left(\nabla\phi^{n+1}_{m,\Delta t}+\nabla\phi^{n}_{m,\Delta t}\right), \nabla\phi^{n+1}_{m,\Delta t}-\nabla\phi^{n}_{m,\Delta t}\right\rangle_{\Omega},\\
I_3 &= \frac{\alpha}{4}\left\langle\left(\widetilde{m}^{n+1}_{RK}+\widetilde{m}^{n}_{RK}\right)\left(\phi^{n+1}_{m,\Delta t}+\phi^{n}_{m,\Delta t}\right), \phi^{n+1}_{m,\Delta t}-\phi^{n}_{m,\Delta t}\right\rangle_{\Gamma^R}.
\end{aligned}$$

For I_1, we use Hypothesis 3 to get

$$I_1 = \frac{1}{2\Delta t}\left|\left|\sqrt{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}+\rho\circ X^{n}_{RK}\det F^{n}_{RK}\right)}\left(\phi^{n+1}_{m,\Delta t}-\phi^n_{m,\Delta t}\right)\right|\right|^2_{\Omega}, \tag{4.21}$$

where we have assumed that $\Delta t<K$, being K the constant appearing in Corollary A.4. For I_2 we first have

$$\begin{aligned}
I_2 &= \frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Omega}-\frac{1}{4}\left|\left|\widetilde{C}^{n}_{RK}\nabla\phi^{n}_{m,\Delta t}\right|\right|^2_{\Omega}\\
&+\frac{1}{4}\left|\left|\widetilde{C}^{n}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Omega}-\frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n}_{m,\Delta t}\right|\right|^2_{\Omega}.
\end{aligned}\tag{4.22}$$

Then we use Corollary A.5, Hypotheses 4 and 7, and equality (4.7) to get

$$\begin{aligned}
\frac{1}{4}\left|\left|\widetilde{C}^{n}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Omega} &\geq \frac{1}{4}\left|\left|C\circ X^{n}_{RK}(F^{n+1}_{RK})^{-T}\nabla\phi^{n+1}_{m,\Delta t}\sqrt{\det F^{n+1}_{RK}}\right|\right|^2_{\Omega}\\
&\quad -c_AC_v\Delta t\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Omega}.
\end{aligned}\tag{4.23}$$

Moreover, since A_{n_1} is symmetric and positive definite, $C_{n_1} = \sqrt{A_{n_1}}$ is a differentiable tensor field . Then by Barrow's rule and the chain rule, the following identity holds,

$$C(X_{RK}^{n+1}(p)) = C(X_{RK}^{n}(p)) + D^n(p) \qquad \text{for a.e. } \ p \in \Omega, \tag{4.24}$$

where we have denoted by D^n the $d \times d$ symmetric tensor field defined by

$$D_{ij}^n(p) := \int_{t_n}^{t_{n+1}} \operatorname{grad} C_{ij}(Y_{RK}^n(p,s)) \cdot \mathbf{v}^{n+\frac{1}{2}}(Y^n(p))\, ds, \tag{4.25}$$

being Y_{RK}^n the mapping defined in the proof of Lemma 4.1. Notice that D is of the form given in (4.10) and verifies $||D^n||_{\infty,\Omega} \leq c_v\sqrt{c_A}\Delta t$. Then, from the previous properties, we have

$$\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} \geq \frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} - c_A C_v \Delta t \left|\left|\widetilde{B}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}. \tag{4.26}$$

Similarly, we obtain the estimate

$$-\frac{1}{4}||\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n}||_{\Omega}^{2} \geq -\frac{1}{4}||\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}||_{\Omega}^{2} - c_A C_v\Delta t||\widetilde{B}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}||_{\Omega}^{2}. \tag{4.27}$$

Thus, by introducing (4.26) and (4.27) in equality (4.22) we obtain the following inequality:

$$\begin{aligned} I_2 \geq{}& \frac{1}{2}\left|\left|\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} - \frac{1}{2}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2} \\ &- c_A C_v\Delta t\left|\left|\widetilde{B}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} - c_A C_v\Delta t\left|\left|\widetilde{B}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2}. \end{aligned} \tag{4.28}$$

For I_3 we first have

$$\begin{aligned} I_3 ={}& \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^{2} - \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^{2} \\ &+ \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^{2} - \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^{2}. \end{aligned} \tag{4.29}$$

Next, by applying Corollaries A.4, A.5, Lemma A.3 and equality (4.7) we obtain

$$\begin{aligned} I_3 \geq{}& \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^{2} - \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^{2} \\ &- C_v\alpha\Delta t\left(\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^{2} + \left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^{2}\right). \end{aligned} \tag{4.30}$$

Then, by summing up (4.21), (4.28) and (4.30), inequality (4.20) follows. □

Now, in order to get error estimates we need to prove stability inequalities for more general right-hand sides; more precisely, for

$$\widehat{Q} = \{Q^n\}_{n=1}^N \in [L^2(\Omega)]^N \text{ and } \widehat{G} = \{G^n\}_{n=1}^N \in [L^2(\Gamma^R)]^N. \tag{4.31}$$

Let us consider the problem:

$$\left\{ \begin{array}{l} \text{Given } \phi_{m,\Delta t}^0, \text{ find } \widehat{\phi_{m,\Delta t}} = \{\phi_{m,\Delta t}^n\}_{n=1}^N \in \left[H_{\Gamma^D}^1(\Omega)\right]^N \text{ such that} \\ \left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}], \psi \right\rangle = \left\langle \mathcal{H}_{\Delta t}^{n+\frac{1}{2}}, \psi \right\rangle \quad \forall \psi \in H_{\Gamma^D}^1(\Omega) \text{ for } n = 0, \ldots, N-1, \end{array} \right. \tag{4.32}$$

with $\left\langle \mathcal{H}_{\Delta t}^{n+\frac{1}{2}}, \psi \right\rangle = \left\langle Q^{n+1}, \psi \right\rangle_{\Omega} + \left\langle G^{n+1}, \psi \right\rangle_{\Gamma^R}$.

THEOREM 4.3. *Let us assume Hypotheses 1, 3 and 4. Let $\widehat{\phi_{m,\Delta t}}$ be the solution of (4.32) subject to the initial value $\phi_{m,\Delta t}^0 \in H^1_{\Gamma^D}(\Omega)$ and $\alpha > 0$ be the constant appearing in the Robin boundary condition (2.10). Then there exist two positive constants J and D, which are independent of the diffusion tensor, such that if $\Delta t < D$ then*

$$\begin{aligned}\sqrt{\gamma}\left|\left|\sqrt{\det \widehat{F_{RK}}}\phi_{m,\Delta t}\right|\right|_{l^\infty(L^2(\Omega))} &+ \sqrt{\frac{\Lambda}{4}}\left|\left|\widetilde{B}_{RK}\widehat{\mathcal{S}[\nabla \phi_{m,\Delta t}]}\right|\right|_{l^2(\mathbf{L}^2(\Omega))}\\ +\sqrt{\frac{\alpha}{8}}\left|\left|\sqrt{\mathcal{S}\,[\widehat{\widetilde{m}_{RK}}]\mathcal{S}}[\phi_{m,\Delta t}]\right|\right|_{l^2(L^2(\Gamma^R))} &\le J\left(\sqrt{\gamma}||\phi^0_{m,\Delta t}||_\Omega\right.\\ &\left.+||\widehat{Q}||_{l^2(L^2(\Omega))} + ||\widehat{G}||_{l^2(L^2(\Gamma^R))}\right).\end{aligned} \tag{4.33}$$

