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# NUMERICAL ANALYSIS OF A SECOND-ORDER PURE LAGRANGE-GALERKIN METHOD FOR CONVECTION-DIFFUSION PROBLEMS. PART II: FULLY DISCRETIZED SCHEME AND NUMERICAL RESULTS\*

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**Abstract.** We analyze a second order pure Lagrange-Galerkin method for variable coefficient convection-(possibly degenerate) diffusion equations with mixed Dirichlet-Robin boundary conditions. In a previous paper the proposed second order pure Lagrangian time discretization scheme has been introduced and analyzed for the same problem. More precisely, the  $l^\infty(H^1)$  stability and  $l^\infty(H^1)$  error estimates of order  $O(\Delta t^2)$  has been obtained. Moreover, for the particular case of incompressible flows, stability inequalities with constants independent of the final time have been stated. In the present paper  $l^\infty(H^1)$  error estimates of order  $O(\Delta t^2) + O(h^k)$  are obtained for the fully discretized pure Lagrange-Galerkin method. To prove these results we use some properties obtained in the previous paper. Finally, numerical tests are presented that confirm the theoretical results.

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

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

**1. Introduction.** For convection-diffusion problems with dominant convection, methods of characteristics for time discretization are extensively used (see the review paper [21]). These methods are based on time discretization of the material time derivative. For space discretization, they has been combined with finite differences [19], finite elements ([27], [9], [11], [25], [33], [32], [28]), spectral finite elements ([34], [1]), discontinuous finite elements ([3], [2], [4]), and so on. When combined with finite elements they are also called Lagrange-Galerkin methods. In particular, when the characteristics methods are formulated in Lagrangian coordinates (respectively, Eulerian coordinates) they are called pure Lagrangian methods (respectively, semi-Lagrangian methods). The Lagrange-Galerkin method has been mathematically analyzed and applied to different problems by several authors, primarily in the semi-Lagrangian version. Numerical solution of convection-diffusion partial differential equations by this kind of methods is addressed in ([19], [27], [33], [18], [5], [17], [13]) among others. In the present paper we will consider the combination of the pure Lagrangian method proposed and analyzed in [8] with a spatial discretization by using finite element spaces. Studying pure Lagrangian methods is quite natural because Lagrangian formulations are very common in mechanics. Moreover, from the numerical results shown in this paper, they do not present oscillations in cases where classical semi-Lagrangian methods do. These results allow us to conclude that the advantages of the (new) pure Lagrangian methods over semi-Lagrangian (classical) ones are that the computational domain is time-independent, they are accurate in zones of strong gradients or discontinuities of the solution (see Ex. 2 in §5) and terms of the form  $O(h^\alpha/\Delta t)$  are not observed in the error (see Ex. 1 in §5) as is typical of

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semi-Lagrangian methods.

There exists an extensive literature studying the classical first order characteristic method combined with finite elements applied to convection-diffusion equations. More precisely, if  $\Delta t$  denotes the time step,  $h$  the mesh-size and  $k$  the degree of the finite elements space, estimates of the form  $O(h^k) + O(\Delta t)$  in the  $l^\infty(L^2(\mathbb{R}^d))$ -norm are shown in [33] ( $d$  denotes the dimension of the spatial domain). In [27] error estimates of the form  $O(h^k) + O(\Delta t) + O(h^{k+1}/\Delta t)$  in the  $l^\infty(L^2(\Omega))$ -norm are obtained under the assumption that the normal velocity vanishes on the boundary of  $\Omega$ . All of these estimates involve constants depending on solution norms. For linear finite elements and for a velocity field vanishing on the boundary, convergence of order  $O(h^2) + O(\min(h, h^2/\Delta t) + O(\Delta t)$  in the  $l^\infty(L^2(\Omega))$ -norm is stated in [5], where the constants only depend on the data. In principle, the method of characteristics has been introduced for evolution equations but an adaption to solve convection-diffusion stationary problems has been proposed in [10].

In order to increase the order of time and space approximations, higher order schemes for the discretization of the material derivative and higher order finite element spaces would be used. In [31] 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  $O(\Delta t^2) + O(h^k)$  error estimates in the  $l^\infty(L^2(\Omega))$ -norm are stated (see also [12] and [13] for further analysis). In [17], semi-Lagrangian and pure Lagrangian methods are proposed and analyzed for convection-diffusion equations. Error estimates for a Galerkin discretization of a pure Lagrangian formulation and for a discontinuous Galerkin discretization of a semi-Lagrangian formulation are obtained. The estimates are written in terms of the projections constructed in [15] and [16].

In the present paper, fully discretized pure Lagrange-Galerkin schemes are used for a more general problem. Specifically, we consider a (possibly degenerate) variable coefficient diffusive term instead of the simpler Laplacian one, a general mixed Dirichlet-Robin boundary condition and a time dependent domain. Moreover, we analyze a scheme involving approximate characteristic curves.

As in [8], the mathematical formalism of continuum mechanics (see for instance [23]) is used to introduce the schemes and to analyze the error. In most cases the exact characteristics curves are not easy to compute analytically, so, as in the first part of this work, our analysis include the case where the characteristics curves are approximated using a second order Runge-Kutta scheme. In [8] a  $l^\infty(L^2)$  stability inequality is stated and  $l^\infty(L^2)$  error estimates of order  $O(\Delta t^2)$  are obtained; these estimates are uniform in the hyperbolic limit. Furthermore, stability and error estimates of order  $O(\Delta t^2)$  are proved in the  $l^\infty(H^1)$ -norm. For incompressible flows the constants in the stability inequalities are independent of the final time. As a logical continuation of [8], fully discretized pure Lagrange-Galerkin scheme with a wide class of finite element spaces is analyzed in the present paper. More precisely,  $l^\infty(L^2)$  error estimates of order  $O(\Delta t^2) + O(h^k)$  are obtained; these estimates are bounded in the hyperbolic limit. Moreover, error estimates of order  $O(\Delta t^2) + O(h^k)$  are proved in the  $l^\infty(H^1)$ -norm.

Usually, the unconditional stability of characteristics methods is only proved under the assumption that the inner products in the Galerkin formulation are exactly calculated. This is rarely possible so in practice they are calculated using numerical

quadrature. In general this adds some terms to the final error estimates and, in some cases, it produces the loss of unconditional stability. There are several papers in the literature analyzing the effect of numerical integration in Lagrange-Galerkin methods (see [25], [33], [29], [22], [35], [13]). In particular, in [25] Fourier analysis is developed for the classical Lagrange-Galerkin method involving piecewise linear finite elements, when it is applied to the one dimensional linear convection equation and combined with several quadrature formulas. Unconditional stability has been shown for the trapezoidal rule and unconditional instability has been proved when the mass matrix is exactly integrated and the term of characteristics is approximated by using the trapezoidal rule (Lemma 2.4 in [25]). In [7] an analogous approach is developed for the classical Lagrange-Galerkin method for piecewise linear finite element applied to the one dimensional linear convection equation. The term of characteristic is decomposed into two parts; one of them is exactly integrated and the other one is approximated using the trapezoidal rule (see also [26] for more details). For this scheme conditional stability depending on the CFL number has been shown when the mass matrix is exactly integrated. Moreover, numerical results showing the influence of several quadrature formulas in the stability are presented. In the present paper, quadrature formulas leading to stable schemes are used for the practical implementation of the introduced methods.

