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

MARTA BENÍTEZ† AND ALFREDO BERMÚDEZ†

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. 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 [20]). In many cases the diffusive term is much smaller than the convective one, giving rise to the so-called convection dominated problems (see [17]). Furthermore, in some cases the diffusive term becomes degenerate, as in some financial models (see, for instance, [26]).

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 [17]). 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 has been applied to time dependent convection-diffusion equations combined with fi-

*This work was supported by Xunta de Galicia under research project INCITE09 207 047 PR, and by Ministerio de Ciencia e Innovación (Spain) under research projects Consolider MATHEMATICA CSD2006-00032 and MTM2008-02483.

†Dep. de Matemática Aplicada, Universidade de Santiago de Compostela, Campus Vida, 15782 Santiago de Compostela, Spain (marta.benitez@usc.es, alfredo.bermudez@usc.es). The first author was supported by Ministerio de Educación.

nite elements ([16], [21]), finite differences ([16]), etc. Its adaptation to steady state convection-diffusion equations has been developed in [8] and, more recently, the combination of the classical first order scheme with disconuous 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 [22] multistep Lagrange-Galerkin methods for convection-diffusion problems are analyzed. In [11] and [12] 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 [25] 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 [9] and [10] for further analysis). In [15] 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 [13] and [14].
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 [18]) 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 [15], 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. More precisely, let $\widehat{\phi_m} = \{\phi_m^n\}_{n=0}^N$ and $\widehat{\phi_{m,\Delta t}} = \{\phi_{m,\Delta t}^n\}_{n=0}^N$ denote, respectively, the exact solution of the continuous problem in Lagrangian coordinates (see §3), and the discrete solution of the pure Lagrangian method proposed and analyzed in this paper (see §4). We prove (Corollary 4.12 and Theorem 4.27) the following inequalities:

$$\begin{aligned}\left|\left|\widehat{\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Omega))} + \sqrt{\frac{\Lambda}{4}}\left|\left|B\mathcal{S}[\widehat{\nabla\phi_{m,\Delta t}}]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} + \left|\left|\mathcal{S}[\widehat{\phi_{m,\Delta t}}]\right|\right|_{l^2(L^2(\Gamma^R))} \\ \leq J_1\left(||\phi_{m,\Delta t}^0||_\Omega + \left|\left|f\circ\widehat{X_{RK}}\right|\right|_{l^2(L^2(\Omega))} + \left|\left|g\circ\widehat{X_{RK}}\right|\right|_{l^2(L^2(\Gamma^R))}\right),\end{aligned} \tag{1.1}$$

and

$$\begin{aligned}||\phi_m\widehat{-\phi_{m,\Delta t}}||_{l^\infty(L^2(\Omega))} + \sqrt{\frac{\Lambda}{4}}\left|\left|B\mathcal{S}\left[\nabla\phi_m\widehat{-\nabla}\phi_{m,\Delta t}\right]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} \\ + \left|\left|\mathcal{S}\left[\phi_m\widehat{-\phi_{m,\Delta t}}\right]\right|\right|_{l^2(L^2(\Gamma^R))} \leq J_2\ \Delta t^2\left(||\phi_m||_{C^3(L^2(\Omega))}\right. \\ \left.+||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))} + ||\nabla\phi_m\cdot\mathbf{m}||_{C^2(L^2(\Gamma^R))} + ||\phi_m||_{C^2(L^2(\Gamma^R))}\right.\end{aligned} \tag{1.2}$$

$$+||f_m||_{C^2(L^2(\Omega))} + ||f||_{C^1(\mathcal{T}^\delta)} + ||g_m||_{C^2(L^2(\Gamma^R))} + ||g||_{C^1(\mathcal{T}^\delta_{\Gamma^R})}\Big),$$

where $\Psi_m := \Psi \circ X_e$ for a spatial field Ψ, being X_e the motion, B is the matrix $B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$, where I_{n_1} is the $n_1 \times n_1$ identity matrix, $\widehat{\mathcal{S}[\psi]} := \{\psi^{n+1} + \psi^n\}_{n=0}^{N-1}$ for a sequence $\widehat{\psi} = \{\psi\}_{n=0}^N$ and $\widehat{X_{RK}} = \{X_{RK}^n\}_{n=0}^N$ is a second order Runge-Kutta approximation of X_e. The diffusion tensor has the form $A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$ and Λ is a uniform lower bound for the eigenvalues of A_{n_1} . Here, J_1 does not depend on the diffusion tensor and J_2 is bounded in the hyperbolic limit. Moreover, for the particular case of Dirichlet boundary conditions, diffusion tensor $A = \epsilon B$ and right-hand side $f = 0$, the $l^\infty(H^1)$ stability estimate is independent of ϵ (see Remark 4.9).

Similar stability and error estimates of order $O(\Delta t^2)$ are proved in the $l^\infty(H^1)$ norm. In particular, we prove (Corollary 4.16 and Theorem 4.28) the inequalities,

$$\begin{aligned} &\left|\left|\widehat{\mathcal{R}_{\Delta t}[\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))} + \sqrt{\frac{\Lambda}{2}}\left|\left|\widehat{B\nabla\phi_{m,\Delta t}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} + \left|\left|\widehat{\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Gamma^R))} \\ &\leq J_3\left(\sqrt{\frac{\Lambda}{2}}\left|\left|B\nabla\phi^0_{m,\Delta t}\right|\right|_\Omega + \left|\left|\phi^0_{m,\Delta t}\right|\right|_{\Gamma^R} + \left|\left|\widehat{f\circ X_{RK}}\right|\right|_{l^2(L^2(\Omega))} + \right. \\ &\qquad \left.\left|\left|\widehat{g\circ X_{RK}}\right|\right|_{l^\infty(L^2(\Gamma^R))} + \left|\left|\widehat{\mathcal{R}_{\Delta t}[g\circ X_{RK}]}\right|\right|_{l^2(L^2(\Gamma^R))}\right), \end{aligned} \tag{1.3}$$

and

$$\begin{aligned} &\left|\left|\widehat{\mathcal{R}_{\Delta t}[\phi_m - \phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))} + \sqrt{\frac{\Lambda}{2}}\left|\left|\widehat{B\left(\nabla\phi_m - \nabla\phi_{m,\Delta t}\right)}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \\ &+ \left|\left|\widehat{\phi_m - \phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Gamma^R))} \leq J_4\ \Delta t^2\left(||\phi_m||_{C^3(L^2(\Omega))} + ||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))} + \right. \\ &||\nabla\phi_m\cdot\mathbf{m}||_{C^3(L^2(\Gamma^R))} + ||\phi_m||_{C^3(L^2(\Gamma^R))} + ||f_m||_{C^2(L^2(\Omega))} \\ &\left.+||f||_{C^1(\mathcal{T}^\delta)} + ||g_m||_{C^3(L^2(\Gamma^R))} + ||g||_{C^2(\mathcal{T}^\delta_{\Gamma^R})}\right), \end{aligned} \tag{1.4}$$

where $\widehat{\mathcal{R}_{\Delta t}[\psi]} := \left\{\dfrac{\psi^{n+1} - \psi^n}{\Delta t}\right\}_{n=0}^{N-1}$ for a sequence $\widehat{\psi} = \{\psi\}_{n=0}^N$. Here, J_3 and J_4 depend on the diffusion tensor; however for the particular case of diffusion tensor of the form $A = \epsilon B$, J_3 does not depend on it and J_4 is bounded in the hyperbolic limit.

To prove these estimates we assume that the exact solution and data of the problem are smooth, and Δt is sufficiently small.

The paper is organized as follows. In Section 2 the convection-diffusion Cauchy problem is stated in a time dependent bounded domain 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 greater 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 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 and functional spaces. 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 [18]. 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 matrix 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 [18] 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.
Let us consider the following initial-boundary value problem.

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

$$\rho(x)\frac{\partial \phi}{\partial t}(x,t) + \rho(x)\mathbf{v}(x,t) \cdot \operatorname{grad}\phi(x,t) - \operatorname{div}\left(A(x)\operatorname{grad}\phi(x,t)\right) = f(x,t), \tag{2.7}$$

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

$$\phi(\cdot,t) = \phi_D(\cdot,t) \ \textit{on}\ \Gamma_t^D, \tag{2.8}$$

$$\alpha\phi(\cdot,t) + A(\cdot)\operatorname{grad}\phi(\cdot,t) \cdot \mathbf{n}(\cdot,t) = g(\cdot,t) \ \textit{on}\ \Gamma_t^R, \tag{2.9}$$

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

$$\phi(x,0) = \phi^0(x) \ \textit{in}\ \Omega. \tag{2.10}$$

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 Lebesque 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 $H^1_{\Gamma^D}(\Omega)$ the closed subspace of $H^1(\Omega)$ defined by

$$H^1_{\Gamma^D}(\Omega) := \left\{\varphi \in H^1(\Omega),\ \varphi|_{\Gamma^D} \equiv 0\right\}. \tag{2.11}$$

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

$$||\mathbf{w}||_{1,\infty,\mathcal{A}} := \max\left\{||\mathbf{w}||_{\infty,\mathcal{A}}, ||\operatorname{div}\mathbf{w}||_{\infty,\mathcal{A}}, ||\nabla\mathbf{w}||_{\infty,\mathcal{A}}\right\}, \tag{2.12}$$

being

$$||\nabla\mathbf{w}||_{\infty,\mathcal{A}} \quad := \quad \operatorname*{ess\,sup}_{x\in\mathcal{A}} ||\nabla\mathbf{w}(x)||_2, \tag{2.13}$$

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

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, [18]):

1. We denote by p the material points in $\overline{\Omega}$, and by x the spatial points in $\overline{\Omega}_t$ with $t > 0$.

2. A material field is a mapping with domain $\overline{\Omega} \times [0,T]$ and a spatial field is a mapping with domain $\mathcal{T}$.

3. We define the material description Ψ_m of a spatial field Ψ by

$$\Psi_m(p,t) = \Psi(X_e(p,t),t). \tag{2.14}$$

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

4. 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 $\dot{\psi}$ the partial derivative with respect to the second argument (time).

5. 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).