Proof. Sequence $\widehat{\phi_{m,\Delta t}} = \{\phi^n_{m,\Delta t}\}_{n=0}^N$ satisfies $\left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right\rangle = \left\langle \mathcal{H}_{\Delta t}^{n+\frac{1}{2}}, \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right\rangle$. We can use Lemma 4.1 to obtain a lower bound of this expression, and Lemma A.8 for $\psi = \phi^{n+1}_{m,\Delta t}$ and $\varphi = \phi^n_{m,\Delta t}$ to obtain an upper bound. By jointly considering both estimates, we get

$$\begin{aligned}&\frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^n_{RK}\det F^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_\Omega\\ &+\frac{1}{4}\left|\left|\widetilde{C}^n_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t} + \nabla\phi^n_{m,\Delta t}\right)\right|\right|^2_\Omega + \frac{\alpha}{8}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}}\left(\phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R}\\ &\le c_s||Q^{n+1}||^2_\Omega + \frac{4c_g}{\alpha}||G^{n+1}||^2_{\Gamma^R}\\ &+\widehat{c}\gamma\left(\left|\left|\sqrt{\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\sqrt{\det F^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_\Omega\right),\end{aligned} \tag{4.34}$$

where $\widehat{c} = \max\{1/\gamma, 2\rho_{1,\infty}(c_v + C_v\Delta t)/\gamma\}$. Let us introduce the notation

$$\theta^1_n := \gamma\left|\left|\sqrt{\det F^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_\Omega, \quad \theta^2_n := \frac{\Lambda}{4}\sum_{s=0}^{n-1}\Delta t\left|\left|\widetilde{B}^s_{RK}\left(\nabla\phi^{s+1}_{m,\Delta t} + \nabla\phi^s_{m,\Delta t}\right)\right|\right|^2_\Omega,$$

$$\overline{\theta}_n := \frac{\alpha}{8}\sum_{s=0}^{n-1}\Delta t\left|\left|\sqrt{\widetilde{m}^{s+1}_{RK} + \widetilde{m}^s_{RK}}\left(\phi^{s+1}_{m,\Delta t} + \phi^s_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R}.$$

Now, for a fixed integer $q \ge 1$, let us sum (4.34) multiplied by Δt from $n = 0$ to $n = q-1$. Then, with the above notation we have

$$(1 - \widehat{c}\Delta t)\theta^1_q + \theta^2_q + \overline{\theta}_q \le 2\widehat{c}\Delta t\sum_{n=0}^{q-1}\theta^1_n + \beta\left(\theta^1_0 + ||\widehat{Q}||^2_{l^2(L^2(\Omega))} + ||\widehat{G}||^2_{l^2(L^2(\Gamma^R))}\right),$$

where we have used Hypotheses 3 and 4. In the above equation β denotes a positive constant and $\widehat{c} = \max\{1/\gamma, 2\rho_{1,\infty}(c_v + C_v\Delta t)/\gamma\}$. For Δt small enough, we can apply the discrete Gronwall inequality (see, for instance, [24]) and take the maximun in $q \in \{1, \ldots, N\}$. Then, estimate (4.33) follows. ∎

THEOREM 4.4. *Let us assume Hypotheses 1, 3, 4, 7 and (4.31), and let* $\widehat{\phi_{m,\Delta t}}$ *be the solution of (4.32) subject to the initial value* $\phi^0_{m,\Delta t} \in H^1_{\Gamma^D}(\Omega)$. *Let* $\alpha > 0$ *be the constant appearing in the Robin boundary condition (2.10). Then, there exist two positive constants* $J(\mathbf{v}, c_A/\Lambda, T)$ *and* $D(\delta, \mathbf{v}, T, c_A/\Lambda)$ *such that if* $\Delta t < D$ *then*

$$\begin{aligned}
&\sqrt{\frac{\gamma}{4}}\left|\left|\sqrt{\mathcal{S}[\widehat{\det F_{RK}}]}\mathcal{R}_{\Delta t}[\phi_{m,\Delta t}]\right|\right|_{l^2(L^2(\Omega))} + \sqrt{\frac{\Lambda}{2}}\left|\left|\widetilde{B}_{RK}\nabla\widehat{\phi_{m,\Delta t}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \\
&+\sqrt{\frac{\alpha}{4}}\left|\left|\sqrt{\widehat{\widetilde{m}_{RK}}}\widehat{\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Gamma^R))} \leq J\left(\sqrt{\frac{\Lambda}{2}}\,||B\nabla\phi^0_{m,\Delta t}||_\Omega\right. \\
&\left.+\sqrt{\frac{\alpha}{4}}\,||\phi^0_{m,\Delta t}||_{\Gamma^R} + ||\widehat{Q}||_{l^2(L^2(\Omega))} + ||\widehat{G}||_{l^\infty(L^2(\Gamma^R))} + \left|\left|\widehat{\mathcal{R}_{\Delta t}[G]}\right|\right|_{l^2(L^2(\Gamma^R))}\right).
\end{aligned} \tag{4.35}$$

Proof. Sequence $\widehat{\phi_{m,\Delta t}} = \{\phi^n_{m,\Delta t}\}_{n=0}^N$ satisfies $\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}\right\rangle = \left\langle \mathcal{H}^{n+\frac{1}{2}}_{\Delta t}, \phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}\right\rangle$. Then, we use Lemma 4.2 and Lemma A.9 for $\psi = \phi^{n+1}_{m,\Delta t}$ and $\varphi = \phi^n_{m,\Delta t}$ to obtain, respectively, a lower and an upper bound for this expression. By jointly considering both estimates, we get

$$\begin{aligned}
&\frac{1}{2\Delta t}\left|\left|\sqrt{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK}\right)}\left(\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}\right)\right|\right|^2_\Omega \\
&+\frac{1}{2}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{2}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^n_{m,\Delta t}\right|\right|^2_\Omega + \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R} \\
&-\frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_{\Gamma^R} \leq \widehat{c}\Delta t\Lambda\left(\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t}\right|\right|^2_\Omega\right) \\
&+\widehat{c}\Delta t\alpha\left(\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R} + \left|\left|\sqrt{\widetilde{m}^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_{\Gamma^R}\right) + \frac{2c_s\Delta t}{\gamma}||Q^{n+1}||^2_\Omega \\
&+\frac{\gamma}{16\Delta t}\left|\left|\sqrt{\det F^{n+1}_{RK} + \det F^n_{RK}}(\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t})\right|\right|^2_\Omega + \left\langle G^{n+1}, \phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}\right\rangle_{\Gamma^R},
\end{aligned} \tag{4.36}$$

with $\widehat{c} = \max\{c_A C_v/\Lambda, C_v\}$. For $n = 0, \ldots, N$, let us introduce the notations

$$\theta^1_n := \frac{\gamma}{4\Delta t}\sum_{s=0}^{n-1}\left|\left|\sqrt{\det F^{s+1}_{RK} + \det F^s_{RK}}\left(\phi^{s+1}_{m,\Delta t} - \phi^s_{m,\Delta t}\right)\right|\right|^2_\Omega,$$

$$\theta^2_n := \frac{\Lambda}{2}\left|\left|\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t}\right|\right|^2_\Omega, \qquad \overline{\theta}_n := \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_{\Gamma^R}.$$