The paper is organized as follows. In Section 2 the convection-diffusion Cauchy problem is posed in a time dependent bounded domain, a weak formulation of this problem in Lagrangian coordinates is written and some notations and hypotheses are stated. In Section 3, we introduce the finite element spaces considered for spatial discretization and pose the corresponding fully discretized schemes. In Section 4, under suitable hypotheses on data and solution,  $l^\infty(L^2)$  and  $l^\infty(H^1)$  error estimates of order  $O(\Delta t^2) + O(h^k)$  for the solution of the fully discretized problem are derived. Finally, in Section 5 numerical examples showing the above theoretical results are presented.

**2. Statement of the problem and weak formulation in Lagrangian coordinates.** Let  $\Omega$  be a bounded domain in  $\mathbb{R}^d$  ( $d = 2, 3$ ) with Lipschitz boundary  $\Gamma$  divided into two parts:  $\Gamma = \Gamma^D \cup \Gamma^R$ , with  $\Gamma^D \cap \Gamma^R = \emptyset$ . Let  $T$  be a positive constant and  $X_e : \bar{\Omega} \times [0, T] \rightarrow \mathbb{R}^d$  be a motion in the sense of Gurtin [23]. In particular,  $X_e \in \mathbf{C}^3(\bar{\Omega} \times [0, T])$  and for each fixed  $t \in [0, T]$ ,  $X_e(\cdot, t)$  is a one-to-one function satisfying

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

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  $\Omega_0 = \Omega$ . We will adopt the notation given in [8] for the trajectory of the motion ( $\mathcal{T}$ ), the velocity ( $\mathbf{v}$ ) and the functional spaces involved (see §2 of [8] for more details). Let us introduce the trajectory of the motion  $\mathcal{T}$  and the set  $\mathcal{O}$  be defined by

$$(2.2) \quad \mathcal{T} := \{(x, t) : x \in \bar{\Omega}_t, t \in [0, T]\}, \quad \mathcal{O} := \bigcup_{t \in [0, T]} \bar{\Omega}_t.$$

We denote by  $L$  the gradient of  $\mathbf{v}$  with respect to the space variables. If  $\Psi$  is a spatial field we define its material description  $\Psi_m$  by

$$(2.3) \quad \Psi_m(p, t) := \Psi(X_e(p, t), t).$$

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

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

value problem:

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

$$(2.4) \quad \rho(x) \frac{\partial \phi}{\partial t}(x, t) + \rho(x) \mathbf{v}(x, t) \cdot \text{grad } \phi(x, t) - \text{div}(A(x) \text{grad } \phi(x, t)) = f(x, t),$$

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

$$(2.5) \quad \phi(\cdot, t) = \phi_D(\cdot, t) \text{ on } \Gamma_t^D,$$

$$(2.6) \quad \alpha \phi(\cdot, t) + A(\cdot) \text{grad } \phi(\cdot, t) \cdot \mathbf{n}(\cdot, t) = g(\cdot, t) \text{ on } \Gamma_t^R,$$

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

$$(2.7) \quad \phi(x, 0) = \phi^0(x) \text{ in } \Omega.$$

In the above equations,  $A : \mathcal{O} \rightarrow \text{Sym}$  denotes the diffusion tensor field, where  $\text{Sym}$  is the space of symmetric tensors in the  $d$ -dimensional space,  $\rho : \mathcal{O} \rightarrow \mathbb{R}$ ,  $f : \mathcal{T} \rightarrow \mathbb{R}$ ,  $\phi^0 : \Omega \rightarrow \mathbb{R}$ ,  $\phi_D(\cdot, t) : \Gamma_t^D \rightarrow \mathbb{R}$  and  $g(\cdot, t) : \Gamma_t^R \rightarrow \mathbb{R}$ ,  $t \in (0, T)$  are given scalar functions and  $\mathbf{n}(\cdot, t)$  is the outward unit normal vector to  $\Gamma_t$ .

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

$$\|\varphi\|_{C^m(X)} := \max_{t \in [0, T]} \left\{ \max_{j=0, \dots, m} \|\varphi^{(j)}(t)\|_X \right\} \cdot \|\varphi\|_{H^m(X)} := \left( \int_0^T \sum_{j=0}^m \|\varphi^{(j)}(t)\|_X^2 dt \right)^{\frac{1}{2}}.$$

In the above definitions,  $\varphi^{(j)}$  denotes the  $j$ -th derivative of  $\varphi$  with respect to time. Throughout this article some of the following assumptions will be made on the data of the problem:

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

$$(2.8) \quad \mathcal{T}^\delta := \bigcup_{t \in [0, T]} \overline{\Omega}_t^\delta \times \{t\}, \text{ being } \Omega_t^\delta := \bigcup_{x \in \overline{\Omega}_t} B(x, \delta).$$

We recall some notations given in [8]

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

*Hypothesis 2.* Function  $\rho$  is defined in  $\mathcal{O}^\delta$  and belongs to  $W^{1, \infty}(\mathcal{O}^\delta)$ . Moreover,  $0 < \gamma \leq \rho(x)$  a.e.  $x \in \mathcal{O}^\delta$ .

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

*Hypothesis 3.* 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:

$$(2.9) \quad A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix},$$

with  $A_{n_1}$  being a positive definite symmetric  $n_1 \times n_1$  tensor ( $n_1 \geq 1$ ) and where  $\Theta$  denotes appropriate zero mappings. Besides, there exists a strictly positive constant,  $\Lambda$ , which is a uniform lower bound for the eigenvalues of  $A_{n_1}$ .

*Hypothesis 4.* Function  $f$  is defined in  $\mathcal{T}^\delta$  and it is continuous with respect to the time variable, in space  $L^2$ .

*Hypothesis 5.* Function  $g$  is defined in  $\mathcal{T}_{\Gamma^R}^\delta$  and it is continuous with respect to the time variable, in space  $H^1$ . Besides, coefficient  $\alpha$  in boundary condition (2.6) is strictly positive.