3. Weak formulation. We are going to develop some formal computations in order to write a weak formulation of 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 (2.7) 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])

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

Then, ϕ_m satisfies

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

Throughout this article, we use the notation

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

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

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

for $(p,t)\in\Gamma\times(0,T)$ and $x = X_e(p,t)$. Thus, from (2.8)-(2.10) 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*

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

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:

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

$\forall\psi\in H^1_{\Gamma^D}(\Omega)$ 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 and obtain some properties. 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 $n = 0, 1/2, 1, \ldots, N$. 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. It arises from approximating the material time derivative at $t = t_{n+\frac{1}{2}}$, for $0 \le n \le N-1$, by a centered formula and using a second order interpolation formula involving values at $t = t_n$ and $t = t_{n+1}$ to approximate the rest of the terms at the same time $t = t_{n+\frac{1}{2}}$. Thus, from (3.8), we have

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

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 $0 \leq n \leq N-1$ 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 §2 is used for the Jacobian tensor of X_{RK}^n, namely,

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

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

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

Now, we state some lemmas concerning properties of the approximate characteristics X_{RK}^n. For this purpose, we require the time step to be upper bounded and the following assumption:

Hypothesis 1. There exists a parameter $\delta > 0$, such that the velocity field $\mathbf{v}$ is defined in

$$\mathcal{T}^\delta := \bigcup_{t\in[0,T]} \overline{\Omega}_t^\delta \times \{t\}, \tag{4.8}$$

being

$$\Omega_t^\delta := \bigcup_{x\in\overline{\Omega}_t} B(x,\delta). \tag{4.9}$$

Moreover $\mathbf{v} \in \mathbf{C}^1(\mathcal{T}^\delta)$.

LEMMA 4.1. *Under Hypothesis 1, there exists a parameter $\eta > 0$ such that if $\Delta t < \eta$ then $X_{RK}^n(p)$ is defined $\forall p \in \overline{\Omega}$ and $\forall n \in \{0,\dots,N\}$, and the following inclusion holds*

$$X_{RK}^n(\overline{\Omega}) \subset \Omega_{t_n}^\delta.$$

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 4.2. *Under Hypothesis 1, if $\Delta t < \eta$ then*

$$||F^n_{RK}||_{\infty,\Omega} \leq e^{T(||L||_{\infty,\mathcal{T}^\delta}+C\Delta t)} \quad \forall\ n \in \{0,\dots,N\}. \tag{4.10}$$

Here constant C depends on $\mathbf{v}$.

Proof. Inequality (4.10) follows by applying norms to (4.7), using the initial condition (4.6) and applying the discrete Gronwall inequality. ∎

LEMMA 4.3. *Under Hypothesis 1 if $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, then*

$$||(F^n_{RK})^{-1}||_{\infty,\Omega} \leq e^{T(||L||_{\infty,\mathcal{T}^\delta}+C\Delta t)} \quad \forall\ n \in \{0,\dots,N\} \tag{4.11}$$

and

$$(F^{n+1}_{RK})^{-1}(p) = (F^n_{RK})^{-1}(p)\left(I - \Delta t L^{n+\frac{1}{2}}(Y^n(p)) + O(\Delta t^2)\right), \tag{4.12}$$

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

Proof. Firstly, we can write

$$F^{n+1}_{RK}(p) = M^n_{RK}(p)F^n_{RK}(p), \tag{4.13}$$

with

$$M^n_{RK}(p) := I + \Delta t L^{n+\frac{1}{2}}(Y^n(p))\left(I + \frac{\Delta t}{2}L^n(X^n_{RK}(p))\right). \tag{4.14}$$

Now, by applying norms to (4.14) 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 (4.12) follows. The proof of (4.11) is analogous to the one of the previous lemma. ∎

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

COROLLARY 4.4. *Under the assumptions of Lemma 4.2, we have*

$$||\det F^n_{RK}||_{\infty,\Omega} \leq e^{T(||\operatorname{div}\mathbf{v}||_{\infty,\mathcal{T}^\delta}+C(\mathbf{v})\Delta t)}, \tag{4.15}$$

$$\det F^n_{RK}(p) > 0 \qquad \text{if } \Delta t < K, \tag{4.16}$$

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

$$\det F^{n+1}_{RK}(p) = \det F^n_{RK}(p)\left(1 + \Delta t \operatorname{div}\mathbf{v}^{n+\frac{1}{2}}(Y^n(p)) + O(\Delta t^2)\right), \tag{4.17}$$

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

COROLLARY 4.5. *Under the assumptions of Lemma 4.3, we have*

$$\det (F^{n+1}_{RK})^{-1}(p) = \det (F^n_{RK})^{-1}(p)\left(1 - \Delta t \operatorname{div}\mathbf{v}^{n+\frac{1}{2}}(Y^n(p)) + O(\Delta t^2)\right), \tag{4.18}$$

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

$$||\det (F^n_{RK})^{-1}||_{\infty,\Omega} \leq e^{T(||\operatorname{div}\mathbf{v}||_{\infty,\mathcal{T}^\delta}+C(\mathbf{v})\Delta t)}. \tag{4.19}$$

LEMMA 4.6. *Under Hypothesis 1 if* $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta}), K\}$, *where* K *is the constant appearing in Corollary 4.4, then,* $\forall p \in \overline{\Omega}$ *and* $\forall n \in \{0,\dots,N\}$, *we have*

$$\widetilde{c_1} \leq \det F^n_{RK}(p) \leq \widetilde{C_1}, \quad \widetilde{c_2} \leq |(F^n_{RK})^{-T}(p)\mathbf{u}| \leq \widetilde{C_2}, \tag{4.20}$$

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 (4.10), (4.11), (4.15), (4.16) and (4.19), and by using the following equality

$$1 = |\mathbf{u}| = \left|(F^n_{RK})^T(p)(F^n_{RK})^{-T}(p)\mathbf{u}\right| \quad \forall \mathbf{u} \in \mathbb{R}^d,\ |\mathbf{u}| = 1. \tag{4.21}$$

∎

Now, we consider a motion satisfying the following assumption:

Hypothesis 2. The motion X_e satisfies

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

Remark 4.2. Notice that, if the motion verifies Hypothesis 2 then

$$\Gamma_t = \Gamma, \quad \mathbf{v}(x,t) = 0 \quad \forall x \in \Gamma\ \forall t \in [0,T].$$

Under Hypothesis 2, Lemma 4.1 can be improved.

LEMMA 4.7. *Let us assume Hypothesis 2. If* $\Delta t < \min\{K, 1/(2||L||_{\infty,\mathcal{T}})\}$, *then,* $X^n_{RK}(p)$ *is defined* $\forall p \in \overline{\Omega}$ *and* $\forall n \in \{0,\dots,N\}$, *and* $X^n_{RK}(\overline{\Omega}) = \overline{\Omega}$.

Proof. See Proposition 1 in [25]. ∎

In order to introduce approximations to the characteristic curves and gradient tensors in scheme (4.1), some additional assumptions are required.

Firstly, we introduce a set containing $X^n_{RK}(\overline{\Omega})$, for every $0 \leq n \leq N$, namely

$$\mathcal{O}^\delta := \bigcup_{t\in[0,T]} \overline{\Omega}^\delta_t. \tag{4.22}$$

Moreover, we define

$$\mathcal{T}^\delta_{\Gamma^R} := \bigcup_{t\in[0,T]} \overline{G}^\delta_t \times \{t\}, \tag{4.23}$$

being

$$G^\delta_t = \bigcup_{x\in\Gamma^R_t} B(x,\delta). \tag{4.24}$$

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 (4.22). Moreover,

$$0 < \gamma \leq \rho(x) \qquad a.e.\ x \in \mathcal{O}^\delta. \tag{4.25}$$

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:

$$A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}, \tag{4.26}$$

with A_{n_1} being a positive definite symmetric $n_1 \times n_1$ tensor ($n_1 \geq 1$) 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 4.3. 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 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 (2.9) is strictly positive.

Let us define the following sequences of functions of p.

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

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,

$$\begin{aligned} &\frac{1}{2}\int_\Omega \left(\rho \circ X^{n+1}_{RK} \det F^{n+1}_{RK} + \rho \circ X^n_{RK} \det F^n_{RK}\right) \frac{\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}}{\Delta t}\, \psi \, dp \\ &+\frac{1}{4}\int_\Omega \left(\widetilde{A}^{n+1}_{RK} + \widetilde{A}^n_{RK}\right)\left(\nabla \phi^{n+1}_{m,\Delta t} + \nabla \phi^n_{m,\Delta t}\right) \cdot \nabla \psi \, dp \\ &+\frac{\alpha}{4}\int_{\Gamma^R} \left(\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}\right)\left(\phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right)\, \psi \, dA_p \\ &= \frac{1}{2}\int_\Omega \left(\det F^{n+1}_{RK} f^{n+1} \circ X^{n+1}_{RK} + \det F^n_{RK} f^n \circ X^n_{RK}\right)\, \psi \, dp \\ &+\frac{1}{2}\int_{\Gamma^R} \left(\widetilde{m}^{n+1}_{RK} g^{n+1} \circ X^{n+1}_{RK} + \widetilde{m}^n_{RK} g^n \circ X^n_{RK}\right)\, \psi \, dA_p. \end{aligned} \tag{4.27}$$

For these computations we have made the assumptions of Lemma 4.3, and Hypothesis 3, 4, 5 and 6.

Notice that we have used a lowest order characteristics approximation formula preserving second order 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

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

$$\left\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \psi \right\rangle := \left\langle \frac{\det F_{RK}^{n+1} f^{n+1} \circ X_{RK}^{n+1} + \det F_{RK}^{n} f^{n} \circ X_{RK}^{n}}{2}, \psi \right\rangle_{\Omega} + \left\langle \frac{\widetilde{m}_{RK}^{n+1} g^{n+1} \circ X_{RK}^{n+1} + \widetilde{m}_{RK}^{n} g^{n} \circ X_{RK}^{n}}{2}, \psi \right\rangle_{\Gamma^R},$$

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

Remark 4.4. Regarding the definitions of $\mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\phi]$ and $\mathcal{F}_{\Delta t}^{n+\frac{1}{2}}$, 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:

$$\text{(4.28)} \quad \begin{cases} \text{Given } \phi_{m,\Delta t}^0, \text{ find } \widehat{\phi_{m,\Delta t}} = \{\phi_{m,\Delta t}^n\}_{n=1}^N \in \left[H_{\Gamma^D}^1(\Omega)\right]^N \text{ such that} \\ \quad \left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}], \psi \right\rangle = \left\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \psi \right\rangle \quad \forall\, \psi \in H_{\Gamma^D}^1(\Omega) \text{ for } n = 0, \ldots, N-1. \end{cases}$$

Remark 4.5. 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 (4.28) by higher order ones or by the exact value.