Now, for a fixed $q \geq 1$, let us sum (4.36) from $n = 0$ to $n = q-1$. With the above notation and by using Lemma A.10 for $\widehat{\psi} = \widehat{\phi_{m,\Delta t}}$, we get

$$\begin{aligned}
&\theta^1_q + (1 - 2\widehat{c}\Delta t)\theta^2_q + (1 - 4\widehat{c}\Delta t)\overline{\theta}_q \leq 4\widehat{c}\Delta t\sum_{n=0}^{q-1}\theta^2_n + 10\widehat{c}\Delta t\sum_{n=0}^{q-1}\overline{\theta}_n \\
&+\beta\left(\theta^2_0 + \overline{\theta}_0 + ||\widehat{Q}||^2_{l^2(L^2(\Omega))} + ||\widehat{G}||^2_{l^\infty(L^2(\Gamma^R))} + \left|\left|\widehat{\mathcal{R}_{\Delta t}[G]}\right|\right|^2_{l^2(L^2(\Gamma^R))}\right),
\end{aligned} \tag{4.37}$$

where we have used Hypotheses 3 and 4. In the above equation $\widehat{c} = \max\{c_A C_v/\Lambda, C_v\}$ and β denotes a positive constant. For Δt small enough, we can apply the discrete

Gronwall inequality (see, for instance, [24]) and take the maximun in $q \in \{1,\dots,N\}$. ∎

Remark 4.4. Stability results for the semidiscretized time scheme (4.9) are obtained by replacing

$$Q^{n+1} \text{ with } 1/2\left(\det F_{RK}^{n+1} f^{n+1} \circ X_{RK}^{n+1} + \det F_{RK}^{n} f^{n} \circ X_{RK}^{n}\right)$$

and G^{n+1} with $1/2\left(\widetilde{m}_{RK}^{n+1} g^{n+1} \circ X_{RK}^{n+1} + \widetilde{m}_{RK}^{n} g^{n} \circ X_{RK}^{n}\right)$ in (4.33) and by replacing

$$Q^{n+1} \text{ with } 1/2\left(\det F_{RK}^{n+1} f^{n+1} \circ X_{RK}^{n+1} + \det F_{RK}^{n} f^{n} \circ X_{RK}^{n}\right)$$

and G^{n+1} with $1/2\left(\widetilde{m}_{RK}^{n+1} g \circ X_{RK}^{n+1} + \widetilde{m}_{RK}^{n} g \circ X_{RK}^{n}\right)$ in (4.35).

Remark 4.5. Notice that, constants J and D appearing in Theorem 4.4 depend on the diffusion tensor, more precisely, on fraction $\dfrac{c_A}{\Lambda}$. In most cases this fraction is bounded in the hyperbolic limit.

Remark 4.6. In the particular case of Dirichlet boundary conditions ($\Gamma^D \equiv \Gamma$), diffusion tensor of the form $A \equiv \epsilon B$ and $f \equiv 0$, a $l^\infty(H^1)$ stability result with constants independent of the diffusion constant ϵ can be obtained. Specifically, by using analogous procedures to the ones in the Theorem 4.4 we can obtain the following $l^\infty(H^1)$ stability result with constants (J and D) independent of ϵ. For $\Delta t < D$,

$$\sqrt{\frac{\gamma}{2}}\left|\left|\sqrt{\mathcal{S}[\widehat{\det F_{RK}]}\mathcal{R}_{\Delta t}[\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))} + \sqrt{\frac{1}{2}}\left|\left|\widetilde{B}_{RK}\widehat{\nabla\phi_{m,\Delta t}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \leq J(1+\sqrt{\epsilon})\sqrt{\frac{1}{2}}\left|\left|B\nabla\phi^0_{m,\Delta t}\right|\right|_{\Omega}. \tag{4.38}$$

Remark 4.7. Notice that, constants appearing in the above stability inequalities depend on T. However, in some particular cases, we can get stability inequalities with constants independent of T as the theorem below shows. Moreover, a possible alternative to obtain a scheme with constants independent of T in stability and error estimates is re-initializing the transformation to the identity after a fixed number of time steps. In this case, by using analogous procedures to the ones in this paper, we could prove the same results but with constants independent of final time.

Let us suppose that motion X_e is incompressible ($\operatorname{div}\mathbf{v} = 0$) and that exact characteristics can be used. Let us assume further that density ρ is constant (we take $\rho \equiv 1$ for simplicity), that diffusion tensor is nondegenerate and that boundary conditions of the problem are Dirichlet everywhere on the boundary, i.e. $\Gamma_D = \Gamma$. Then we can prove a stability result with constants independent of T. For this purpose, let us first introduce the following notation:

$$\phi_{\Delta t}^{n,l}(x) = \phi_{m,\Delta t}^{n}((X_e^l)^{-1}(x)) \quad \forall x \in \overline{\Omega},\ 0 \leq n, l \leq N.$$

THEOREM 4.5. *For $\Delta t < D$ we have,*

$$\left|\left|\widehat{\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Omega))} + \left(\frac{\Lambda}{8}\sum_{s=0}^{N-1}\Delta t\left(\left|\left|\operatorname{grad}\phi_{\Delta t}^{s+1,s+1} + \operatorname{grad}\phi_{\Delta t}^{s,s+1}\right|\right|_{\Omega}^2 + \left|\left|\operatorname{grad}\phi_{\Delta t}^{s+1,s} + \operatorname{grad}\phi_{\Delta t}^{s,s}\right|\right|_{\Omega}^2\right)\right)^{1/2} \leq J\left(||\phi^0_{m,\Delta t}||_\Omega + \left|\left|\widehat{f_m}\right|\right|_{l^2(L^2(\Omega))}\right), \tag{4.39}$$

being J and D independent of T.

Proof. For this particular case it is easy to prove that

$$
\begin{aligned}
&\left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}], \phi_{m,\Delta t}^{n+1} + \phi_{m,\Delta t}^{n} \right\rangle \\
&= \frac{1}{\Delta t} \left|\left|\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} - \frac{1}{\Delta t} \left|\left|\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2} \\
&+\frac{1}{4} \left|\left|\widetilde{C}^{n+1} \left(\nabla\phi_{m,\Delta t}^{n+1} + \nabla\phi_{m,\Delta t}^{n}\right)\right|\right|_{\Omega}^{2} + \frac{1}{4} \left|\left|\widetilde{C}^{n} \left(\nabla\phi_{m,\Delta t}^{n+1} + \nabla\phi_{m,\Delta t}^{n}\right)\right|\right|_{\Omega}^{2},
\end{aligned} \tag{4.40}
$$

being $\widetilde{C}^{l} := C \circ X_e^l (F^l)^{-T}$, $0 \leq l \leq N$. By using the change of variable $x = X_e^{n+1}(p)$ and the chain rule, we obtain

$$
\int_{\Omega} \left| \operatorname{grad} \phi_{\Delta t}^{n+1,n+1} + \operatorname{grad} \phi_{\Delta t}^{n,n+1} \right|^{2} dx = \int_{\Omega} \left| (F^{n+1})^{-T} \left(\nabla\phi_{m,\Delta t}^{n+1} + \nabla\phi_{m,\Delta t}^{n}\right) \right|^{2} dp. \tag{4.41}
$$