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

$$(2.10) \quad B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix},$$

where  $I_{n_1}$  is the  $n_1 \times n_1$  identity tensor. Clearly, under Hypothesis 3 we have

$$(2.11) \quad \Lambda \|B\mathbf{w}\|_\Omega^2 \leq \langle A\mathbf{w}, \mathbf{w} \rangle_\Omega \quad \forall \mathbf{w} \in \mathbb{R}^d.$$

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

*Hypothesis 6.* The velocity field satisfies

$$(2.12) \quad (I - B)L(x, t)B = 0 \quad \forall (x, t) \in \mathcal{T}^\delta.$$

*Remark 2.1.* For any  $d \times d$  tensor  $E$  of the form given in (2.9) it is easy to check that

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

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

In [8] the following Lagrangian formulation of the initial-boundary value problem (SP) has been deduced:

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

$$(2.13) \quad \rho_m(p, t)\dot{\phi}_m(p, t) \det F(p, t) - \text{Div} \left[ \tilde{A}_m(p, t)\nabla\phi_m(p, t) \right] = f_m(p, t) \det F(p, t),$$

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

$$(2.14) \quad \phi_m(p, t) = \phi_D(X_e(p, t), t) \text{ on } \Gamma^D \times (0, T),$$

$$(2.15) \quad \alpha \tilde{m}(p, t)\phi_m(p, t) + \tilde{A}_m(p, t)\nabla\phi_m(p, t) \cdot \mathbf{m}(p) = \tilde{m}(p, t)g(X_e(p, t), t) \text{ on } \Gamma^R \times (0, T),$$

and the initial condition

$$(2.16) \quad \phi_m(p, 0) = \phi^0(p) \text{ in } \Omega,$$

where  $\tilde{A}_m$  and  $\tilde{m}$  are defined by:

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

$$\tilde{m}(p, t) := |F^{-T}(p, t)\mathbf{m}(p)| \det F(p, t) \quad \forall (p, t) \in \Gamma \times [0, T],$$

being  $\mathbf{m}$  the outward unit normal vector to  $\Gamma$ .

Moreover, the standard weak problem associated with this Lagrangian strong problem has been considered:

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

$$(2.17) \quad \int_{\Omega} \rho_m(p, t) \dot{\phi}_m(p, t) \psi(p) \det F(p, t) dp + \int_{\Omega} \tilde{A}_m(p, t) \nabla \phi_m(p, t) \cdot \nabla \psi(p) dp \\ + \alpha \int_{\Gamma^R} \tilde{m}(p, t) \phi_m(p, t) \psi(p) dA_p = \int_{\Omega} f_m(p, t) \psi(p) \det F(p, t) dp \\ + \int_{\Gamma^R} \tilde{m}(p, t) g_m(p, t) \psi(p) dA_p,$$

$\forall \psi \in H_{\Gamma^D}^1(\Omega)$  and  $t \in (0, T)$ .

**3. Space discretization. Finite element method.** In [8] a second order pure Lagrangian time semidiscretized scheme have been proposed and analyzed. Stability and error estimates has been obtained. We introduce the number of time steps,  $N$ , the time step  $\Delta t = T/N$ , and the mesh-points,  $t_n = n\Delta t$  for  $n = 0, 1/2, 1, \dots, N$ . In what follows we use the notations:  $\psi^n(y) := \psi(y, t_n)$ , for a function  $\psi(y, t)$ , and

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

for a sequence  $\widehat{\psi} = \{\psi^n\}_{n=0}^N$ . Let us define the following sequences of functions of  $p$

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

for  $0 \leq n \leq N$ .

We propose a space discretization of the time semidiscretized problem introduced in [8] by using finite elements spaces  $V_h^k$ , where  $h$  denotes the mesh-size and the positive integer  $k$  is the ‘‘approximation degree’’ in the following sense:

*Hypothesis 7.* There exists an interpolation operator  $\pi_h : C^0(\overline{\Omega}) \rightarrow V_h^k$  satisfying

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

for a positive constant  $Q$  independent of  $h$ .

In order to obtain fully discrete schemes of the time semidiscretized problem proposed in [8] (see §4 for more details), we use space  $V_h^k$  to approximate space  $H_{\Gamma^D}^1(\Omega)$ . Thus, we obtain the following fully discrete problem:

$$(3.1) \quad \left\{ \begin{array}{l} \text{Given } \phi_{m, \Delta t, h}^0 \in V_h^k, \text{ find } \widehat{\phi_{m, \Delta t, h}} = \{\phi_{m, \Delta t, h}^n\}_{n=1}^N \in [V_h^k]^N \text{ such that} \\ \langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\phi_{m, \Delta t, h}}], \psi_h \rangle = \langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \psi_h \rangle \quad \forall \psi_h \in V_h^k, \text{ for } n = 0, \dots, N-1. \end{array} \right.$$

Mappings  $\mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\phi] \in (H^1(\Omega))'$  and  $\mathcal{F}_{\Delta t}^{n+\frac{1}{2}} \in (H^1(\Omega))'$  are defined by

$$\left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\phi], \psi \right\rangle := \left\langle \frac{\rho \circ X_{RK}^{n+1} \det F_{RK}^{n+1} + \rho \circ X_{RK}^n \det F_{RK}^n}{2} \frac{\phi^{n+1} - \phi^n}{\Delta t}, \psi \right\rangle_{\Omega}$$

$$\begin{aligned}
& + \left\langle \frac{(\tilde{A}_{RK}^{n+1} + \tilde{A}_{RK}^n)}{2} \frac{(\nabla \phi^{n+1} + \nabla \phi^n)}{2}, \nabla \psi \right\rangle_{\Omega} \\
& + \alpha \left\langle \frac{(\tilde{m}_{RK}^{n+1} + \tilde{m}_{RK}^n)}{2} \frac{(\phi^{n+1} + \phi^n)}{2}, \psi \right\rangle_{\Gamma^R}, \\
\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}}, \psi \rangle & := \left\langle \frac{\det F_{RK}^{n+1} f^{n+1} \circ X_{RK}^{n+1} + \det F_{RK}^n f^n \circ X_{RK}^n}{2}, \psi \right\rangle_{\Omega} \\
& + \left\langle \frac{\tilde{m}_{RK}^{n+1} g^{n+1} \circ X_{RK}^{n+1} + \tilde{m}_{RK}^n g^n \circ X_{RK}^n}{2}, \psi \right\rangle_{\Gamma^R},
\end{aligned}$$

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

*Remark 3.1.* 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  $\phi$  at discrete time steps  $\{t_n\}_{n=0}^N$  are required. Thus, the above definitions can also be stated for a sequence of functions  $\widehat{\phi} = \{\phi^n\}_{n=0}^N \in [H^1(\Omega)]^{N+1}$ .

*Remark 3.2.* By using the same procedures as the ones employed in [8] to get stability results of the semidiscretized scheme we can obtain similar stability estimates for the fully discretized scheme, with  $H_{\Gamma^D}^1(\Omega)$  replaced with  $V_h^k$ . In particular, for incompressible flows we can get a stability inequality with constants independent of  $T$ .