4.3. Stability of the semidiscretized scheme. In order to prove stability estimates for problem (4.28), the assumptions considered in the previous section are required.
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

$$\text{(4.29)} \qquad C = \begin{pmatrix} C_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}.$$

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

$$\text{(4.30)} \qquad c_A = \max\{||G||^2_{\infty,\mathcal{O}^\delta}, ||C||^2_{\infty,\mathcal{O}^\delta}\},$$

and the sequence of tensor fields

$$\widetilde{C}_{RK}^n := C \circ X_{RK}^n (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n} \quad \forall n \in \{0, \ldots, N\}.$$

Next, let us denote by B the $d \times d$ tensor

$$\text{(4.31)} \qquad B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix},$$

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

$$\text{(4.32)} \qquad \Lambda ||B\mathbf{w}||^2_\Omega \le \langle A\mathbf{w}, \mathbf{w} \rangle_\Omega \quad \forall \mathbf{w} \in \mathbb{R}^d.$$

Let us introduce the sequence of tensor fields

$$\widetilde{B}_{RK}^n := B (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n} \quad \forall n \in \{0, \ldots, N\}.$$

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

$$(I-B)L(x,t)B=0 \quad \forall (x,t)\in \mathcal{T}^{\delta}. \tag{4.33}$$

Remark 4.6. 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 4.7. For any $d\times d$ tensor E of the form given in (4.26) it is easy to check that

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

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. Moreover, under Hypothesis 7, if $\Delta t<\min\{\eta,1/(2||L||_{\infty,\mathcal{T}^\delta})\}$ it is easy to prove that

$$|B(F^n_{RK})^{-T}(p)\mathbf{w}|\geq D|B\mathbf{w}|,$$

for $p\in\overline{\Omega}$, $\mathbf{w}\in\mathbb{R}^d$, $n=0,\dots,N$, and D depending on $\mathbf{v}$ and T.

Now, it is convenient to notice that Hypothesis 4 also covers the nondegenerate case. This hypothesis is usual in ultraparabolic equations (see, for instance, [24]), which represent a wide class of degenerate diffusion equations arising from many applications (see, for instance, [5]). Furthermore, as stated in [19], 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

$$c_v:=\max_{t\in[0,T]}||\mathbf{v}(\cdot,t)||_{1,\infty,\Omega^\delta_t}, \tag{4.34}$$

where $||\cdot||_{1,\infty,\Omega^\delta_t}$ is the norm given in (2.12). 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.

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 $l^\infty(L^2(\Omega))$ and $l^2(L^2(\Omega))$ equipped with their respective usual norms:

$$\left|\left|\widehat{\psi}\right|\right|_{l^\infty(L^2(\Omega))}:=\max_{0\leq n\leq N}||\psi^n||_\Omega\,,\quad \left|\left|\widehat{\psi}\right|\right|_{l^2(L^2(\Omega))}:=\sqrt{\Delta t\sum_{n=0}^N||\psi^n||^2_\Omega}. \tag{4.35}$$

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 $l^\infty(\mathbf{L}^2(\Omega))$ and $l^2(\mathbf{L}^2(\Omega))$. Moreover, let us introduce the notations

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

We denote by $\widehat{f\circ X_{RK}}$ and by $\widehat{g\circ X_{RK}}$ the following sequences of functions

$$\widehat{f\circ X_{RK}}:=\{f^n\circ X^n_{RK}\}_{n=0}^N\,,\quad \widehat{g\circ X_{RK}}:=\{g^n\circ X^n_{RK}\}_{n=0}^N\,.$$

Before establishing some technical lemmas, let us recall the Young's inequality

$$ab \leq \frac{1}{2}\left(\epsilon a^2 + \frac{1}{\epsilon}b^2\right), \tag{4.36}$$

for $a,\ b \in \mathbb{R}$ and $\epsilon > 0$, which will be extensively used in what follows.

LEMMA 4.8. *Let us assume Hypotheses 1, 3 and 4. Let $\{\phi^n_{m,\Delta t}\}_{n=1}^N$ be the solution of (4.28). Then, there exist a positive constant $c(\mathbf{v}, T, \delta)$ such that, for $\Delta t < c$, we have*

$$\begin{aligned}
&\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right\rangle \\
&\geq \frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n}_{RK}\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega \\
&+\frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t} + \nabla\phi^n_{m,\Delta t}\right)\right|\right|^2_\Omega + \frac{1}{4}\left|\left|\widetilde{C}^{n}_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t} + \nabla\phi^n_{m,\Delta t}\right)\right|\right|^2_\Omega \\
&+\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}}\left(\phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R} \\
&-\widehat{c}\gamma\left(\left|\left|\sqrt{\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\sqrt{\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega\right),
\end{aligned} \tag{4.37}$$

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

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

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

Let K be the constant appearing in Corollary 4.4. If $\Delta t < K$, we first have

$$\begin{aligned}
I_1 &= \left\langle \frac{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK}\right)}{2}\frac{\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}}{\Delta t}, \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right\rangle_\Omega \\
&= \frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X^{n}_{RK}\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega \\
&+ \frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X^{n}_{RK}\det F^{n}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{2\Delta t}\left|\left|\sqrt{\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega,
\end{aligned} \tag{4.38}$$

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

$$\rho(X^n_{RK}(p)) = \rho(X^{n+1}_{RK}(p)) - \zeta^n(p) \quad \text{for a.e. } p \in \Omega, \tag{4.39}$$

where

$$\zeta^n(p) := \int_{t_n}^{t_{n+1}} \operatorname{grad}\rho(Y^n_{RK}(p,s))\cdot \mathbf{v}^{n+\frac{1}{2}}(Y^n(p))\,ds \quad \text{for a.e. } p\in\Omega, \tag{4.40}$$

verifies $|\zeta^n(p)|\le \rho_{1,\infty}c_v\Delta t$. Then, by using (4.17), (4.18) and (4.39) in (4.38), we get

$$\begin{aligned} I_1 \ge{}& \frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n}_{RK}\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega \\ &-\rho_{1,\infty}\left(c_v+C_v\Delta t\right)\left\{\left|\left|\sqrt{\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\sqrt{\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega\right\}. \end{aligned} \tag{4.41}$$

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

$$\begin{aligned} I_2 :=& \frac{1}{4}\left\langle\left(\widetilde{A}^{n+1}_{RK}+\widetilde{A}^{n}_{RK}\right)\left(\nabla\phi^{n+1}_{m,\Delta t}+\nabla\phi^{n}_{m,\Delta t}\right),\nabla\phi^{n+1}_{m,\Delta t}+\nabla\phi^{n}_{m,\Delta t}\right\rangle_\Omega \\ =& \frac{1}{4}\left|\left|\widetilde{C}^{n+1}_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t}+\nabla\phi^{n}_{m,\Delta t}\right)\right|\right|^2_\Omega + \frac{1}{4}\left|\left|\widetilde{C}^{n}_{RK}\left(\nabla\phi^{n}_{m,\Delta t}+\nabla\phi^{n}_{m,\Delta t}\right)\right|\right|^2_\Omega. \end{aligned} \tag{4.42}$$

For I_3 we have

$$I_3 = \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}+\widetilde{m}^{n}_{RK}}\left(\phi^{n+1}_{m,\Delta t}+\phi^{n}_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R}. \tag{4.43}$$

Then, by summing up (4.41), (4.42) and (4.43) we get inequality (4.37). ∎

LEMMA 4.9. *Let us assume Hypotheses 1, 3, 4 and 7. Let $\{\phi^n_{m,\Delta t}\}_{n=1}^N$ be the solution of (4.28) and $\alpha>0$ be the constant appearing in the Robin boundary condition (2.9). Then, there exist a positive constant $c(\mathbf{v},T,\delta)$ such that, for $\Delta t<c$, we have*

$$\begin{aligned} &\left\langle\mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}],\phi^{n+1}_{m,\Delta t}-\phi^{n}_{m,\Delta t}\right\rangle \\ &\ge \frac{1}{2\Delta t}\left|\left|\sqrt{\left(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}+\rho\circ X^{n}_{RK}\det F^{n}_{RK}\right)}\left(\phi^{n+1}_{m,\Delta t}-\phi^{n}_{m,\Delta t}\right)\right|\right|^2_\Omega \\ &+\frac{1}{2}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{2}\left|\left|\widetilde{C}^{n}_{RK}\nabla\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega \\ &+\frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R} - \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_{\Gamma^R} \\ &-\widehat{c}\Delta t\Lambda\left(\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\widetilde{B}^{n}_{RK}\nabla\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega\right) \\ &-\widehat{c}\Delta t\alpha\left(\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R} + \left|\left|\sqrt{\widetilde{m}^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_{\Gamma^R}\right), \end{aligned} \tag{4.44}$$

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

$$I_1 = \frac{1}{2\Delta t}\left|\left|\sqrt{\left(\rho\circ X_{RK}^{n+1}\det F_{RK}^{n+1}+\rho\circ X_{RK}^{n}\det F_{RK}^{n}\right)}\left(\phi_{m,\Delta t}^{n+1}-\phi_{m,\Delta t}^{n}\right)\right|\right|_{\Omega}^{2}, \tag{4.45}$$

where we have assumed that $\Delta t < K$, being K the constant appearing in Corollary 4.4. For I_2 we first have

$$\begin{aligned} I_2 = &\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}-\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2}\\ &+\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}-\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2}. \end{aligned} \tag{4.46}$$

Then we use Corollary 4.5, Hypotheses 4 and 7, and equality (4.7) to get

$$\begin{aligned} \frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} \geq &\frac{1}{4}\left|\left|C\circ X_{RK}^{n}(F_{RK}^{n+1})^{-T}\nabla\phi_{m,\Delta t}^{n+1}\sqrt{\det F_{RK}^{n+1}}\right|\right|_{\Omega}^{2}\\ &-c_A C_v\Delta t\left|\left|\widetilde{B}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}. \end{aligned} \tag{4.47}$$

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,

$$C(X_{RK}^{n+1}(p)) = C(X_{RK}^{n}(p)) + D^{n}(p) \qquad \text{for a.e. } p\in\Omega, \tag{4.48}$$

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

$$D_{ij}^{n}(p) := \int_{t_n}^{t_{n+1}} \operatorname{grad} C_{ij}(Y_{RK}^{n}(p,s))\cdot\mathbf{v}^{n+\frac{1}{2}}(Y^{n}(p))\,ds, \tag{4.49}$$

being Y_{RK}^n the mapping defined in the proof of Lemma 4.8. Notice that D is of the form given in (4.29) and verifies $||D^n||_{\infty,\Omega}\leq c_v\sqrt{c_A}\Delta t$. Then, from the previous properties, we have

$$\frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} \geq \frac{1}{4}\left|\left|\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2} - c_A C_v\Delta t\left|\left|\widetilde{B}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}. \tag{4.50}$$