Similarly, but by using the change of variable $x = X_e^n(p)$, we have

$$
\int_{\Omega} \left| \operatorname{grad} \phi_{\Delta t}^{n+1,n} + \operatorname{grad} \phi_{\Delta t}^{n,n} \right|^{2} dx = \int_{\Omega} \left| (F^{n})^{-T} \left(\nabla\phi_{m,\Delta t}^{n+1} + \nabla\phi_{m,\Delta t}^{n}\right) \right|^{2} dp. \tag{4.42}
$$

By applying the Cauchy-Schwarz inequality, the Young's inequality and a change of variable we obtain an upper bound for $\left\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \phi_{m,\Delta t}^{n+1} + \phi_{m,\Delta t}^{n} \right\rangle$, namely

$$
\begin{aligned}
&\left\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \phi_{m,\Delta t}^{n+1} + \phi_{m,\Delta t}^{n} \right\rangle \leq \frac{C}{2\Lambda} \left(||f_m^{n+1}||_{\Omega}^2 + ||f_m^n||_{\Omega}^2 \right) \\
&+\frac{\Lambda}{8} || \operatorname{grad} \phi_{\Delta t}^{n+1,n+1} + \operatorname{grad} \phi_{\Delta t}^{n,n+1} ||_{\Omega}^2 + \frac{\Lambda}{8} || \operatorname{grad} \phi_{\Delta t}^{n+1,n} + \operatorname{grad} \phi_{\Delta t}^{n,n} ||_{\Omega}^2,
\end{aligned} \tag{4.43}
$$

where we have used that the H^1-norm and the $\mathbf{L}^2$-norm of the gradient are equivalent on $H^1_\Gamma(\Omega)$. Sequence $\widehat{\phi_{m,\Delta t}} = \{\phi_{m,\Delta t}^n\}_{n=0}^N$ satisfies

$$
\left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}], \phi_{m,\Delta t}^{n+1} + \phi_{m,\Delta t}^{n} \right\rangle = \left\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \phi_{m,\Delta t}^{n+1} + \phi_{m,\Delta t}^{n} \right\rangle.
$$

We use (4.40), Hypothesis 4, (4.41) and (4.42) to obtain a lower bound of this expression and (4.43) to get an upper bound. By jointly considering both estimates we obtain an inequality which we sum up from $n = 0$ to $n = q - 1$. Then, by taking the maximum in $q \in \{1, \ldots, N\}$, we get the result. ∎

Remark 4.8. Now, let us suppose that we use approximate characteristics. By assuming Dirichlet boundary conditions, $\operatorname{div} \mathbf{v} = 0$, $\rho \equiv 1$, nondegenerate diffusion tensor and Hypothesis 2, and by using analogous procedures to the ones in the previous theorem, we can prove a stability result with constants independent of T for the semidiscretized time scheme similar to (4.9) obtained by replacing $\det F_{RK}$ with 1 in the mass term. We notice that this replacement is plausible because for incompressible motion $\det F = 1$.

Remark 4.9. Let us suppose $f \equiv 0$, $\operatorname{div} \mathbf{v} = 0$, $\rho \equiv 1$ and Hypothesis 2. Then, by using analogous procedures to the ones in the Theorem 4.3, one can also prove a stability result with constants independent of T for the semidiscretized time scheme (4.9).

4.4. Error estimate for the semidiscretized scheme. The aim of the present section is to estimate the difference between the *discrete solution* of (4.9), $\widehat{\phi_{m,\Delta t}} := \{\phi^n_{m,\Delta t}\}_{n=0}^N$, and the exact solution of the continuous problem, $\widehat{\phi_m} := \{\phi^n_m\}_{n=0}^N$. According to (3.8) for $t_{n+\frac{1}{2}}$, with $0 \leq n \leq N-1$, the latter solves the problem

$$\left\langle \mathcal{L}^{n+\frac{1}{2}}[\widehat{\phi_m}], \psi \right\rangle = \left\langle \mathcal{F}^{n+\frac{1}{2}}, \psi \right\rangle \quad \forall \psi \in H^1_{\Gamma^D}(\Omega), \tag{4.44}$$

where $\mathcal{L}^{n+\frac{1}{2}}[\widehat{\phi_m}] \in (H^1(\Omega))'$ and $\mathcal{F}^{n+\frac{1}{2}} \in (H^1(\Omega))'$ are defined by

$$\begin{aligned}
\left\langle \mathcal{L}^{n+\frac{1}{2}}[\widehat{\phi_m}], \psi \right\rangle :=& \left\langle \rho \circ X_e^{n+\frac{1}{2}} \det F^{n+\frac{1}{2}} \left(\dot{\phi}_m\right)^{n+\frac{1}{2}}, \psi \right\rangle_\Omega \\
&+ \left\langle \widetilde{A}_m^{n+\frac{1}{2}} \nabla \phi_m^{n+\frac{1}{2}}, \nabla \psi \right\rangle_\Omega + \alpha \left\langle \widetilde{m}^{n+\frac{1}{2}} \phi_m^{n+\frac{1}{2}}, \psi \right\rangle_{\Gamma^R}, \\
\left\langle \mathcal{F}^{n+\frac{1}{2}}, \psi \right\rangle :=& \left\langle \det F^{n+\frac{1}{2}} f^{n+\frac{1}{2}} \circ X_e^{n+\frac{1}{2}}, \psi \right\rangle_\Omega + \left\langle \widetilde{m}^{n+\frac{1}{2}} g^{n+\frac{1}{2}} \circ X_e^{n+\frac{1}{2}}, \psi \right\rangle_{\Gamma^R},
\end{aligned}$$

$\forall \psi \in H^1(\Omega)$.
The error estimate in the $l^\infty(L^2(\Omega))$-norm, to be stated in Theorem 4.8, is proved by means of Theorem 4.3 and the forthcoming Lemmas 4.6 and 4.7. On the other hand, the error estimate for the gradient in the $l^\infty(\mathbf{L}^2(\Omega))$-norm, to be stated in Theorem 4.9, is proved by means of Theorem 4.4 and the forthcoming Lemmas 4.6 and 4.7. Before doing this, we recall some properties satisfied by exact and approximate characteristics. If $\mathbf{v}$ is smooth enough and Δt is small enough, it is easy to prove that F, F^{-1}, $\det F$ and their partial derivatives, as well as the ones of $(F^n_{RK})^{-1}$ and $\det F^n_{RK}$ can be bounded by constants depending only on $\mathbf{v}$ and T, moreover

$$\begin{aligned}
||X_e^n - X^n_{RK}||_{1,\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2, ||(F^n)^{-T} - (F^n_{RK})^{-T}||_{1,\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2 \\
|| \det F^n - \det F^n_{RK}||_{1,\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2.
\end{aligned}$$

The following lemmas can be easily proved by using Taylor expansions, the above estimates and the ones obtained in Appendix A for F^n_{RK}, $(F^n_{RK})^{-1}$ and $\det F^n_{RK}$ (see [6] for further details).