**4. Error estimates for the fully discretized scheme.** The aim of the present section is to estimate the difference between the *discrete solution* of (3.1),  $\widehat{\phi}_{m,\Delta t,h} := \{\phi_{m,\Delta t,h}^n\}_{n=0}^N$ , and the exact solution of the continuous problem,  $\widehat{\phi}_m := \{\phi_m^n\}_{n=0}^N$ . For this, let us introduce the notations  $\widehat{e}_{m,\Delta t,h} := \widehat{\phi}_{m,\Delta t,h} - \widehat{\pi}_h \widehat{\phi}_m$ ,  $\vartheta_{m,h} := \phi_m - \pi_h \phi_m$ . Then,  $\widehat{\phi}_m - \widehat{\phi}_{m,\Delta t,h} = \widehat{\vartheta}_{m,h} - \widehat{e}_{m,\Delta t,h}$  and, since  $\widehat{\vartheta}_{m,h}$  can be estimated by Hypothesis 7, the problem is reduced to establish a bound for  $\widehat{e}_{m,\Delta t,h}$ . Notice that, according to (2.17), for  $t_{n+\frac{1}{2}}$  with  $0 \leq n \leq N-1$ ,  $\widehat{\phi}_m$  solves the problem

$$(4.1) \quad \left\langle \mathcal{L}^{n+\frac{1}{2}}[\widehat{\phi}_m], \psi \right\rangle = \left\langle \mathcal{F}^{n+\frac{1}{2}}, \psi \right\rangle \quad \forall \psi \in H_{\Gamma^D}^1(\Omega),$$

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

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

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

We notice that, as a consequence of Hypothesis 3, 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

$$(4.2) \quad C = \begin{pmatrix} C_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}.$$

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

$$(4.3) \quad c_A = \max\{\|G\|_{\infty, \mathcal{O}^\delta}^2, \|C\|_{\infty, \mathcal{O}^\delta}^2\},$$



and the sequences of tensor fields

$$\tilde{C}_{RK}^n := C \circ X_{RK}^n (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n}, \quad \tilde{B}_{RK}^n := B(F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n},$$

for  $0 \leq n \leq N$ , where tensor  $B$  has been defined in (2.10).

In what follows,  $c_v$  denotes the positive constant  $c_v := \max_{t \in [0, T]} \|\mathbf{v}(\cdot, t)\|_{1, \infty, \Omega_t^\delta}$ . 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 problem data), not necessarily the same at each occurrence.

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

*Hypothesis 8. Functions appearing in problem (2.4)-(2.7) satisfy:*

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

*Hypothesis 9. Functions appearing in problem (2.4)-(2.7) satisfy:*

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

LEMMA 4.1. *Assume Hypotheses 1, 2, 3, 7. Let  $\phi_m \in C^1(C^0(\overline{\Omega})) \cap C^0(H^{k+1}(\Omega)) \cap H^1(H^k(\Omega))$  be the solution of (4.1) and  $\widehat{\phi_{m, \Delta t, h}}$  be the solution of (3.1). Then there exist a positive constant  $c(\mathbf{v}, T, \delta)$  such that, for  $\Delta t < c$ , the following inequality holds:*

$$(4.4) \quad \left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\vartheta_{m, h}}], e_{m, \Delta t, h}^{n+1} + e_{m, \Delta t, h}^n \right\rangle \\ \leq \frac{1}{8} \left\| \tilde{C}_{RK}^{n+1} \left( \nabla e_{m, \Delta t, h}^{n+1} + \nabla e_{m, \Delta t, h}^n \right) \right\|_{\Omega}^2 \\ + \frac{1}{8} \left\| \tilde{C}_{RK}^n \left( \nabla e_{m, \Delta t, h}^{n+1} + \nabla e_{m, \Delta t, h}^n \right) \right\|_{\Omega}^2 \\ + \frac{\alpha}{16} \left\| \sqrt{\tilde{m}_{RK}^{n+1} + \tilde{m}_{RK}^n} \left\{ e_{m, \Delta t, h}^{n+1} + e_{m, \Delta t, h}^n \right\} \right\|_{\Gamma^R}^2 \\ + \gamma \left\| \sqrt{\det F_{RK}^{n+1}} e_{m, \Delta t, h}^{n+1} \right\|_{\Omega}^2 + \gamma \left\| \sqrt{\det F_{RK}^n} e_{m, \Delta t, h}^n \right\|_{\Omega}^2 \\ + \tilde{c} Q^2 h^{2k} \left( \frac{1}{\Delta t} \left\| \dot{\phi}_m \right\|_{L^2((t_n, t_{n+1}), H^k(\Omega))}^2 + \left\| \phi_m^{n+1} \right\|_{k+1, 2, \Omega}^2 + \left\| \phi_m^n \right\|_{k+1, 2, \Omega}^2 \right),$$

being  $\tilde{c}$  a positive constant,  $n \in \{0, \dots, N-1\}$  and where  $\alpha > 0$  is the constant appearing in the Robin boundary condition (2.6).

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

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

For  $I_1^n$ , applying Cauchy-Schwarz inequality, Young's inequality and Corollary A.4 in [8], we first have

$$(4.5) \quad I_1^n \leq \tilde{c} \left\| \frac{\vartheta_{m,h}^{n+1} - \vartheta_{m,h}^n}{\Delta t} \right\|_{\Omega}^2 + \gamma \left\| \sqrt{\det F_{RK}^{n+1}} e_{m,\Delta t,h}^{n+1} \right\|_{\Omega}^2 + \gamma \left\| \sqrt{\det F_{RK}^n} e_{m,\Delta t,h}^n \right\|_{\Omega}^2,$$

where we have assumed that  $\Delta t < K$ , being  $K$  the constant appearing in Corollary A.4 in [8]. Here  $\tilde{c}$  is a positive constant depending on  $\mathbf{v}$ ,  $T$  and  $\rho_{1,\infty}/\gamma$ . Moreover, from Barrow's rule and by applying Cauchy-Schwarz inequality, we deduce

$$(4.6) \quad \begin{aligned} \left\| \frac{\vartheta_{m,h}^{n+1} - \vartheta_{m,h}^n}{\Delta t} \right\|_{\Omega}^2 &\leq \frac{1}{\Delta t} \int_{\Omega} \int_{t_n}^{t_{n+1}} \left( \dot{\vartheta}_{m,h}(p, s) \right)^2 ds dp \\ &= \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \int_{\Omega} \left( \dot{\vartheta}_{m,h}(p, s) \right)^2 dp ds = \frac{1}{\Delta t} \left\| \dot{\vartheta}_{m,h} \right\|_{L^2((t_n, t_{n+1}), L^2(\Omega))}^2. \end{aligned}$$

Finally, by using Hypothesis 7 for  $s = 0$  and  $r = k$  we obtain

$$(4.7) \quad \begin{aligned} I_1^n &\leq \frac{\tilde{c}Q^2 h^{2k}}{\Delta t} \left\| \dot{\phi}_m \right\|_{L^2((t_n, t_{n+1}), H^k(\Omega))}^2 + \gamma \left\| \sqrt{\det F_{RK}^{n+1}} e_{m,\Delta t,h}^{n+1} \right\|_{\Omega}^2 \\ &\quad + \gamma \left\| \sqrt{\det F_{RK}^n} e_{m,\Delta t,h}^n \right\|_{\Omega}^2. \end{aligned}$$