Similarly, we obtain the estimate

$$-\frac{1}{4}||\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n}||_{\Omega}^{2} \geq -\frac{1}{4}||\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}||_{\Omega}^{2} - c_A C_v\Delta t||\widetilde{B}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}||_{\Omega}^{2}. \tag{4.51}$$

Thus, by introducing (4.50) and (4.51) in equality (4.46) we obtain the following inequality:

$$\begin{aligned} I_2 \geq &\frac{1}{2}\left|\left|\widetilde{C}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}-\frac{1}{2}\left|\left|\widetilde{C}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2}\\ &-c_A C_v\Delta t\left|\left|\widetilde{B}_{RK}^{n+1}\nabla\phi_{m,\Delta t}^{n+1}\right|\right|_{\Omega}^{2}-c_A C_v\Delta t\left|\left|\widetilde{B}_{RK}^{n}\nabla\phi_{m,\Delta t}^{n}\right|\right|_{\Omega}^{2}. \end{aligned} \tag{4.52}$$

For I_3 we first have

$$\begin{aligned} I_3 = &\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^{2}-\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^{2}\\ &+\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^{2}-\frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^{2}. \end{aligned} \tag{4.53}$$

Next, by applying Corollaries 4.4, 4.5, Lemma 4.3 and equality (4.7) we obtain

$$
\begin{aligned}
I_3 \geq & \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^2 - \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^2 \\
& - C_v\alpha\Delta t\left(\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}}\phi_{m,\Delta t}^{n+1}\right|\right|_{\Gamma^R}^2 + \left|\left|\sqrt{\widetilde{m}_{RK}^{n}}\phi_{m,\Delta t}^{n}\right|\right|_{\Gamma^R}^2\right).
\end{aligned} \tag{4.54}
$$

Then, by summing up (4.45), (4.52) and (4.54), inequality (4.44) follows. ∎

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

$$
\begin{cases}
\text{Given } \phi_{m,\Delta t}^0, \text{ find } \widehat{\phi_{m,\Delta t}} = \{\phi_{m,\Delta t}^n\}_{n=1}^N \in \left[H_{\Gamma^D}^1(\Omega)\right]^N \text{ such that} \\
\left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m,\Delta t}}], \psi\right\rangle = \left\langle \mathcal{H}_{\Delta t}^{n+\frac{1}{2}}, \psi\right\rangle \quad \forall \psi \in H_{\Gamma^D}^1(\Omega) \text{ for } n = 0, \ldots, N-1,
\end{cases} \tag{4.55}
$$

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

Hypothesis 8. $\widehat{S} = \{S^n\}_{n=1}^N \in [L^2(\Omega)]^N$ and $\widehat{G} = \{G^n\}_{n=1}^N \in [L^2(\Gamma^R)]^N$.

LEMMA 4.10. *Let us assume Hypotheses 1 and 8. Let us suppose $\alpha > 0$ and $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^s}), K\}$, being η and K the constants appearing, respectively, in Lemma 4.1 and in Corollary 4.4. Then, we have*

$$
\begin{aligned}
\langle S^{n+1}, \psi+\varphi\rangle_\Omega + \langle G^{n+1}, \psi+\varphi\rangle_{\Gamma^R} \leq & \, c_s||S^{n+1}||_\Omega^2 \\
+\frac{1}{2}\left(\left|\left|\sqrt{\det F_{RK}^{n+1}}\psi\right|\right|_\Omega^2 + \left|\left|\sqrt{\det F_{RK}^{n}}\varphi\right|\right|_\Omega^2\right) + & \frac{4c_g}{\alpha}||G^{n+1}||_{\Gamma^R}^2 \\
+\frac{\alpha}{32}\left|\left|\sqrt{\widetilde{m}_{RK}^{n+1}+\widetilde{m}_{RK}^{n}}\,(\varphi+\psi)\right|\right|_{\Gamma^R}^2 & ,
\end{aligned} \tag{4.56}
$$

$\forall \varphi, \psi \in H^1(\Omega)$, 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 4.6.

Proof. The estimate follows directly by applying the Cauchy-Schwarz inequality to the left-hand side of (4.56), and using inequality (4.36) and Lemma 4.6. ∎

THEOREM 4.11. *Let us assume Hypotheses 1, 3, 4 and 8. Let $\widehat{\phi_{m,\Delta t}}$ be the solution of (4.55) subject to the initial value $\phi_{m,\Delta t}^0 \in H_{\Gamma^D}^1(\Omega)$ and $\alpha > 0$ be the constant appearing in the Robin boundary condition (2.9). Then there exist two positive constants J and D, which are independent of the diffusion tensor, such that if $\Delta t < D$ then*

$$
\begin{aligned}
\sqrt{\gamma}\left|\left|\widehat{\sqrt{\det F_{RK}}}\phi_{m,\Delta t}\right|\right|_{l^\infty(L^2(\Omega))} + & \sqrt{\frac{\Lambda}{4}}\left|\left|\widetilde{B}_{RK}\widehat{\mathcal{S}[\nabla\phi}_{m,\Delta t}]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} \\
+\sqrt{\frac{\alpha}{8}}\left|\left|\widehat{\sqrt{\mathcal{S}\,[\widetilde{m}_{RK}]}\mathcal{S}}[\phi_{m,\Delta t}]\right|\right|_{l^2(L^2(\Gamma^R))} \leq & \, J\left(\sqrt{\gamma}||\phi_{m,\Delta t}^0||_\Omega\right. \\
& \left.+||\widehat{S}||_{l^2(L^2(\Omega))} + ||\widehat{G}||_{l^2(L^2(\Gamma^R))}\right).
\end{aligned} \tag{4.57}
$$

where $\widehat{S} = \{S^n\}_{n=1}^N$, $\widehat{G} = \{G^n\}_{n=1}^N$.

Proof. Sequence $\widehat{\phi_{m,\Delta t}} = \{\phi^n_{m,\Delta t}\}_{n=0}^N$ satisfies $\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{\phi_{m,\Delta t}}], \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t} \right\rangle = \left\langle \mathcal{H}^{n+\frac{1}{2}}_{\Delta t}, \phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t} \right\rangle$. We can use Lemma 4.8 to obtain a lower bound of this expression, and Lemma 4.10 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

$$\begin{aligned}
&\frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{\Delta t}\left|\left|\sqrt{\rho\circ X^{n}_{RK}\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega \\
&+\frac{1}{4}\left|\left|\widetilde{C}^n_{RK}\left(\nabla\phi^{n+1}_{m,\Delta t} + \nabla\phi^n_{m,\Delta t}\right)\right|\right|^2_\Omega + \frac{\alpha}{8}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK} + \widetilde{m}^n_{RK}}\left(\phi^{n+1}_{m,\Delta t} + \phi^n_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R} \\
&\qquad \le c_s||S^{n+1}||^2_\Omega + \frac{4c_g}{\alpha}||G^{n+1}||^2_{\Gamma^R} \\
&\qquad +\widehat{c}\gamma\left(\left|\left|\sqrt{\det F^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\sqrt{\det F^{n}_{RK}}\phi^{n}_{m,\Delta t}\right|\right|^2_\Omega\right),
\end{aligned} \tag{4.58}$$

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

$$\begin{aligned}
\theta^1_n &:= \gamma\left|\left|\sqrt{\det F^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_\Omega, \\
\theta^2_n &:= \frac{\Lambda}{4}\sum_{s=0}^{n-1}\Delta t\left|\left|\widetilde{B}^s_{RK}\left(\nabla\phi^{s+1}_{m,\Delta t} + \nabla\phi^s_{m,\Delta t}\right)\right|\right|^2_\Omega, \\
\overline{\theta}_n &:= \frac{\alpha}{8}\sum_{s=0}^{n-1}\Delta t\left|\left|\sqrt{\widetilde{m}^{s+1}_{RK} + \widetilde{m}^s_{RK}}\left(\phi^{s+1}_{m,\Delta t} + \phi^s_{m,\Delta t}\right)\right|\right|^2_{\Gamma^R}.
\end{aligned}$$

Now, for a fixed integer $q \ge 1$, let us sum (4.58) multiplied by Δt from $n = 0$ to $n = q-1$. Then, with the above notation we have

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

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, [23]) and take the maximun in $q \in \{1, \dots, N\}$. Then, estimate (4.57) follows. ∎

COROLLARY 4.12. *Let us assume Hypotheses 1, 3, 4, 5 and 6. Let $\widehat{\phi_{m,\Delta t}}$ be the solution of (4.28) subject to the initial value $\phi^0_{m,\Delta t} \in H^1_{\Gamma^D}(\Omega)$. Then, there exist two positive constants J and D, independent of the diffusion tensor and such that, for $\Delta t < D$, we have*

$$\begin{aligned}
&\sqrt{\gamma}\left|\left|\widehat{\sqrt{\det F_{RK}}\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Omega))} + \sqrt{\frac{\Lambda}{4}}\left|\left|\widetilde{B}_{RK}\widehat{\mathcal{S}[\nabla\phi_{m,\Delta t}]}\right|\right|_{l^2(\mathbf{L}^2(\Omega))} \\
&\qquad +\sqrt{\frac{\alpha}{8}}\left|\left|\widehat{\sqrt{\mathcal{S}\,[\widetilde{m}_{RK}]}\mathcal{S}[\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Gamma^R))} \le J\left(\sqrt{\gamma}||\phi^0_{m,\Delta t}||_\Omega\right. \\
&\qquad \left. + \left|\left|\widehat{\det F f}\circ X_{RK}\right|\right|_{l^2(L^2(\Omega))} + \left|\left|\widehat{\widetilde{m}_{RK}g\circ X_{RK}}\right|\right|_{l^2(L^2(\Gamma^R))}\right).
\end{aligned} \tag{4.59}$$

Proof. The result follows directly by replacing

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

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 (4.57). ∎

LEMMA 4.13. *Let us assume Hypotheses 1 and 8. Let $\Delta t < \min\{\eta, K\}$, being η and K the constants appearing in Lemma 4.1 and in Corollary 4.4, respectively. Then, we have*

$$\left\langle S^{n+1}, \psi-\varphi\right\rangle_{\Omega} \leq \frac{2c_s\Delta t}{\gamma}||S^{n+1}||_{\Omega}^2 + \frac{\gamma}{16\Delta t}\left|\left|\sqrt{\det F_{RK}^{n+1} + \det F_{RK}^{n}}(\psi-\varphi)\right|\right|_{\Omega}^2, \tag{4.60}$$

$\forall \varphi, \psi \in L^2(\Omega)$, where c_s is the constant appearing in Lemma 4.10.