LEMMA 4.6. *Assume Hypotheses 1, 3 and 4 hold. Moreover, suppose that* $X_e \in \mathbf{C}^5(\overline{\Omega} \times [0,T])$ *and that the coefficients of problem (2.8)-(2.11) satisfy,*

$$\mathbf{v} \in \mathbf{C}^3(\mathcal{T}^\delta), \quad \rho_m \in C^2(L^\infty(\Omega)), \quad A \in \mathbb{W}^{2,\infty}(\mathcal{O}^\delta), \quad A_m \in C^2(\mathbb{W}^{1,\infty}(\Omega)).$$

Let the solution of (4.44) satisfy,

$$\phi_m \in C^3(L^2(\Omega)), \quad \nabla\phi_m \in C^2(\mathbf{H}^1(\Omega)), \quad \phi_m|_{\Gamma^R} \in C^2(L^2(\Gamma^R)).$$

Finally, assume that $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$. *Then, for each* $0 \leq n \leq N-1$, *there exist two functions* $\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega} : \Omega \longrightarrow \mathbb{R}$ *and* $\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma} : \Gamma^R \longrightarrow \mathbb{R}$, *such that*

$$\left\langle \left(\mathcal{L}^{n+\frac{1}{2}} - \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}\right)[\widehat{\phi_m}], \psi \right\rangle = \left\langle \xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega}, \psi \right\rangle_\Omega + \left\langle \xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma}, \psi \right\rangle_{\Gamma^R}, \tag{4.45}$$

$\forall \psi \in H^1_{\Gamma^D}(\Omega)$. *Moreover,* $\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega} \in L^2(\Omega)$, $\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma} \in L^2(\Gamma^R)$ *and the following estimates hold:*

$$\begin{aligned}
\left|\left|\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega}\right|\right|_\Omega &\leq \Delta t^2 C(T,\mathbf{v},\rho,A)\left(||\phi_m||_{C^3(L^2(\Omega))} + ||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))}\right), \\
\left|\left|\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma}\right|\right|_{\Gamma^R} &\leq \Delta t^2 C(T,\mathbf{v},A)\left(||\nabla\phi_m \cdot \mathbf{m}||_{C^2(L^2(\Gamma^R))} + \alpha||\phi_m||_{C^2(L^2(\Gamma^R))}\right),
\end{aligned} \tag{4.46}$$

where $\alpha > 0$ appears in (2.10).

LEMMA 4.7. *Assume Hypothesis 1, $\mathbf{v} \in \mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$ and $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, being η the constant appearing in Lemma A.1. Let $f_m \in C^2(L^2(\Omega))$, $f \in C^1(\mathcal{T}^\delta)$, $g_m \in C^2(L^2(\Gamma^R))$, $g \in C^1(\mathcal{T}^\delta_{\Gamma^R})$. Then, for each $n \in \{0, \ldots, N-1\}$, there exist $\xi_f^{n+\frac{1}{2}} : \Omega \longrightarrow \mathbb{R}$ and $\xi_g^{n+\frac{1}{2}} : \Gamma^R \longrightarrow \mathbb{R}$, satisfying*

$$\left\langle \left(\mathcal{F}^{n+\frac{1}{2}} - \mathcal{F}^{n+\frac{1}{2}}_{\Delta t}\right), \psi \right\rangle = \left\langle \xi_f^{n+\frac{1}{2}}, \psi \right\rangle_\Omega + \left\langle \xi_g^{n+\frac{1}{2}}, \psi \right\rangle_{\Gamma^R} \quad \forall \psi \in H^1(\Omega). \tag{4.47}$$

Moreover, $\xi_f^{n+\frac{1}{2}} \in L^2(\Omega)$ and $\xi_g \in L^2(\Gamma^R)$ and the following estimates hold:

$$\begin{aligned} \left|\left|\xi_f^{n+\frac{1}{2}}\right|\right|_\Omega &\leq \Delta t^2 C(T, \mathbf{v}, \mathcal{T}^\delta) \left(|| \det F f_m||_{C^2(L^2(\Omega))} + ||f||_{C^1(\mathcal{T}^\delta)}\right), \\ \left|\left|\xi_g^{n+\frac{1}{2}}\right|\right|_{\Gamma^R} &\leq \Delta t^2 C(T, \mathbf{v}, \mathcal{T}^\delta_{\Gamma^R}) \left(||\widetilde{m} g_m||_{C^2(L^2(\Gamma^R))} + ||g||_{C^1(\mathcal{T}^\delta_{\Gamma^R})}\right). \end{aligned} \tag{4.48}$$

Now let us introduce some regularity assumptions on the data of the problem needed to prove the error estimates below.

Hypothesis 8. Functions appearing in problem (2.8)-(2.11) satisfy,

- $\rho_m \in C^2(L^\infty(\Omega))$, $A \in \mathbb{W}^{2,\infty}(\mathcal{O}^\delta)$, $A_m \in C^2(\mathbb{W}^{1,\infty}(\Omega))$,
- $\mathbf{v} \in \mathbf{C}^3(\mathcal{T}^\delta)$,
- $f_m \in C^2(L^2(\Omega))$, $f \in C^1(\mathcal{T}^\delta)$, $g_m \in C^2(L^2(\Gamma^R))$, $g \in C^1(\mathcal{T}^\delta_{\Gamma^R})$ *and* $\alpha > 0$.

Hypothesis 9. Functions appearing in problem (2.8)-(2.11) satisfy,

- $\rho_m \in C^2(L^\infty(\Omega))$, $A \in \mathbb{W}^{2,\infty}(\mathcal{O}^\delta)$, $A_m \in C^3(\mathbb{W}^{1,\infty}(\Omega))$,
- $\mathbf{v} \in \mathbf{C}^3(\mathcal{T}^\delta)$,
- $f_m \in C^2(L^2(\Omega))$, $f \in C^1(\mathcal{T}^\delta)$, $g_m \in C^3(L^2(\Gamma^R))$, $g \in C^2(\mathcal{T}^\delta_{\Gamma^R})$ *and* $\alpha > 0$.

THEOREM 4.8. *Assume Hypotheses 1, 3, 4, 5, 6, 7 and 8, and $X_e \in \mathbf{C}^5(\overline{\Omega}\times[0,T])$. Let*

$$\phi_m \in C^3(L^2(\Omega)), \quad \nabla\phi_m \in C^2(\mathbf{H}^1(\Omega)), \quad \phi_m|_{\Gamma^R} \in C^2(L^2(\Gamma^R)),$$

be the solution of (4.44) and let $\widehat{\phi_{m,\Delta t}}$ be the solution of (4.9) subject to the initial value $\phi^0_{m,\Delta t} = \phi^0_m = \phi^0 \in H^1(\Omega)$. Then, there exist two positive constants J and D, the latter being independent of the diffusion tensor, such that, if $\Delta t < D$ we have

$$\begin{aligned} &\sqrt{\gamma}||\widehat{\sqrt{\det F_{RK}}\,(\phi_m} - \phi_{m,\Delta t})||_{l^\infty(L^2(\Omega))} \\ &+\sqrt{\frac{\Lambda}{4}}\left|\left|\widetilde{B}_{RK}\mathcal{S}\,[\widehat{\nabla\phi_m - \nabla\phi_{m,\Delta t}}]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} \\ &+\sqrt{\frac{\alpha}{8}}\left|\left|\widehat{\sqrt{\mathcal{S}\,[\widetilde{m}_{RK}]}\mathcal{S}\,[\phi_m} - \phi_{m,\Delta t}]\right|\right|_{l^2(L^2(\Gamma^R))} \leq J\ \Delta t^2 \left(||\phi_m||_{C^3(L^2(\Omega))}\right. \\ &+||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))} + ||\nabla\phi_m\cdot\mathbf{m}||_{C^2(L^2(\Gamma^R))} + ||\phi_m||_{C^2(L^2(\Gamma^R))} \\ &\left.+|| \det F f_m||_{C^2(L^2(\Omega))} + ||f||_{C^1(\mathcal{T}^\delta)} + ||\widetilde{m} g_m||_{C^2(L^2(\Gamma^R))} + ||g||_{C^1(\mathcal{T}^\delta_{\Gamma^R})}\right). \end{aligned} \tag{4.49}$$