For  $I_2^n$ , we apply Cauchy-Schwarz inequality and Young's inequality, obtaining

$$(4.8) \quad \begin{aligned} I_2^n &\leq \tilde{c}Q^2 h^{2k} \left( \|\phi_m^{n+1}\|_{k+1,2,\Omega}^2 + \|\phi_m^n\|_{k+1,2,\Omega}^2 \right) \\ &\quad + \frac{1}{8} \left\| \tilde{C}_{RK}^{n+1} \left( \nabla e_{m,\Delta t,h}^{n+1} + \nabla e_{m,\Delta t,h}^n \right) \right\|_{\Omega}^2 + \frac{1}{8} \left\| \tilde{C}_{RK}^n \left( \nabla e_{m,\Delta t,h}^{n+1} + \nabla e_{m,\Delta t,h}^n \right) \right\|_{\Omega}^2, \end{aligned}$$

where we have used inequalities (A.2) and (A.4) from [8] and Hypothesis 7 for  $s = 1$  and  $r = k+1$ . Here  $\tilde{c}$  is a positive constant depending on  $\mathbf{v}$ ,  $T$  and  $c_A$  and is bounded in the hyperbolic limit. For  $I_3^n$  we apply Cauchy-Schwarz inequality, Young's inequality, inequalities (A.2) and (A.4) from [8] and Hypothesis 7 for  $s = 1$  and  $r = k+1$ , getting

$$(4.9) \quad \begin{aligned} I_3^n &\leq \tilde{c}Q^2 h^{2k} \left( \|\phi_m^{n+1}\|_{k+1,2,\Omega}^2 + \|\phi_m^n\|_{k+1,2,\Omega}^2 \right) \\ &\quad + \frac{\alpha}{16} \left\| \sqrt{\tilde{m}_{RK}^{n+1} + \tilde{m}_{RK}^n} \left\{ e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n \right\} \right\|_{\Gamma^R}^2, \end{aligned}$$

where we have used the continuity of the trace mapping, i.e., there exist a positive constant  $c_{\Omega}$  such that  $\|\vartheta_{m,h}^l\|_{\Gamma^R}^2 \leq c_{\Omega} \|\vartheta_{m,h}^l\|_{1,2,\Omega}^2$ , for  $l = n, n+1$ . Finally, summing up (4.7), (4.8) and (4.9) we get inequality (4.4).  $\square$

**THEOREM 4.2.** *Let us assume Hypotheses 1, 2, 3, 4, 5, 8 and 7, and  $X_e \in \mathbf{C}^5(\bar{\Omega} \times [0, T])$ . Let*

$$(4.10) \quad \begin{aligned} \phi_m &\in C^3(L^2(\Omega)) \cap C^1(C^0(\bar{\Omega})) \cap C^0(H^{k+1}(\Omega)) \cap H^1(H^k(\Omega)), \\ \nabla \phi_m &\in C^2(\mathbf{H}^1(\Omega)), \quad \phi_m|_{\Gamma^R} \in C^2(L^2(\Gamma^R)), \end{aligned}$$

be the solution of (4.1) and let  $\widehat{\phi_{m,\Delta t,h}}$  be the solution of (3.1) subject to the initial value  $\phi_{m,\Delta t,h}^0 = \pi_h \phi_m^0$ . Then, there exist two positive constants  $J$  and  $D$ , being the

latter independent of the diffusion tensor, such that, if  $\Delta t < D$  we have

$$\begin{aligned}
& \sqrt{\frac{\gamma}{2}} \left\| \sqrt{\widehat{\det F_{RK}}} (\phi_m - \phi_{m,\Delta t,h}) \right\|_{L^\infty(L^2(\Omega))} \\
& + \sqrt{\frac{\Lambda}{8}} \left\| \widetilde{B}_{RK} \mathcal{S} [\widehat{\nabla \phi_m - \nabla \phi_{m,\Delta t,h}}] \right\|_{L^2(\mathbf{L}^2(\Omega))} \\
(4.11) \quad & + \sqrt{\frac{\alpha}{8}} \left\| \sqrt{\mathcal{S}[\widetilde{m}_{RK}]} \widehat{\mathcal{S}} [\phi_m - \phi_{m,\Delta t,h}] \right\|_{L^2(L^2(\Gamma^R))} \leq J \Delta t^2 (\|\phi_m\|_{C^3(L^2(\Omega))}) \\
& + \|\nabla \phi_m\|_{C^2(\mathbf{H}^1(\Omega))} + \|\nabla \phi_m \cdot \mathbf{m}\|_{C^2(L^2(\Gamma^R))} + \|\phi_m\|_{C^2(L^2(\Gamma^R))} \\
& + \|\det F f_m\|_{C^2(L^2(\Omega))} + \|f\|_{C^1(\mathcal{T}^\delta)} + \|\widetilde{m} g_m\|_{C^2(L^2(\Gamma^R))} + \|g\|_{C^1(\mathcal{T}_{\Gamma^R}^\delta)} \\
& + J h^k \left( \left\| \dot{\phi}_m \right\|_{L^2(H^k(\Omega))} + \|\phi_m\|_{C^0(H^{k+1}(\Omega))} \right).
\end{aligned}$$

*Proof.* First, recall that  $\widehat{e_{m,\Delta t,h}} = \widehat{\vartheta_{m,h}} - \widehat{\phi_m} + \widehat{\phi_{m,\Delta t,h}} \in [V_h^k]^{N+1}$ . Then, by using (4.1) and (3.1) we have

$$\begin{aligned}
& \left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}} [\widehat{e_{m,\Delta t,h}}], e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n \right\rangle = \left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}} [\widehat{\vartheta_{m,h}}], e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n \right\rangle \\
& + \left\langle \left( \mathcal{L}^{n+\frac{1}{2}} - \mathcal{L}_{\Delta t}^{n+\frac{1}{2}} \right) [\widehat{\phi_m}], e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n \right\rangle + \left\langle \mathcal{F}_{\Delta t}^{n+\frac{1}{2}} - \mathcal{F}^{n+\frac{1}{2}}, e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n \right\rangle,
\end{aligned} \tag{4.12}$$

for  $n \in \{0, \dots, N-1\}$ . A lower bound for (4.12) is given by Lemma 4.1 in [8]. Moreover, by applying Lemmas 4.6, 4.7 and A.8 in [8], we have an upper bound for (4.12). By jointly considering these lower and upper bounds of (4.12) and inequality (4.4) we deduce