Proof. The result easily follows by applying the Cauchy-Schwarz inequality, inequality (4.36) with $\epsilon = 8\Delta t/\gamma$ and Lemma 4.6. ∎

LEMMA 4.14. *Let us assume Hypotheses 1 and 8. 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:*

$$\left|\sum_{n=0}^{q-1}\langle G^{n+1}, \psi^{n+1}-\psi^n\rangle_{\Gamma^R}\right| \leq \frac{4c_g}{\alpha}||G^q||_{\Gamma^R}^2 + \frac{\alpha}{16}||\sqrt{\widetilde{m}_{RK}^q}\psi^q||_{\Gamma^R}^2 + \frac{1}{2\alpha}||G^1||_{\Gamma^R}^2$$
$$+\frac{\alpha}{2}||\psi^0||_{\Gamma^R}^2 + \frac{\Delta t c_g}{2\alpha}\sum_{n=1}^{q-1}\left|\left|\frac{G^{n+1}-G^n}{\Delta t}\right|\right|_{\Gamma^R}^2 + \frac{\Delta t\alpha}{2}\sum_{n=1}^{q-1}||\sqrt{\widetilde{m}_{RK}^n}\psi^n||_{\Gamma^R}^2. \tag{4.61}$$

Proof. The result follows from the equality

$$\sum_{n=0}^{q-1}\langle G^{n+1}, \psi^{n+1}-\psi^n\rangle_{\Gamma^R} = \langle G^q, \psi^q\rangle_{\Gamma^R} - \langle G^1, \psi^0\rangle_{\Gamma^R} - \Delta t\sum_{n=1}^{q-1}\left\langle \frac{G^{n+1}-G^n}{\Delta t}, \psi^n\right\rangle_{\Gamma^R}. \tag{4.62}$$

Indeed, the three terms on the right-hand side can be bounded by using the Cauchy-Schwarz inequality, inequality (4.36) and Lemma 4.6. ∎

THEOREM 4.15. *Let us assume Hypotheses 1, 3, 4, 7 and 8, and let $\widehat{\phi_{m,\Delta t}}$ be the solution of (4.55) subject to the initial value $\phi_{m,\Delta t}^0 \in H_{\Gamma^D}^1(\Omega)$. Let $\alpha > 0$ be the constant appearing in the Robin boundary condition (2.9). 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*

$$\sqrt{\frac{\gamma}{4}}\left|\left|\widehat{\sqrt{\mathcal{S}[\det F_{RK}]}\mathcal{R}_{\Delta t}[\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))} + \sqrt{\frac{\Lambda}{2}}\left|\left|\widetilde{B}_{RK}\widehat{\nabla\phi_{m,\Delta t}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))}$$
$$+\sqrt{\frac{\alpha}{4}}\left|\left|\widehat{\sqrt{\widetilde{m}_{RK}}\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Gamma^R))} \leq J\left(\sqrt{\frac{\Lambda}{2}}\left|\left|B\nabla\phi_{m,\Delta t}^0\right|\right|_{\Omega}\right. \tag{4.63}$$
$$\left.+\sqrt{\frac{\alpha}{4}}\left|\left|\phi_{m,\Delta t}^0\right|\right|_{\Gamma^R} + ||\widehat{S}||_{l^2(L^2(\Omega))} + ||\widehat{G}||_{l^\infty(L^2(\Gamma^R))} + \left|\left|\widehat{\mathcal{R}_{\Delta t}[G]}\right|\right|_{l^2(L^2(\Gamma^R))}\right).$$

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 4.9 and Lemma 4.13 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

$$\begin{aligned}
&\frac{1}{2\Delta t}\left|\left|\sqrt{(\rho\circ X^{n+1}_{RK}\det F^{n+1}_{RK} + \rho\circ X^n_{RK}\det F^n_{RK})}\left(\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}\right)\right|\right|^2_\Omega \\
&+\frac{1}{2}\left|\left|\widetilde{C}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega - \frac{1}{2}\left|\left|\widetilde{C}^n_{RK}\nabla\phi^n_{m,\Delta t}\right|\right|^2_\Omega + \frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R} \\
&-\frac{\alpha}{2}\left|\left|\sqrt{\widetilde{m}^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_{\Gamma^R} \le \widehat{c}\Delta t\Lambda\left(\left|\left|\widetilde{B}^{n+1}_{RK}\nabla\phi^{n+1}_{m,\Delta t}\right|\right|^2_\Omega + \left|\left|\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t}\right|\right|^2_\Omega\right) \\
&+\widehat{c}\Delta t\alpha\left(\left|\left|\sqrt{\widetilde{m}^{n+1}_{RK}}\phi^{n+1}_{m,\Delta t}\right|\right|^2_{\Gamma^R} + \left|\left|\sqrt{\widetilde{m}^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_{\Gamma^R}\right) + \frac{2c_s\Delta t}{\gamma}||S^{n+1}||^2_\Omega \\
&+\frac{\gamma}{16\Delta t}\left|\left|\sqrt{\det F^{n+1}_{RK} + \det F^n_{RK}}(\phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t})\right|\right|^2_\Omega + \left\langle G^{n+1}, \phi^{n+1}_{m,\Delta t} - \phi^n_{m,\Delta t}\right\rangle_{\Gamma^R},
\end{aligned} \tag{4.64}$$

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

$$\begin{aligned}
\theta^1_n &:= \frac{\gamma}{4\Delta t}\sum_{s=0}^{n-1}\left|\left|\sqrt{\det F^{s+1}_{RK} + \det F^s_{RK}}\left(\phi^{s+1}_{m,\Delta t} - \phi^s_{m,\Delta t}\right)\right|\right|^2_\Omega, \\
\theta^2_n &:= \frac{\Lambda}{2}\left|\left|\widetilde{B}^n_{RK}\nabla\phi^n_{m,\Delta t}\right|\right|^2_\Omega, \qquad \overline{\theta}_n := \frac{\alpha}{4}\left|\left|\sqrt{\widetilde{m}^n_{RK}}\phi^n_{m,\Delta t}\right|\right|^2_{\Gamma^R}.
\end{aligned}$$

Now, for a fixed $q \ge 1$, let us sum (4.64) from $n = 0$ to $n = q-1$. With the above notation and by using Lemma 4.14 for $\widehat{\psi} = \widehat{\phi_{m,\Delta t}}$, we get

$$\begin{aligned}
&\theta^1_q + (1 - 2\widehat{c}\Delta t)\theta^2_q + (1 - 4\widehat{c}\Delta t)\overline{\theta}_q \le 4\widehat{c}\Delta t\sum_{n=0}^{q-1}\theta^2_n + 10\widehat{c}\Delta t\sum_{n=0}^{q-1}\overline{\theta}_n \\
&+\beta\left(\theta^2_0 + \overline{\theta}_0 + ||\widehat{S}||^2_{l^2(L^2(\Omega))} + ||\widehat{G}||^2_{l^\infty(L^2(\Gamma^R))} + \left|\left|\widehat{\mathcal{R}_{\Delta t}[G]}\right|\right|^2_{l^2(L^2(\Gamma^R))}\right),
\end{aligned} \tag{4.65}$$

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, [23]) and take the maximun in $q \in \{1, \dots, N\}$. Thus, estimate (4.63) follows. ∎

COROLLARY 4.16. *Let us assume Hypotheses 1, 3, 4, 5, 6 and 7, and let* $\widehat{\phi_{m,\Delta t}}$ *be the solution of (4.28) subject to the initial value* $\phi^0_{m,\Delta t} \in H^1_{\Gamma_D}(\Omega)$. *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*

$$\begin{aligned}\sqrt{\frac{\gamma}{4}}\left|\left|\widehat{\sqrt{\mathcal{S}[\det F_{RK}]}\mathcal{R}_{\Delta t}[\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))}+\sqrt{\frac{\Lambda}{2}}\left|\left|\widehat{\widetilde{B}_{RK}\nabla\phi_{m,\Delta t}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))}\\ +\sqrt{\frac{\alpha}{4}}\left|\left|\widehat{\sqrt{\widetilde{m}_{RK}}\phi_{m,\Delta t}}\right|\right|_{l^\infty(L^2(\Gamma^R))}\leq J\left(\sqrt{\frac{\Lambda}{2}}\left|\left|B\nabla\phi^0_{m,\Delta t}\right|\right|_\Omega\right.\\ +\sqrt{\frac{\alpha}{4}}\left|\left|\phi^0_{m,\Delta t}\right|\right|_{\Gamma^R}+\left|\left|\widehat{\det F_{RK}f}\circ X_{RK}\right|\right|_{l^2(L^2(\Omega))}+\left|\left|\widehat{\widetilde{m}_{RK}g\circ X_{RK}}\right|\right|_{l^\infty(L^2(\Gamma^R))}\\ \left.+\left|\left|\widehat{\mathcal{R}_{\Delta t}[\widetilde{m}_{RK}g\circ X_{RK}]}\right|\right|_{l^2(L^2(\Gamma^R))}\right).\end{aligned}\tag{4.66}$$

Proof. The result follows directly by replacing

$$S^{n+1}\text{ with }1/2\left(\det F^{n+1}_{RK}f^{n+1}\circ X^{n+1}_{RK}+\det F^n_{RK}f^n\circ X^n_{RK}\right)$$

and G^{n+1} with $1/2\left(\widetilde{m}^{n+1}_{RK}g\circ X^{n+1}_{RK}+\widetilde{m}^n_{RK}g\circ X^n_{RK}\right)$ in (4.63). ∎

Remark 4.8. Notice that, constants J and D appearing in Theorem 4.15 and Corollary 4.16 depend on the diffusion tensor, more precisely they depend on fraction $\frac{c_A}{\Lambda}$. In most cases this fraction is bounded in the hyperbolic limit.