Proof. We denote by $\widehat{e_{m,\Delta t}}$ the difference between the continuous and the discrete solution, that is, $\widehat{e_{m,\Delta t}} = \left\{\phi^n_m - \phi^n_{m,\Delta t}\right\}_{n=0}^N$. Then, by using (4.9) and (4.44) we have

$$\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{e_{m,\Delta t}}], \psi \right\rangle = \left\langle \left(\mathcal{L}^{n+\frac{1}{2}}_{\Delta t} - \mathcal{L}^{n+\frac{1}{2}}\right)[\widehat{\phi_m}], \psi \right\rangle + \left\langle \mathcal{F}^{n+\frac{1}{2}} - \mathcal{F}^{n+\frac{1}{2}}_{\Delta t}, \psi \right\rangle, \tag{4.50}$$

$\forall\psi \in H^1_{\Gamma^D}(\Omega)$ and $0 \le n \le N-1$. Then, as a consequence of Lemmas 4.6 and 4.7, we deduce

$$\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{e_{m,\Delta t}}], \psi \right\rangle = \left\langle \xi_f^{n+\frac{1}{2}} - \xi_{\mathcal{L}_\Omega}^{n+\frac{1}{2}}, \psi \right\rangle_\Omega + \left\langle \xi_g^{n+\frac{1}{2}} - \xi_{\mathcal{L}_\Gamma}^{n+\frac{1}{2}}, \psi \right\rangle_{\Gamma^R}, \tag{4.51}$$

$\forall\psi \in H^1_{\Gamma^D}(\Omega)$. Now the result follows by applying Theorem 4.3 to (4.51), noting that $e^0_{m,\Delta t} = 0$ and using the upper bounds for $\xi_{\mathcal{L}_\Omega}$, ξ_f, $\xi_{\mathcal{L}_\Gamma}$ and ξ_g given in Lemmas 4.6 and 4.7. ∎

Remark 4.10. Notice that constant J appearing in the previous theorem is bounded in the limit when the diffusion tensor vanishes. In particular, Theorem 4.8 is also valid when $A \equiv 0$.

THEOREM 4.9. *Let us assume Hypotheses 1, 3, 4, 5, 6, 7 and 9, and $X_e \in \mathbf{C}^5(\overline{\Omega} \times [0,T])$. Let ϕ_m with*

$$\phi_m \in C^3(L^2(\Omega)), \quad \nabla\phi_m \in C^3(\mathbf{H}^1(\Omega)), \quad \phi_m|_{\Gamma^R} \in C^3(L^2(\Gamma^R)),$$

be the solution of (4.44) and $\widehat{\phi_{m,\Delta t}}$ be the solution of (4.9) subject to the initial value $\phi^0_{m,\Delta t} = \phi^0_m = \phi^0 \in H^1(\Omega)$. Then, there exist two positive constants J and D such that, for $\Delta t < D$ we have

$$\begin{aligned}
&\sqrt{\frac{\gamma}{4}}\left|\left|\sqrt{\mathcal{S}[\det F_{RK}]}\widehat{\mathcal{R}_{\Delta t}[\phi_m - \phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))} \\
&\quad + \sqrt{\frac{\Lambda}{2}}\left|\left|\widetilde{B}_{RK}\,(\widehat{\nabla\phi_m - \nabla\phi_{m,\Delta t}})\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \\
&+\sqrt{\frac{\alpha}{4}}\left|\left|\sqrt{\widetilde{m}_{RK}}\,(\widehat{\phi_m - \phi_{m,\Delta t}})\right|\right|_{l^\infty(L^2(\Gamma^R))} \le J\,\Delta t^2 \big(||\phi_m||_{C^3(L^2(\Omega))} \\
&\quad + ||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))} + ||\nabla\phi_m\cdot\mathbf{m}||_{C^3(L^2(\Gamma^R))} + ||\phi_m||_{C^3(L^2(\Gamma^R))} \\
&\quad + ||\det F f_m||_{C^2(L^2(\Omega))} + ||f||_{C^1(\mathcal{T}^\delta)} + ||\widetilde{m}g_m||_{C^3(L^2(\Gamma^R))} + ||g||_{C^2(\mathcal{T}^\delta_{\Gamma^R})}\Big).
\end{aligned} \tag{4.52}$$

Proof. It is analogous to the one of the previous theorem, but using Theorem 4.4 instead of Theorem 4.3 and noting that

$$\begin{aligned}
\left|\left|\widehat{\mathcal{R}_{\Delta t}[\xi_{\mathcal{L}_\Gamma}]}\right|\right|_{l^2(L^2(\Gamma^R))} + \left|\left|\widehat{\mathcal{R}_{\Delta t}[\xi_g]}\right|\right|_{l^2(L^2(\Gamma^R))} &\le \widetilde{C}\Delta t^2 \Big(||\nabla\phi_m\cdot\mathbf{m}||_{C^3(L^2(\Gamma^R))} \\
&+ ||\phi_m||_{C^3(L^2(\Gamma^R))} + ||\widetilde{m}g_m||_{C^3(L^2(\Gamma^R))} + ||g||_{C^2(\mathcal{T}^\delta_{\Gamma^R})}\Big).
\end{aligned}$$

This estimate follows by using Taylor expansions and

$$\begin{aligned}
\left|\big(X_e^{n+1}(p) - X_{RK}^{n+1}(p)\big) - (X_e^n(p) - X_{RK}^n(p))\right| &\le \widetilde{C}\Delta t^3, \\
\left|\big((F^{n+1})^{-1}(p) - (F_{RK}^{n+1})^{-1}(p)\big) - \big((F^n)^{-1}(p) - (F_{RK}^n)^{-1}(p)\big)\right| &\le \widetilde{C}\Delta t^3, \\
\left|\big(\det F^{n+1}(p) - \det F_{RK}^{n+1}(p)\big) - (\det F^n(p) - \det F_{RK}^n(p))\right| &\le \widetilde{C}\Delta t^3.
\end{aligned}$$ ∎

Remark 4.11. In the particular case of diffusion tensor of the form $A = \epsilon B$ with $\epsilon > 0$, constants J and D appearing in the previous theorem are bounded as $\epsilon \to 0$.

Remark 4.12. Notice that, from the obtained estimates and by using a change of variable, we can deduce similar ones in Eulerian coordinates (see [6] for further details).