$$\begin{aligned}
& \frac{1}{\Delta t} \left\| \sqrt{\rho \circ X_{RK}^{n+1} \det F_{RK}^{n+1}} e_{m,\Delta t,h}^{n+1} \right\|_{\Omega}^2 - \frac{1}{\Delta t} \left\| \sqrt{\rho \circ X_{RK}^n \det F_{RK}^n} e_{m,\Delta t,h}^n \right\|_{\Omega}^2 \\
& + \frac{1}{8} \left\| \widetilde{C}_{RK}^{n+1} (\nabla e_{m,\Delta t,h}^{n+1} + \nabla e_{m,\Delta t,h}^n) \right\|_{\Omega}^2 + \frac{1}{8} \left\| \widetilde{C}_{RK}^n (\nabla e_{m,\Delta t,h}^{n+1} + \nabla e_{m,\Delta t,h}^n) \right\|_{\Omega}^2 \\
& + \frac{\alpha}{8} \left\| \sqrt{\widetilde{m}_{RK}^{n+1} + \widetilde{m}_{RK}^n} (e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n) \right\|_{\Gamma^R}^2 \\
(4.13) \quad & \leq c_s \left( \left\| \xi_{\mathcal{L}\Omega}^{n+\frac{1}{2}} \right\|_{\Omega}^2 + \left\| \xi_f^{n+\frac{1}{2}} \right\|_{\Omega}^2 \right) + \frac{4c_g}{\alpha} \left( \left\| \xi_{\mathcal{L}\Gamma}^{n+\frac{1}{2}} \right\|_{\Gamma^R}^2 + \left\| \xi_g^{n+\frac{1}{2}} \right\|_{\Gamma^R}^2 \right) \\
& + 3\widehat{c}\gamma \left( \left\| \sqrt{\det F_{RK}^{n+1}} e_{m,\Delta t,h}^{n+1} \right\|_{\Omega}^2 + \left\| \sqrt{\det F_{RK}^n} e_{m,\Delta t,h}^n \right\|_{\Omega}^2 \right) \\
& + \widetilde{c}Q^2 h^{2k} \left( \frac{1}{\Delta t} \left\| \dot{\phi}_m \right\|_{L^2((t_n, t_{n+1}), H^k(\Omega))}^2 + \|\phi_m^{n+1}\|_{k+1,2,\Omega}^2 + \|\phi_m^n\|_{k+1,2,\Omega}^2 \right),
\end{aligned}$$

where  $\widehat{c} = \max\{1, 1/\gamma, \rho_{1,\infty}(c_v + C_v \Delta t)/\gamma\}$ ,  $\widetilde{c}$  is a positive constant and  $c_s$  and  $c_g$  are the positive constants appearing in Lemma A.8 from [8]. For  $n = 0, \dots, N$ , let us introduce the notations

$$\begin{aligned}
\theta_n^1 & := \gamma \left\| \sqrt{\det F_{RK}^n} e_{m,\Delta t,h}^n \right\|_{\Omega}^2 \\
\theta_n^2 & := \frac{\Lambda}{8} \sum_{s=0}^{n-1} \Delta t \left\| \widetilde{B}_{RK}^s (\nabla e_{m,\Delta t,h}^{s+1} + \nabla e_{m,\Delta t,h}^s) \right\|_{\Omega}^2,
\end{aligned}$$

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

Now, for fixed  $q$ ,  $1 \leq q \leq N$ , let us sum (4.13) multiplied by  $\Delta t$  from  $n = 0$  to  $n = q - 1$ . We have,

$$(4.14) \quad (1 - 3\widehat{c}\Delta t)\theta_q^1 + \theta_q^2 + \bar{\theta}_q \leq 6\widehat{c}\Delta t \sum_{n=0}^{q-1} \theta_n^1 + \frac{\rho_{1,\infty}}{\gamma} \theta_0^1 \\ + c_s \Delta t \sum_{n=1}^q \left( \left\| \xi_{\mathcal{L}\Omega}^{n-\frac{1}{2}} \right\|_{\Omega}^2 + \left\| \xi_f^{n-\frac{1}{2}} \right\|_{\Omega}^2 \right) + \frac{4c_g \Delta t}{\alpha} \sum_{n=1}^q \left( \left\| \xi_{\mathcal{L}\Gamma}^{n-\frac{1}{2}} \right\|_{\Gamma^R}^2 + \left\| \xi_g^{n-\frac{1}{2}} \right\|_{\Gamma^R}^2 \right) \\ + \widetilde{c}Q^2 h^{2k} \sum_{n=0}^{q-1} \left( \left\| \dot{\phi}_m \right\|_{L^2((t_n, t_{n+1}), H^k(\Omega))}^2 + \Delta t \left( \left\| \phi_m^{n+1} \right\|_{k+1,2,\Omega}^2 + \left\| \phi_m^n \right\|_{k+1,2,\Omega}^2 \right) \right),$$

by using Hypotheses 2 and 3. Some of the terms on the right hand side of (4.14) can also be bounded. More precisely, by using Lemmas 4.6 and 4.7 in [8] we get

$$(1 - 3\widehat{c}\Delta t)\theta_q^1 + \theta_q^2 + \bar{\theta}_q \leq 6\widehat{c}\Delta t \sum_{n=0}^{q-1} \theta_n^1 + \widetilde{c} \left( \theta_0^1 + \widetilde{C} \right)$$

where  $\widetilde{C}$  contains the constant terms multiplied by  $h^{2k}$  and  $\Delta t^4$ . For  $\Delta t$  small enough, we can apply the discrete Gronwall inequality (see, for instance, [30]) and take the maximum in  $q \in \{1, \dots, N\}$ . Then, noting that  $e_{m,\Delta t,h}^0 = 0$ ,  $\widehat{\phi}_m - \widehat{\phi_{m,\Delta t,h}} = \widehat{\vartheta_{m,h}} - \widehat{e_{m,\Delta t,h}}$ , using Hypothesis 7, and bounds A.2 and A.4 from [8] the result follows.  $\square$

*Remark 4.1.* Notice that constant  $J$  appearing in the previous theorem is bounded in the limit when the diffusion tensor vanishes. In particular, Theorem 4.2 is also valid when  $A \equiv 0$ .

*Remark 4.2.* In the particular case of pure convection problems, that is  $A \equiv 0$ , and assuming Dirichlet boundary conditions ( $\Gamma^D \equiv \Gamma$ ), an error estimate of the form  $O(h^{k+1}) + O(\Delta t^2)$  in the  $l^\infty(L^2(\Omega))$ -norm can be obtained by using analogous procedures to the ones in the previous theorem.

*Remark 4.3.* Notice that in the previous theorem, an error estimate of order  $O(\Delta t^2) + O(h^k)$  for the semi-sum of the gradient in  $l^2(\mathbf{L}^2(\Omega))$  norm is obtained. Assuming additional regularity this estimate can be improved. Specifically, in the following theorem we state an error estimate of order  $O(\Delta t^2) + O(h^k)$  for the gradient in  $l^\infty(\mathbf{L}^2(\Omega))$  norm. Furthermore, an error estimate of order  $O(\Delta t^2) + O(h^k)$  for the time derivative is established.