Remark 4.9. In the particular case of Dirichlet boundary conditions ($\Gamma^D \equiv \Gamma$), diffusion tensor of the form $A = \epsilon B$ and $f = 0$, the previous corollary can be improved. Specifically, by using analogous procedures to the ones in the previous corollary we can obtain the following $l^\infty(H^1)$ stability result with constants (J and D) independent of the diffusion constant ϵ

$$\begin{aligned}\sqrt{\frac{\gamma}{2}}\left|\left|\widehat{\sqrt{\mathcal{S}[\det F_{RK}]}\mathcal{R}_{\Delta t}[\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))}+\sqrt{\frac{1}{2}}\left|\left|\widehat{\widetilde{B}_{RK}\nabla\phi_{m,\Delta t}}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))}\\ \leq J(1+\sqrt{\epsilon})\sqrt{\frac{1}{2}}\left|\left|B\nabla\phi^0_{m,\Delta t}\right|\right|_\Omega.\end{aligned}\tag{4.67}$$

for $\Delta t < D$.

4.4. Error estimate for the semidiscretized scheme. The aim of the present section is to estimate the difference between the *discrete solution* of (4.28), $\widehat{\phi_{m,\Delta t}} := \{\phi^n_{m,\Delta t}\}_{n=0}^N$, 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

$$\left\langle \mathcal{L}^{n+\frac{1}{2}}[\widehat{\phi_m}], \psi\right\rangle = \left\langle \mathcal{F}^{n+\frac{1}{2}}, \psi\right\rangle \quad \forall\psi \in H^1_{\Gamma^D}(\Omega),\tag{4.68}$$

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 4.27, is proved by means of Theorem 4.11 and the forthcoming Lemmas 4.25 and 4.26. On the other hand, the error estimate for the gradient in the $l^\infty(\mathbf{L}^2(\Omega))$-norm, to be stated in Theorem 4.28, is proved by means of Theorem 4.15 and the forthcoming Lemmas 4.25 and 4.26. Before doing this we give some results with sketched proofs (see [6] for further details). Some auxiliary mappings will be introduced. They will be denoted by ξ, $\mathbf{u}$ and Ψ depending on whether they are scalar, vector or tensor mappings, respectively. Moreover, if $\mathbf{v}$ is smooth 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. These estimates and the ones obtained in §4.2 for F^n_{RK}, $(F^n_{RK})^{-1}$ and $\det F^n_{RK}$ will be used below without explicitly stated (see [6] for further details).

LEMMA 4.17. *Let us assume Hypotheses 1 and 3. Let us suppose that* $\mathbf{v} \in \mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$, $\Delta t < \eta$, $\varphi \in C^3(L^2(\Omega))$ *and* $\rho_m \in C^2(L^\infty(\Omega))$. *Let us define the function* $\xi^{n+\frac{1}{2}} : \Omega \longrightarrow \mathbb{R}$, *for* $n \in \{0, \ldots, N-1\}$, *by*

$$\xi^{n+\frac{1}{2}}(p) := \rho \circ X_e^{n+\frac{1}{2}}(p) \det F^{n+\frac{1}{2}}(p) \dot{\varphi}^{n+\frac{1}{2}}(p)$$
$$-\frac{1}{2}\left(\rho \circ X^{n+1}_{RK}(p) \det F^{n+1}_{RK}(p) + \rho \circ X^n_{RK}(p) \det F^n_{RK}(p)\right) \frac{\varphi^{n+1}(p) - \varphi^n(p)}{\Delta t},$$

for a.e. $p \in \Omega$. *Then* $\xi^{n+\frac{1}{2}} \in L^2(\Omega)$ *and* $||\xi^{n+\frac{1}{2}}||_\Omega \leq C(T, \mathbf{v}, \rho)\Delta t^2 ||\varphi||_{C^3(L^2(\Omega))}$, $n = 0, \ldots, N-1$.

Proof. The result follows by using Taylor expansions and noting that if $X_e \in \mathbf{C}^3(\overline{\Omega} \times [0,T])$ and $\mathbf{v} \in \mathbf{C}^1(\mathcal{T}^\delta)$ then $|X^n_e(p) - X^n_{RK}(p)| \leq C(\mathbf{v}, T)\Delta t^2$, and if $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$ and $\mathbf{v} \in \mathbf{C}^2(\mathcal{T}^\delta)$ then $|\det F^n(p) - \det F^n_{RK}(p)| \leq C(\mathbf{v}, T)\Delta t^2$. ∎

LEMMA 4.18. *Let us assume that* $A_m \in C^2(\mathbb{L}^\infty(\Omega))$. *Let* $\mathbf{w} \in C^2(\mathbf{L}^2(\Omega))$ *be a given mapping and* $\mathbf{u}^{n+\frac{1}{2}} : \Omega \longrightarrow \mathbb{R}^d$, *for* $n \in \{0, \ldots, N-1\}$, *be defined by*

$$\mathbf{u}^{n+\frac{1}{2}}(p) := \widetilde{A}^{n+\frac{1}{2}}_m(p)\mathbf{w}^{n+\frac{1}{2}}(p) - \left(\frac{\widetilde{A}^{n+1}_m(p) + \widetilde{A}^n_m(p)}{2}\right)\left(\frac{\mathbf{w}^{n+1}(p) + \mathbf{w}^n(p)}{2}\right),$$

for a.e. $p \in \Omega$. *Then,* $\mathbf{u}^{n+\frac{1}{2}} \in \mathbf{L}^2(\Omega)$ *and* $||\mathbf{u}^{n+\frac{1}{2}}||_\Omega \leq C(T, \mathbf{v}, A)\Delta t^2 ||\mathbf{w}||_{C^2(\mathbf{L}^2(\Omega))}$, $n \in \{0, \ldots, N-1\}$. *Moreover, if* $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$, $A_m \in C^2(\mathbb{W}^{1,\infty}(\Omega))$ *and* $\mathbf{w} \in C^2(\mathbf{H}^1(\Omega))$ *then* $\mathbf{u}^{n+\frac{1}{2}} \in \mathbf{H}^1(\Omega)$ *and* $||\operatorname{Div} \mathbf{u}^{n+\frac{1}{2}}||_\Omega \leq C(T, \mathbf{v}, A)\Delta t^2 ||\mathbf{w}||_{C^2(\mathbf{H}^1(\Omega))}$, $n \in \{0, \ldots, N-1\}$.

Proof. The result follows by writing Taylor expansions in the time variable for $\mathbf{w}$ and the tensor field $\widetilde{A}_m(p,s) := \det F(p,s) F^{-1}(p,s) A \circ X_e(p,s) F^{-T}(p,s)$, $s \in [0,T]$. ∎

LEMMA 4.19. *Let us assume Hypotheses 1 and 4. Let us suppose that* $\mathbf{v} \in \mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$ *and* $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, *being* η *the constant appearing in Lemma 4.1. Let* $\mathbf{w} \in \mathbf{L}^2(\Omega)$ *be a given function and* $\mathbf{u}^n : \Omega \longrightarrow \mathbb{R}^d$ *be defined by*

$$\mathbf{u}^n(p) := \widetilde{A}^n_m(p)\mathbf{w}(p) - \widetilde{A}^n_{RK}(p)\mathbf{w}(p), \ 0 \leq n \leq N. \tag{4.69}$$

Then, $\mathbf{u}^n \in \mathbf{L}^2(\Omega)$ *and* $||\mathbf{u}^n||_\Omega \leq C(T, \mathbf{v}, A)\Delta t^2 ||\mathbf{w}||_\Omega$. *Moreover, if* $\mathbf{v} \in \mathbf{C}^3(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^5(\overline{\Omega} \times [0,T])$, $A \in \mathbb{W}^{2,\infty}(\mathcal{O}^\delta)$ *and* $\mathbf{w} \in \mathbf{H}^1(\Omega)$, *then* $\mathbf{u}^n \in \mathbf{H}^1(\Omega)$ *and*

$||\operatorname{Div}\mathbf{u}^n||_\Omega \leq C(T,\mathbf{v},A)\Delta t^2||\mathbf{w}||_{1,2,\Omega}$.

Proof. The result follows by applying Taylor expansions, noting that if $X_e \in \mathbf{C}^4(\overline{\Omega}\times[0,T])$ and $\mathbf{v}\in\mathbf{C}^2(\mathcal{T}^\delta)$ then $||X_e^n - X_{RK}^n||_{1,\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2$, $||(F^n)^{-T} - (F_{RK}^n)^{-T}||_{\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2$ and $||\det F^n - \det F_{RK}^n||_{\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2$, and if $X_e \in \mathbf{C}^5(\overline{\Omega}\times[0,T])$ and $\mathbf{v}\in\mathbf{C}^3(\mathcal{T}^\delta)$ then $||(F^n)^{-T} - (F_{RK}^n)^{-T}||_{1,\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2$ and $||\det F^n - \det F_{RK}^n||_{1,\infty,\Omega} \leq C(\mathbf{v},T)\Delta t^2$. ∎

LEMMA 4.20. *Let $\varphi \in C^2(L^2(\Gamma^R))$ be a given mapping and $\xi_1^{n+\frac{1}{2}} : \Gamma^R \longrightarrow \mathbb{R}$, $\xi_2^{n+\frac{1}{2}} : \Gamma^R \longrightarrow \mathbb{R}$ be defined by*

$$\xi_1^{n+\frac{1}{2}}(p) := \widetilde{m}^{n+\frac{1}{2}}(p)\varphi^{n+\frac{1}{2}}(p) - \left(\frac{\widetilde{m}^{n+1}(p)+\widetilde{m}^n(p)}{2}\right)\left(\frac{\varphi^{n+1}(p)+\varphi^{n+1}(p)}{2}\right),$$
$$\xi_2^{n+\frac{1}{2}}(p) := \widetilde{m}^{n+\frac{1}{2}}(p)\varphi^{n+\frac{1}{2}}(p) - \left(\frac{\widetilde{m}^{n+1}(p)\varphi^{n+1}(p)+\widetilde{m}^n(p)\varphi^n(p)}{2}\right).$$

Then $\xi_1^{n+\frac{1}{2}}$, $\xi_2^{n+\frac{1}{2}} \in L^2(\Gamma^R)$ and

$$||\xi_1^{n+\frac{1}{2}}||_{\Gamma^R} \leq \frac{\Delta t^2}{8}||\widetilde{m}\varphi||_{C^2(L^2(\Gamma^R))} \leq C(T,\mathbf{v})\Delta t^2||\varphi||_{C^2(L^2(\Gamma^R))},$$
$$||\xi_2^{n+\frac{1}{2}}||_{\Gamma^R} \leq C(T,\mathbf{v})\Delta t^2||\varphi||_{C^2(L^2(\Gamma^R))}.$$

Proof. The result follows by using Taylor expansions in the time variable. ∎

LEMMA 4.21. *Let us assume Hypothesis 1. Let us suppose that $\mathbf{v}\in\mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega}\times[0,T])$ and $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, being η the constant appearing in Lemma 4.1. Let $\varphi\in L^2(\Gamma^R)$ be a given function and $\xi^n : \Gamma^R \longrightarrow \mathbb{R}$ be defined by*

$$\xi^n(p) := \widetilde{m}^n(p)\varphi(p) - \widetilde{m}_{RK}^n(p)\varphi(p),\ 0\leq n\leq N. \tag{4.70}$$

Then $\xi^n \in L^2(\Gamma^R)$ and $||\xi^n||_{\Gamma^R} \leq C(T,\mathbf{v})\Delta t^2||\varphi||_{\Gamma^R}$.