5. Conclusions. We have performed the numerical analysis of a second-order pure Lagrangian method for convection-diffusion equations with degenerate diffusion tensor and non-divergence-free velocity fields. Moreover, we have considered general Dirichlet-Robin boundary conditions. The method has been introduced and analyzed by using the formalism of continuum mechanics. Although our analysis considers any velocity field and use approximate characteristic curves, second order error estimates have been obtained when smooth enough data and solutions are available. In the second part of this paper ([7]), we analyze a fully discretized pure Lagrange-Galerkin scheme and present numerical examples showing the predicted behavior (see also [6]).

Appendix A. In this section, firstly we prove some technical results which are used throughout this paper. Then, we introduce a summary table of the main notations.

Lemma A.1. *Under Hypothesis 1, there exists a parameter $\eta > 0$ such that if $\Delta t < \eta$ then $X^n_{RK}(p)$ is defined $\forall p \in \overline{\Omega}$ and $\forall n \in \{0, \dots, N\}$, and the following inclusion holds*

$$X^n_{RK}(\overline{\Omega}) \subset \Omega^\delta_{t_n}.$$

Proof. The result can be easily proved by applying Taylor expansion to X_e in the time variable and using the regularity of $\mathbf{v}$. ∎

Lemma A.2. *Under Hypothesis 1, if $\Delta t < \eta$, η being the number introduced in the previous lemma, there exists a constant C depending on $\mathbf{v}$ such that*

$$||F^n_{RK}||_{\infty,\Omega} \leq e^{T(||L||_{\infty,\mathcal{T}^\delta}+C\Delta t)} \quad \forall\, n \in \{0, \dots, N\}. \tag{A.1}$$

Proof. The inequality follows by applying norms to (4.7), using the initial condition (4.6) and applying the discrete Gronwall inequality. ∎

Lemma A.3. *Under Hypothesis 1 if $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, then*

$$||(F^n_{RK})^{-1}||_{\infty,\Omega} \leq e^{T(||L||_{\infty,\mathcal{T}^\delta}+C\Delta t)} \quad \forall\, n \in \{0, \dots, N\} \tag{A.2}$$

and

$$(F^{n+1}_{RK})^{-1}(p) = (F^n_{RK})^{-1}(p) \left(I - \Delta t L^{n+\frac{1}{2}}(Y^n(p)) + O(\Delta t^2) \right), \tag{A.3}$$

being the term $O(\Delta t^2)$ depending on $\mathbf{v}$, $p \in \overline{\Omega}$ and $0 \leq n \leq N-1$.

Proof. Firstly, we can write $F^{n+1}_{RK}(p) = M^n_{RK}(p)F^n_{RK}(p)$, with $M^n_{RK}(p) := I + \Delta t L^{n+\frac{1}{2}}(Y^n(p))\,(I + \Delta t/2 L^n(X^n_{RK}(p)))$. Now, by applying norms we have that $||I - M^n_{RK}||_{\infty,\Omega} < 1$. Thus, $M^n_{RK}(p)$ is invertible for $0 \leq n \leq N-1$ and then, by induction, we deduce that $F^{n+1}_{RK}(p)$ is invertible too, with $(F^{n+1}_{RK})^{-1}(p) = (F^n_{RK})^{-1}(p)(M^n_{RK})^{-1}(p)$. Moreover, $(M^n_{RK})^{-1}(p) = \sum_{j=0}^\infty (I - M^n_{RK}(p))^j$ so (A.3) follows. The proof of (A.2) is analogous to the one of the previous lemma. ∎

The following corollaries can be easily proved (see [6] for further details).

Corollary A.4. *Under the assumptions of Lemma A.2, we have*

$$||\det F^n_{RK}||_{\infty,\Omega} \leq e^{T(||\operatorname{div}\mathbf{v}||_{\infty,\mathcal{T}^\delta}+C(\mathbf{v})\Delta t)}, \tag{A.4}$$

$$\det F^n_{RK}(p) > 0 \qquad \text{if } \Delta t < K, \tag{A.5}$$

with K depending on $\mathbf{v}$ and $0 \leq n \leq N$. Moreover, $\forall p \in \overline{\Omega}$ $\det F^{n+1}_{RK}(p)$ satisfies

$$\det F^{n+1}_{RK}(p) = \det F^n_{RK}(p) \left(1 + \Delta t \operatorname{div} \mathbf{v}^{n+\frac{1}{2}}(Y^n(p)) + O(\Delta t^2) \right), \tag{A.6}$$

being $O(\Delta t^2)$ depending on $\mathbf{v}$ and $0 \leq n \leq N-1$.

COROLLARY A.5. *Under the assumptions of Lemma A.3, we have*

$$\det(F_{RK}^{n+1})^{-1}(p) = \det(F_{RK}^{n})^{-1}(p)\left(1 - \Delta t \operatorname{div} \mathbf{v}^{n+\frac{1}{2}}(Y^n(p)) + O(\Delta t^2)\right), \tag{A.7}$$

$\forall p \in \overline{\Omega}$, $\forall n \in \{0,\ldots,N-1\}$, with $O(\Delta t^2)$ depending on $\mathbf{v}$. Moreover, $\forall n \in \{0,\ldots,N\}$, we have

$$||\det(F_{RK}^{n})^{-1}||_{\infty,\Omega} \leq e^{T(||\operatorname{div}\mathbf{v}||_{\infty,\mathcal{T}^\delta} + C(\mathbf{v})\Delta t)}. \tag{A.8}$$

LEMMA A.6. *Under Hypothesis 1 if $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta}), K\}$, where K is the constant appearing in Corollary A.4, then, $\forall p \in \overline{\Omega}$ and $\forall n \in \{0,\ldots,N\}$, we have*

$$\widetilde{c_1} \leq \det F_{RK}^n(p) \leq \widetilde{C_1}, \quad \widetilde{c_2} \leq |(F_{RK}^n)^{-T}(p)\mathbf{u}| \leq \widetilde{C_2}, \tag{A.9}$$

being $\widetilde{c_j} > 0$, $\widetilde{C_j} > 0$, $j = 1,2$, constants depending on $\mathbf{v}$ and T, and $\mathbf{u} \in \mathbb{R}^d$ with $|\mathbf{u}| = 1$.

Proof. The result follows from expressions (A.1), (A.2), (A.4), (A.5) and (A.8), and by using the following equality

$$1 = |\mathbf{u}| = \left|(F_{RK}^n)^T(p)(F_{RK}^n)^{-T}(p)\mathbf{u}\right| \quad \forall \mathbf{u} \in \mathbb{R}^d,\ |\mathbf{u}| = 1. \qquad \square \tag{A.10}$$

Under Hypothesis 2, Lemma A.1 can be improved.