**THEOREM 4.3.** *Let us assume Hypotheses 1, 2, 3, 6, 4, 5, 9 and 7, and  $X_e \in \mathbf{C}^5(\overline{\Omega} \times [0, T])$ . Let*

$$(4.15) \quad \phi_m \in C^3(L^2(\Omega)) \cap C^1(C^1(\overline{\Omega})) \cap C^0(H^{k+1}(\Omega)) \cap H^1(H^{k+1}(\Omega)) \text{ with} \\ \nabla \phi_m \in C^3(\mathbf{H}^1(\Omega)) \text{ and } \phi_m|_{\Gamma^R} \in C^3(L^2(\Gamma^R)),$$

be the solution of (4.1) and  $\widehat{\phi_{m,\Delta t,h}}$  the solution of (3.1) subject to the initial value  $\phi_{m,\Delta t,h}^0 = \pi_h \phi_m^0$ . Then, there exist two positive constants  $J$  and  $D$  such that, if

$\Delta t < D$ , we have

$$\begin{aligned}
& \sqrt{\frac{\gamma}{8}} \left\| \sqrt{\mathcal{S}[\det F_{RK}] \widehat{\mathcal{R}}_{\Delta t}[\phi_m - \phi_{m,\Delta t,h}]} \right\|_{L^2(L^2(\Omega))} \\
& + \sqrt{\frac{\Lambda}{4}} \left\| \widetilde{B}_{RK}(\nabla \widehat{\phi_m} - \nabla \phi_{m,\Delta t,h}) \right\|_{L^\infty(L^2(\Omega))} \\
(4.16) \quad & + \sqrt{\frac{\alpha}{4}} \left\| \sqrt{\widetilde{m}_{RK}}(\widehat{\phi_m} - \phi_{m,\Delta t,h}) \right\|_{L^\infty(L^2(\Gamma^R))} \leq J \Delta t^2 (\|\phi_m\|_{C^3(L^2(\Omega))}) \\
& + \|\nabla \phi_m\|_{C^2(\mathbf{H}^1(\Omega))} + \|\nabla \phi_m \cdot \mathbf{m}\|_{C^3(L^2(\Gamma^R))} + \|\phi_m\|_{C^3(L^2(\Gamma^R))} \\
& + \|\det F f_m\|_{C^2(L^2(\Omega))} + \|f\|_{C^1(\mathcal{T}^\delta)} + \|\widetilde{m} g_m\|_{C^3(L^2(\Gamma^R))} + \|g\|_{C^2(\mathcal{T}_{\Gamma^R}^\delta)} \\
& + J h^k \left( \|\dot{\phi}_m\|_{L^2(H^{k+1}(\Omega))} + \|\phi_m\|_{C^0(H^{k+1}(\Omega))} \right).
\end{aligned}$$

*Proof.* This result can be proved by using similar procedures to the ones of the previous theorem but applying (4.1) and (3.1) for  $e_{m,\Delta t,h}^{n+1} - e_{m,\Delta t,h}^n$  instead of  $e_{m,\Delta t,h}^{n+1} + e_{m,\Delta t,h}^n$ , Lemmas 4.2, A.9, A.10 from [8] instead of Lemmas 4.1, A.8 from [8], and the following bound instead of (4.4) (see [6] for further details):

$$\begin{aligned}
& \sum_{n=0}^{q-1} \left\langle \mathcal{L}_{\Delta t}^{n+\frac{1}{2}}[\widehat{\vartheta}_{m,h}], e_{m,\Delta t,h}^{n+1} - e_{m,\Delta t,h}^n \right\rangle \\
& \leq \frac{1}{4\Delta t} \sum_{n=0}^{q-1} \left\| \sqrt{\rho \circ X_{RK}^{n+1} \det F_{RK}^{n+1} + \rho \circ X_{RK}^n \det F_{RK}^n} (e_{m,\Delta t,h}^{n+1} - e_{m,\Delta t,h}^n) \right\|_{\Omega}^2 \\
& + \frac{\Lambda}{4} \left\| \widetilde{B}_{RK}^q \nabla e_{m,h}^q \right\|_{\Omega}^2 + \frac{\alpha}{8} \left\| \sqrt{\widetilde{m}_{RK}^q} e_{m,\Delta t,h}^q \right\|_{\Gamma^R}^2 \\
(4.17) \quad & + \widehat{c} \Delta t \Lambda \sum_{n=1}^{q-1} \left\| \widetilde{B}_{RK}^n \nabla e_{m,\Delta t,h}^n \right\|_{\Omega}^2 + \widehat{c} \alpha \Delta t \sum_{n=1}^{q-1} \left\| \sqrt{\widetilde{m}_{RK}^n} e_{m,\Delta t,h}^n \right\|_{\Gamma^R}^2 \\
& - \frac{1}{4} \left\langle (\widetilde{A}_{RK}^1 + A) (\nabla \vartheta_{m,h}^1 + \nabla \vartheta_{m,h}^0), \nabla e_{m,\Delta t,h}^0 \right\rangle_{\Omega} \\
& - \frac{\alpha}{4} \left\langle (\widetilde{m}_{RK}^1 + 1) (\vartheta_{m,h}^1 + \vartheta_{m,h}^0), e_{m,\Delta t,h}^0 \right\rangle_{\Gamma^R} \\
& + \widetilde{c} Q^2 h^{2k} \left( \|\dot{\phi}_m\|_{L^2(H^{k+1}(\Omega))}^2 + \|\phi_m\|_{C^0(H^{k+1}(\Omega))}^2 \right),
\end{aligned}$$

where  $\widehat{c} = \max\{C_v c_A / \Lambda, C_v\}$ ,  $\Delta t < c(\mathbf{v}, T, \delta)$ ,  $\widetilde{c}$  is a positive constant,  $\alpha > 0$  is the constant appearing in the Robin boundary condition (2.6) and  $q \in \{1, \dots, N\}$ .  $\square$

*Remark 4.4.* 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  $\epsilon \rightarrow 0$ .

### Approximate solution in Eulerian coordinates

In order to obtain an approximate solution of  $\phi^n$  in Eulerian coordinates, we are going to calculate the spatial description of material field  $\phi_{m,\Delta t,h}^n$ . To do this, we distinguish two cases:

- $X_e$  known. In this case, we calculate  $\widehat{\phi}_{\Delta t,h} \sim \widehat{\phi}$  as follows

$$(4.18) \quad \phi_{\Delta t,h}^n(x) := \phi_{m,\Delta t,h}^n(P(x, t_n)) \quad \forall x \in \overline{\Omega}_{t_n}, \quad 0 \leq n \leq N,$$

where  $P$  is the *reference map* of motion  $X_e$  (see [8] for more details).