Proof. The result follows noting that $|\det F^n(p) - \det F_{RK}^n(p)| \leq C(\mathbf{v},T)\Delta t^2$ and $\left|\left|(F^n)^{-T}(p) - (F_{RK}^n)^{-T}(p)\right|\right|_2 \leq C(\mathbf{v},T)\Delta t^2$. ∎

LEMMA 4.22. *Let us assume Hypotheses 1. Let us suppose $\mathbf{v}\in\mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega}\times[0,T])$ and $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, being η the constant appearing in Lemma 4.1. Let $\varphi\in H^1(G_{t_n}^\delta)$ be a given function, being $G_{t_n}^\delta$ the set defined in (4.24), and let $\xi^n : \Gamma^R \longrightarrow \mathbb{R}$ be defined by*

$$\xi^n(p) := \widetilde{m}^n(p)\varphi(X_e^n(p)) - \widetilde{m}_{RK}^n(p)\varphi(X_{RK}^n(p)),\ 0\leq n\leq N. \tag{4.71}$$

Then $\xi^n \in L^2(\Gamma^R)$ and $||\xi^n||_{\Gamma^R} \leq C(T,\mathbf{v})\Delta t^2||\varphi||_{1,2,G_{t_n}^\delta}$.

Proof. The result follows by applying Taylor expansions, noting that $|X_e^n(p) - X_{RK}^n(p)| \leq C(\mathbf{v},T)\Delta t^2$, $|(F^n)^{-T}(p) - (F_{RK}^n)^{-T}(p)| \leq C(\mathbf{v},T)\Delta t^2$ and $|\det F^n(p) - \det F_{RK}^n(p)| \leq C(\mathbf{v},T)\Delta t^2$. ∎

LEMMA 4.23. *Let $\varphi\in C^2(L^2(\Omega))$ be a given function and $\xi^{n+\frac{1}{2}} : \Omega \longrightarrow \mathbb{R}$, for $n\in\{0,\ldots,N-1\}$, be defined by*

$$\xi^{n+\frac{1}{2}}(p) := \det F^{n+\frac{1}{2}}(p)\varphi^{n+\frac{1}{2}}(p) - \frac{\det F^{n+1}(p)\varphi^{n+1}(p) + \det F^n(p)\varphi^n(p)}{2}.$$

Then, $\xi^{n+\frac{1}{2}} \in L^2(\Omega)$ *and*

$$\left|\left|\xi^{n+\frac{1}{2}}\right|\right|_\Omega \leq \frac{\Delta t^2}{8} ||\det F\varphi||_{C^2(L^2(\Omega))} \leq C(T,\mathbf{v})\Delta t^2 ||\varphi||_{C^2(L^2(\Omega))}.$$

Proof. The result follows by applying Taylor expansions. ∎

LEMMA 4.24. *Let us assume Hypothesis 1. Let us suppose that* $\mathbf{v} \in \mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$ *and* $\Delta t < \eta$, *being* η *the constant appearing in Lemma 4.1. Let* $\varphi \in H^1(\Omega^\delta_{t_n})$ *be a given function, being* $\Omega^\delta_{t_n}$ *the set defined in (4.9), and let* $\xi^n : \Omega \longrightarrow \mathbb{R}$ *be defined by*

$$\xi^n(p) := \det F^n(p)\varphi(X^n_e(p)) - \det F^n_{RK}(p)\varphi(X^n_{RK}(p)),\ 0 \leq n \leq N.$$

Then $\xi^n \in L^2(\Omega)$ *and* $||\xi^n||_\Omega \leq C(T,\mathbf{v})\Delta t^2 ||\varphi||_{1,2,\Omega^\delta_{t_n}}$.

Proof. The result follows by using Taylor expansions, noting that $|X^n_e(p) - X^n_{RK}(p)| \leq C(\mathbf{v},T)\Delta t^2$ and $|\det F^n(p) - \det F^n_{RK}(p)| \leq C(\mathbf{v},T)\Delta t^2$. ∎

LEMMA 4.25. *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 (2.7)-(2.10) 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 (4.68) 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*

$$\left\langle \left(\mathcal{L}^{n+\frac{1}{2}} - \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}\right)[\widehat{\phi_m}], \psi \right\rangle = \left\langle \xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega}, \psi \right\rangle_\Omega + \left\langle \xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma}, \psi \right\rangle_{\Gamma^R}, \tag{4.72}$$

$\forall \psi \in H^1_{\Gamma^D}(\Omega)$. *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:*

$$\begin{aligned} &\left|\left|\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega}\right|\right|_\Omega \leq \Delta t^2 C(T,\mathbf{v},\rho,A)\left(||\phi_m||_{C^3(L^2(\Omega))} + ||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))}\right), \\ &\left|\left|\xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma}\right|\right|_{\Gamma^R} \leq \Delta t^2 C(T,\mathbf{v},A)\left(||\nabla\phi_m \cdot \mathbf{m}||_{C^2(L^2(\Gamma^R))} + \alpha||\phi_m||_{C^2(L^2(\Gamma^R))}\right), \end{aligned} \tag{4.73}$$

where $\alpha > 0$ *appears in (2.9).*

Proof. The left-hand side of (4.72) is equal to $I_1 + I_2 + I_3$, with

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

The bound for I_1 directly follows from Lema 4.17 for $\varphi = \phi_m$, so we can define a function $\xi_{I_1}^{n+\frac{1}{2}} \in L^2(\Omega)$ such that

$$I_1 = \left\langle \xi_{I_1}^{n+\frac{1}{2}}, \psi \right\rangle_\Omega, \text{ with } \left|\left|\xi_{I_1}^{n+\frac{1}{2}}\right|\right|_\Omega \leq C(T, \mathbf{v}, \rho)\Delta t^2 ||\phi_m||_{C^3(L^2(\Omega))}. \tag{4.74}$$

In order to estimate I_2 we apply Lemmas 4.18 and 4.19 for $\mathbf{w} = \nabla\phi_m$ and $\mathbf{w} = \nabla\phi_m^{n+1} + \nabla\phi_m^n$, respectively, so $I_2 = \left\langle \mathbf{u}_{I_2}^{n+\frac{1}{2}}, \nabla\psi \right\rangle_\Omega$, with $\mathbf{u}_{I_2}^{n+\frac{1}{2}} \in \mathbf{H}^1(\Omega)$. Then, by using a Green's formula, we deduce

$$I_2 = \left\langle \mathbf{u}_{I_2}^{n+\frac{1}{2}} \cdot \mathbf{m}, \psi \right\rangle_{\Gamma^R} - \left\langle \operatorname{Div} \mathbf{u}_{I_2}^{n+\frac{1}{2}}, \psi \right\rangle_\Omega,$$

where, the involved functions are bounded as follows:

$$\begin{aligned} \left|\left|\mathbf{u}_{I_2}^{n+\frac{1}{2}} \cdot \mathbf{m}\right|\right|_{\Gamma^R} &\leq C(T, \mathbf{v}, A)\Delta t^2 ||\nabla\phi_m \cdot \mathbf{m}||_{C^2(L^2(\Gamma^R))}, \\ \left|\left|\operatorname{Div} \mathbf{u}_{I_2}^{n+\frac{1}{2}}\right|\right|_\Omega &\leq C(T, \mathbf{v}, A)\Delta t^2 ||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))}. \end{aligned} \tag{4.75}$$

The estimate for I_3 follows by applying Lemmas 4.20 and 4.21 for $\varphi = \alpha\phi_m|_{\Gamma^R}$ and $\varphi = \alpha(\phi_m^{n+1} + \phi_m^n)|_{\Gamma^R}$, respectively:

$$I_3 = \left\langle \xi_{I_3}^{n+\frac{1}{2}}, \psi \right\rangle_{\Gamma^R} \text{ with } \left|\left|\xi_{I_3}^{n+\frac{1}{2}}\right|\right|_{\Gamma^R} \leq C(T, \mathbf{v})\alpha\Delta t^2 ||\phi_m||_{C^2(L^2(\Gamma^R))}. \tag{4.76}$$

Finally, partial results (4.74), (4.75) and (4.76) imply (4.72). ∎

LEMMA 4.26. *Assume Hypothesis 1, and* $\mathbf{v} \in \mathbf{C}^2(\mathcal{T}^\delta)$, $X_e \in \mathbf{C}^4(\overline{\Omega} \times [0,T])$ *and* $\Delta t < \min\{\eta, 1/(2||L||_{\infty,\mathcal{T}^\delta})\}$, *being* η *the constant appearing in Lemma 4.1. 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*

$$\left\langle \left(\mathcal{F}^{n+\frac{1}{2}} - \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}\right), \psi \right\rangle = \left\langle \xi_f^{n+\frac{1}{2}}, \psi \right\rangle_\Omega + \left\langle \xi_g^{n+\frac{1}{2}}, \psi \right\rangle_{\Gamma^R} \quad \forall \psi \in H^1(\Omega). \tag{4.77}$$

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

$$\begin{aligned} \left|\left|\xi_f^{n+\frac{1}{2}}\right|\right|_\Omega &\leq \Delta t^2 C(T, \mathbf{v}, \mathcal{T}^\delta) \left(||\det F f_m||_{C^2(L^2(\Omega))} + ||f||_{C^1(\mathcal{T}^\delta)}\right), \\ \left|\left|\xi_g^{n+\frac{1}{2}}\right|\right|_{\Gamma^R} &\leq \Delta t^2 C(T, \mathbf{v}, \mathcal{T}^\delta_{\Gamma^R}) \left(||\widetilde{m} g_m||_{C^2(L^2(\Gamma^R))} + ||g||_{C^1(\mathcal{T}^\delta_{\Gamma^R})}\right). \end{aligned} \tag{4.78}$$

Proof. The proof follows from Lemmas 4.20, 4.22, 4.23 and 4.24. ∎

Hypothesis 9. Functions appearing in problem (2.7)-(2.10) 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 10. Functions appearing in problem (2.7)-(2.10) 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 $\alpha > 0$.