LEMMA A.7. *Let us assume Hypothesis 2. If $\Delta t < \min\{K, 1/(2||L||_{\infty,\mathcal{T}})\}$, then, $X_{RK}^n(p)$ is defined $\forall p \in \overline{\Omega}$ and $\forall n \in \{0,\ldots,N\}$, and $X_{RK}^n(\overline{\Omega}) = \overline{\Omega}$.*

Proof. See Proposition 1 in [26]. $\square$

LEMMA A.8. *Let us assume Hypotheses 1 and (4.31). Let us suppose $\alpha > 0$ and $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta}), K\}$, being η and K the constants appearing, respectively, in Lemma A.1 and in Corollary A.4. Then, we have*

$$\begin{aligned}\langle Q^{n+1}, \psi + \varphi\rangle_\Omega + \langle G^{n+1}, \psi+\varphi\rangle_{\Gamma^R} &\leq c_s||Q^{n+1}||_\Omega^2 + \frac{4c_g}{\alpha}||G^{n+1}||_{\Gamma^R}^2 \\ + \frac{1}{2}\left(\left|\left|\sqrt{\det F_{RK}^{n+1}}\psi\right|\right|_\Omega^2 + \left|\left|\sqrt{\det F_{RK}^{n}}\varphi\right|\right|_\Omega^2\right) &+ \frac{\alpha}{32}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1} + \widetilde{m}_{RK}^{n}}\,(\varphi+\psi)\right|\right|_{\Gamma^R}^2,\end{aligned}$$

$\forall \varphi, \psi \in H^1(\Omega)$, with $c_s = 1/\widetilde{c_1}$ and $c_g = 1/(\widetilde{c_1}\widetilde{c_2})$, where $\widetilde{c_1}$ and $\widetilde{c_2}$ are the constants appearing in Lemma A.6.

Proof. The estimate follows directly by applying the Cauchy-Schwarz inequality to the left-hand side of the inequality, and using Young's inequality and Lemma A.6. $\square$

LEMMA A.9. *Let us assume Hypotheses 1 and (4.31). Let $\Delta t < \min\{\eta, K\}$, being η and K the constants appearing in Lemma A.1 and in Corollary A.4, respectively. Then, we have*

$$\left\langle Q^{n+1}, \psi - \varphi\right\rangle_\Omega \leq \frac{2c_s\Delta t}{\gamma}||Q^{n+1}||_\Omega^2 + \frac{\gamma}{16\Delta t}\left|\left|\sqrt{\det F_{RK}^{n+1} + \det F_{RK}^n}(\psi-\varphi)\right|\right|_\Omega^2,$$

$\forall \varphi, \psi \in L^2(\Omega)$, where c_s is the constant appearing in Lemma A.8.

Proof. The result easily follows by applying the Cauchy-Schwarz inequality, Young's inequality and Lemma A.6. ∎

LEMMA A.10. *Let us assume Hypotheses 1 and (4.31). Suppose that* $\alpha > 0$ *and* $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta}), K\}$. *Then, for any sequence* $\{\psi^n\}_{n=0}^N \in [L^2(\Gamma^R)]^{N+1}$ *and any* $q \in \{1, \dots, N\}$*, the following inequality holds:*

$$\left|\sum_{n=0}^{q-1}\langle G^{n+1}, \psi^{n+1} - \psi^n\rangle_{\Gamma^R}\right| \leq \frac{4c_g}{\alpha}||G^q||^2_{\Gamma^R} + \frac{\alpha}{16}||\sqrt{\widetilde{m}^q_{RK}}\psi^q||^2_{\Gamma^R} + \frac{1}{2\alpha}||G^1||^2_{\Gamma^R}$$
$$+\frac{\alpha}{2}||\psi^0||^2_{\Gamma^R} + \frac{\Delta t c_g}{2\alpha}\sum_{n=1}^{q-1}\left|\left|\frac{G^{n+1} - G^n}{\Delta t}\right|\right|^2_{\Gamma^R} + \frac{\Delta t\alpha}{2}\sum_{n=1}^{q-1}||\sqrt{\widetilde{m}^n_{RK}}\psi^n||^2_{\Gamma^R}.$$

Proof. The result follows from the equality

$$\sum_{n=0}^{q-1}\langle G^{n+1}, \psi^{n+1} - \psi^n\rangle_{\Gamma^R} = \langle G^q, \psi^q\rangle_{\Gamma^R} - \langle G^1, \psi^0\rangle_{\Gamma^R}$$
$$-\Delta t\sum_{n=1}^{q-1}\left\langle\frac{G^{n+1} - G^n}{\Delta t}, \psi^n\right\rangle_{\Gamma^R}.$$

Indeed, the three terms on the right-hand side can be bounded by using the Cauchy-Schwarz inequality, Young's inequality and Lemma A.6. ∎

Ω: bounded domain	X_e: motion
$\Omega_t := X_e(\Omega, t)$	$\mathcal{T}$: trajectory of the motion
$\mathcal{O} := \bigcup_{t\in[0,T]} \overline{\Omega}_t$	$F = \nabla X_e$: Jacobian matrix of the deformation
P: reference map of X_e	$\mathbf{v}$: spatial description of the velocity
$L :=$ grad $\mathbf{v}$	Ψ_m: material description of a spatial field Ψ
$A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$: diffusion tensor field	$\widetilde{A}_m(p,t) := F^{-1}(p,t)A_m(p,t)F^{-T}(p,t)\det F(p,t)$
$\mathbf{m}$: the outward unit normal vector to $\Gamma := \partial\Omega$	$\widetilde{m}(p,t) := \lvert F^{-T}(p,t)\mathbf{m}(p)\rvert \det F(p,t)$
X^n_{RK}: second order Runge-Kutta approximation of X^n_e	$F^n_{RK} := \nabla X^n_{RK}$
$\Omega^\delta_t := \bigcup_{x\in\overline{\Omega}_t} B(x,\delta)$	$\mathcal{O}^\delta := \bigcup_{t\in[0,T]} \overline{\Omega}^\delta_t$
ρ: density	γ: lower bound for ρ
$\rho_{1,\infty} = \lvert\lvert\rho\rvert\rvert_{1,\infty,\mathcal{O}^\delta}$	Λ: lower bound for the eigenvalues of A_{n_1}
$\widetilde{A}^n_{RK} := (F^n_{RK})^{-1} A\circ X^n_{RK}(F^n_{RK})^{-T}\det F^n_{RK}$	$\widetilde{m}^n_{RK} = \lvert(F^n_{RK})^{-T}\mathbf{m}\rvert \det F^n_{RK}$
$C = \sqrt{A}$	$c_A = \max\{\lvert\lvert G\rvert\rvert^2_{\infty,\mathcal{O}^\delta}, \lvert\lvert C\rvert\rvert^2_{\infty,\mathcal{O}^\delta}\}$, $G_{ij} = \lvert \operatorname{grad} C_{ij}\rvert$
$c_v := \max_{t\in[0,T]} \lvert\lvert\mathbf{v}(\cdot,t)\rvert\rvert_{1,\infty,\Omega^\delta_t}$	$\widetilde{C}^n_{RK} := C\circ X^n_{RK}(F^n_{RK})^{-T}\sqrt{\det F^n_{RK}}$
$B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$, I_{n_1} is the $n_1 \times n_1$ identity matrix	$\widetilde{B}^n_{RK} = B(F^n_{RK})^{-T}\sqrt{\det F^n_{RK}}$
$\widehat{\mathcal{S}[\psi]} := \{\psi^{n+1} + \psi^n\}^{N-1}_{n=0}$	$\widehat{\mathcal{R}_{\Delta t}[\psi]} := \left\{\dfrac{\psi^{n+1} - \psi^n}{\Delta t}\right\}^{N-1}_{n=0}$

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