Lemmas in this section hold under Hypotheses 1, 3 and 4 and the previous ones.

THEOREM 4.27. *Assume Hypotheses 1, 3, 4, 5, 6, 7 and 9, 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 (4.68) and let $\widehat{\phi_{m,\Delta t}}$ *be the solution of (4.28) 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*

$$\begin{aligned}
&\sqrt{\gamma}||\widehat{\sqrt{\det F_{RK}}\,(\phi_m} - \phi_{m,\Delta t})||_{l^\infty(L^2(\Omega))} \\
&+\sqrt{\frac{\Lambda}{4}}\left|\left|\widetilde{B}_{RK}\mathcal{S}\,[\widehat{\nabla\phi_m} - \nabla\phi_{m,\Delta t}]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} \\
&+\sqrt{\frac{\alpha}{8}}\left|\left|\widehat{\sqrt{\mathcal{S}\,[\widetilde{m}_{RK}]}\mathcal{S}\,[\phi_m} - \phi_{m,\Delta t}]\right|\right|_{l^2(L^2(\Gamma^R))} \leq J\ \Delta t^2\left(||\phi_m||_{C^3(L^2(\Omega))}\right. \\
&+||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))} + ||\nabla\phi_m\cdot\mathbf{m}||_{C^2(L^2(\Gamma^R))} + ||\phi_m||_{C^2(L^2(\Gamma^R))} \\
&\left.+||\det F f_m||_{C^2(L^2(\Omega))} + ||f||_{C^1(\mathcal{T}^\delta)} + ||\widetilde{m}g_m||_{C^2(L^2(\Gamma^R))} + ||g||_{C^1(\mathcal{T}^\delta_{\Gamma^R})}\right).
\end{aligned} \tag{4.79}$$

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 (4.28) and (4.68) we have

$$\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{e_{m,\Delta t}}], \psi\right\rangle = \left\langle \left(\mathcal{L}^{n+\frac{1}{2}}_{\Delta t} - \mathcal{L}^{n+\frac{1}{2}}\right)[\widehat{\phi_m}], \psi\right\rangle + \left\langle \mathcal{F}^{n+\frac{1}{2}} - \mathcal{F}^{n+\frac{1}{2}}_{\Delta t}, \psi\right\rangle, \tag{4.80}$$

$\forall\psi \in H^1_{\Gamma^D}(\Omega)$ and $0 \leq n \leq N-1$. Then, as a consequence of Lemmas 4.25 and 4.26, we deduce

$$\left\langle \mathcal{L}^{n+\frac{1}{2}}_{\Delta t}[\widehat{e_{m,\Delta t}}], \psi\right\rangle = \left\langle \xi_f^{n+\frac{1}{2}} - \xi^{n+\frac{1}{2}}_{\mathcal{L}_\Omega}, \psi\right\rangle_\Omega + \left\langle \xi_g^{n+\frac{1}{2}} - \xi^{n+\frac{1}{2}}_{\mathcal{L}_\Gamma}, \psi\right\rangle_{\Gamma^R}, \tag{4.81}$$

$\forall\psi \in H^1_{\Gamma^D}(\Omega)$. Now the result follows by applying Theorem 4.11 to (4.81), 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 4.25 and 4.26. ∎

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 4.27 is also valid when $A \equiv 0$.

THEOREM 4.28. *Let us assume Hypotheses 1, 3, 4, 5, 6, 7 and 10, 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 (4.68) and $\widehat{\phi_{m,\Delta t}}$ *be the solution of (4.28) 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

$$
\begin{aligned}
&\sqrt{\frac{\gamma}{4}}\left|\left|\widehat{\sqrt{\mathcal{S}[\det F_{RK}]}\mathcal{R}_{\Delta t}[\phi_m-\phi_{m,\Delta t}]}\right|\right|_{l^2(L^2(\Omega))}\\
&\qquad+\sqrt{\frac{\Lambda}{2}}\left|\left|\widetilde{B}_{RK}\,\widehat{(\nabla\phi_m-\nabla\phi_{m,\Delta t})}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))}\\
&\qquad+\sqrt{\frac{\alpha}{4}}\left|\left|\sqrt{\widetilde{m}_{RK}}\,\widehat{(\phi_m-\phi_{m,\Delta t})}\right|\right|_{l^\infty(L^2(\Gamma^R))}\le J\ \Delta t^2\left(||\phi_m||_{C^3(L^2(\Omega))}\right.\\
&\qquad+||\nabla\phi_m||_{C^2(\mathbf{H}^1(\Omega))}+||\nabla\phi_m\cdot\mathbf{m}||_{C^3(L^2(\Gamma^R))}+||\phi_m||_{C^3(L^2(\Gamma^R))}\\
&\qquad\left.+||\det F f_m||_{C^2(L^2(\Omega))}+||f||_{C^1(\mathcal{T}^\delta)}+||\widetilde{m}g_m||_{C^3(L^2(\Gamma^R))}+||g||_{C^2(\mathcal{T}^\delta_{\Gamma^R})}\right).
\end{aligned}
\tag{4.82}
$$

Proof. It is analogous to the one of the previous theorem, but using Theorem 4.15 instead of Theorem 4.11 and noting that

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

This estimate follows by using Taylor expansions and

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

□

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]).

REFERENCES

[1] R.A. Adams. Sobolev Spaces. *Academic Press, New York*, 1975.

[2] J. Baranger, D. Esslaoui, and A. Machmoum. Error estimate for convection problem with characteristics method. *Numer. Algorithms*, 21 (1999):49–56. Numerical methods for partial differential equations (Marrakech, 1998).

[3] J. Baranger and A. Machmoum. Une norme "naturelle" pour la méthode des caractéristiques en éléments finis discontinus: cas 1-D. *RAIRO Modél. Math. Anal. Numér.*, 30:549–574, 1996.
[4] J. Baranger and A. Machmoum. A "natural" norm for the method of characteristics using discontinuous finite elements: 2D and 3D case. *Math. Model. Numer. Anal.*, 33:1223–1240, 1999.
[5] E. Barucci, S. Pilodoro, and V. Vespri. Some results on partial differential equations and Asian options. *Math. Models Methods Appl. Sci.*, 11:475–497, 2001.
[6] M. Benítez. Métodos numéricos para problemas de convección difusión. Aplicación a la convección natural, Ph.D. Thesis, Universidade de Santiago de Compostela. 2009.
[7] M. Benítez and A. Bermúdez. Numerical Analysis of a second-order pure Lagrange-Galerkin method for convection-diffusion problems. Part II: fully discretized scheme and numerical results. *Submitted*.
[8] A. Bermúdez and J. Durany. La méthode des charactéristiques pour les problèmes de convection-diffusion stationnaires. *Math. Model. Numer. Anal.*, 21:7–26, 1987.
[9] A. Bermúdez, M.R. Nogueiras, and C. Vázquez. Numerical solution of (degenerated) convection-diffusion-reaction problems with higher order characteristics/finite elements. Part I: Time discretization. *SIAM. J. Numer. Anal.*, 44:1829–1853, 2006.
[10] A. Bermúdez, M.R. Nogueiras, and C. Vázquez. Numerical solution of (degenerated) convection-diffusion-reaction problems with higher order characteristics/finite elements. Part II: Fully Discretized Scheme and Quadrature Formulas. *SIAM. J. Numer. Anal.*, 44:1854–1876, 2006.
[11] K. Boukir, Y. Maday, and B. Métivet. A high-order characteristics method for the incompressible Navier-Stokes equations. *Comput. Methods Appl. Mech. Engrg.*, 116:211–218, 1994. ICOSAHOM'92 (Montpellier, 1992).
[12] K. Boukir, Y. Maday, B. Métivet, and E. Razafindrakoto. A high-order characteristics/finite element method for the incompressible Navier-Stokes equations. *Internat. J. Numer. Methods Fluids*, 25:1421–1454, 1997.
[13] K. Chrysafinos and N. J. Walkington. Error estimates for discontinuous Galerkin approximations of implicit parabolic equations. *SIAM J. Numer. Anal.*, 43:2478–2499 (electronic), 2006.
[14] K. Chrysafinos and N. J. Walkington. Error estimates for the discontinuous Galerkin methods for parabolic equations. *SIAM J. Numer. Anal.*, 44:349–366 (electronic), 2006.
[15] K. Chrysafinos and N. J. Walkington. Lagrangian and moving mesh methods for the convection diffusion equation. *M2AN Math. Model. Numer. Anal.*, 42:25–55, 2008.
[16] J. Douglas, Jr., and T.F. Russell. Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures. *SIAM J. Numer. Anal.*, 19:871–885, 1982.
[17] R.E. Ewing and H. Wang. A summary of numerical methods for time-dependent advection-dominated partial differential equations. *J. Comput. Appl. Math.*, 128:423–445, 2001.
[18] M.E. Gurtin. An Introduction to Continuum Mechanics. *Mathematics in Science and Engineering*, 158, Academic Press, San Diego, 1981.
[19] L. Hörmander. Hypoelliptic second order differential equations. *Acta Math.*, 119:147–171, 1967.
[20] K. W. Morton. Numerical solution of convection-diffusion problems. *Appl. Math. Comput.*, 12, Chapman Hall, London, 1996.
[21] O. Pironneau. On the Transport-Diffusion Algorithm and Its Applications to the Navier-Stokes Equations. *Numer. Math.*, 38:309–332, 1982.
[22] O. Pironneau, J. Liou, and T. Tezduyar. Characteristic-Galerkin and Galerkin/least-squares space-time formulations for the advection-diffusion equations with time-dependent domains. *Comput. Methods Appl. Mech. Engrg.*, 100:117–141, 1992.
[23] A. Quarteroni and A. Valli. Numerical approximation of partial differential equations. *Springer Series in Computational Mathematics, Springer-Verlag*, 23, Berlin, 1994.
[24] M. A. Ragusa. On weak solutions of ultraparabolic equations. *Nonlinear Anal.*, 47:503–511, 2001.
[25] H. Rui and M. Tabata. A second order characteristic finite element scheme for convection-diffusion problems. *Numer. Math.*, 92:161–177, 2002.
[26] P. Wilmot, J. Dewynne, and S. Howison. Option pricing. mathematical models and computation. *Oxford Financial Press*, Oxford, 1993.