- $X_e$  unknown. In this case, we use accurate enough approximations of  $P$  preserving the error order of the method. More precisely, we use the second order Runge-Kutta method considered to approximate the characteristics curves. Then, we calculate  $\widehat{\phi}_{\Delta t, h}$  as follows

$$(4.19) \quad \phi_{\Delta t, h}^n(x) := \phi_{m, \Delta t, h}^n(P_{RK}^n(x)) \quad \forall x \in \overline{\Omega}_{t_n}, \quad 0 \leq n \leq N.$$

being  $P_{RK}^n$  the second order Runge-Kutta approximation of  $P^n$ . Notice that, for a general velocity field, point  $P_{RK}^n(x)$  can go out of the computational domain. In this case, we approximate  $\phi_{\Delta t, h}^n(P_{RK}^n(x))$  by

$$(4.20) \quad \phi_{\Delta t, h}^n(P_{RK}^n(x)) \simeq \phi_{m, \Delta t, h}^n(x_f),$$

being  $x_f$  the nearest point on the boundary to  $P_{RK}^n(x)$ . Notice that, if the velocity vanishes on the boundary of  $\Omega$  and  $\Delta t$  is small enough, then  $P_{RK}^n(\overline{\Omega}) = \overline{\Omega}$  (see Lemma A.7 in [8]). In Example 2 below  $\mathbf{v}$  satisfies this property.

*Remark 4.5.* Notice that, from the estimates obtained in Lagrangian coordinates and by using appropriate changes of variable, we can deduce analogous estimates in Eulerian coordinates (see [6] for further details).

**5. Numerical results.** In order to assess the performance of the above numerical method and to check the convergence behavior predicted by the above theory, we solve two test problems in two space dimensions. The first one is the *rotating Gaussian hill*, for which we verify rates of convergence for the second order pure Lagrangian method described in the present paper and the analogous one of first order in time. The second example has a solution developing a steep layer and a velocity field which is not divergence-free. For this problem, we compare the numerical results obtained from the pure Lagrangian method proposed in this paper, with the analogous one of first order in time and with semi-Lagrangian methods. In Example 1, we calculate the error between discrete solution  $\phi_{h, \Delta t}$ , given in (4.18), and exact solution  $\phi$ . For this, we approximate the theoretical  $H^1(\Omega_{t_n})$  and  $L^2(\Omega_{t_n})$  norms by using a quadrature formula exact for polynomials of degree 5. The functional spaces endowed with these norms are denoted by  $H_h^1(\Omega_{t_n})$  and  $L_h^2(\Omega_{t_n})$ , respectively. Thus, we denote by  $l^\infty(\mathcal{A})$ , being  $\mathcal{A} = H_h^1(\Omega_{t_n}), L_h^2(\Omega_{t_n})$ , and  $l^2(L_h^2(\Omega))$  the spaces equipped with the norms

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

Firstly, we show numerical results for the problem of the rotating Gaussian hill and then for the problem including a steep layer.

### Example 1

This is a convection-diffusion problem (see, for instance [31] and [13]), aiming to check the properties of the numerical solution obtained with the scheme analyzed in this paper. We also make comparisons with some variations of it by changing the time discretization and the method to compute the characteristics. We also compare our method with the standard first order characteristics one combined with piecewise linear finite elements.

The spatial domain is  $\Omega = (-1, 1) \times (-1, 1)$  and  $T = 2\pi$ . The diffusion tensor is  $A = aI$  with  $a$  given below. Moreover,  $\mathbf{v} = (-x_2, x_1)$ ,  $\rho = 1$  and the right-hand side  $f = 0$ . We also impose appropriate Dirichlet boundary and initial conditions such that the solution of the problem is

$$(5.1) \quad \phi(x_1, x_2, t) = \frac{b}{b + 4at} \exp \left\{ -\frac{(\bar{x}(t) - x_c)^2 + (\bar{y}(t) - y_c)^2}{b + 4at} \right\}$$

where

$$\begin{aligned} \bar{x} &= x_1 \cos t + x_2 \sin t, \quad \bar{y} = -x_1 \sin t + x_2 \cos t, \\ (x_c, y_c) &= (0.25, 0), \quad a = 0.001, \quad b = 0.01. \end{aligned}$$

We solve this problem by using several pure Lagrangian methods. More precisely, let us denote by  $(\mathcal{LG})_1$  the method which arises from the Lagrangian weak problem (2.17), by approximating the material derivative at  $t = t_{n+1}$  by a first order backward formula and the characteristics by a first order Euler formula (see [8] for more details), combined with continuous piecewise-quadratic finite elements for space discretization. Similarly, we denote by  $(\mathcal{LG})_3$  the method which arises from replacing in (3.1) the second order Runge-Kutta approximation of  $X_e$  by a third order Runge-Kutta approximation. Finally, we denote by  $(\mathcal{LG})_2$  the second order scheme given by (3.1). We have also chosen for space discretization of problems  $(\mathcal{LG})_2$  and  $(\mathcal{LG})_3$  piecewise quadratic finite elements, that is  $k = 2$ . Moreover, we have solved the pure convection problem (i.e.  $a = 0$ ) with the  $(\mathcal{LG})_2$  scheme. All these methods were combined with an exact quadrature formula for polynomials of degree 2 in all the terms. It is well-known (see, for instance, [25], [33], [29], [35], [13], [7]) that the numerical quadrature may add terms to the final error of the form  $O(h^\alpha/\Delta t)$  and, in some cases, it produces the loss of unconditional stability. We do not address this issue in the present paper. Anyway, for this particular example, neither these errors nor an unstable behaviour are observed (see Figure 5.1). Moreover, it is easy to prove the following properties:

$$\det F_{RK}^n - \det F^n = O(\Delta t^3), \quad \tilde{A}_{RK}^n - \tilde{A}_m^n = O(\Delta t^3).$$

Therefore, for this example, the error estimates for  $(\mathcal{LG})_2$  scheme are of the form  $O(\Delta t^3) + O(\Delta t^2) + O(h^2)$ . This fact can be observed in the Figures below. In

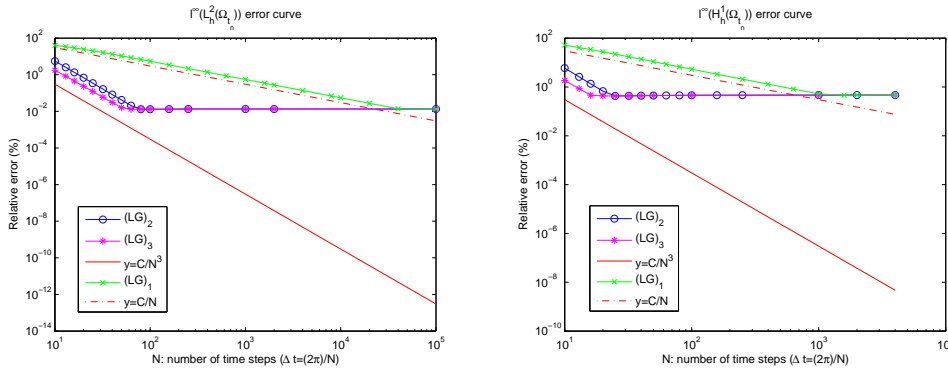


FIG. 5.1. Example 1: computed  $l^\infty(L_h^2(\Omega_{t_n}))$  (left) and  $l^\infty(H_h^1(\Omega_{t_n}))$  (right) errors, in log-log scale, for  $a = 0.001$  versus the number of time steps, for a fixed spatial mesh of  $133 \times 133$  vertices.

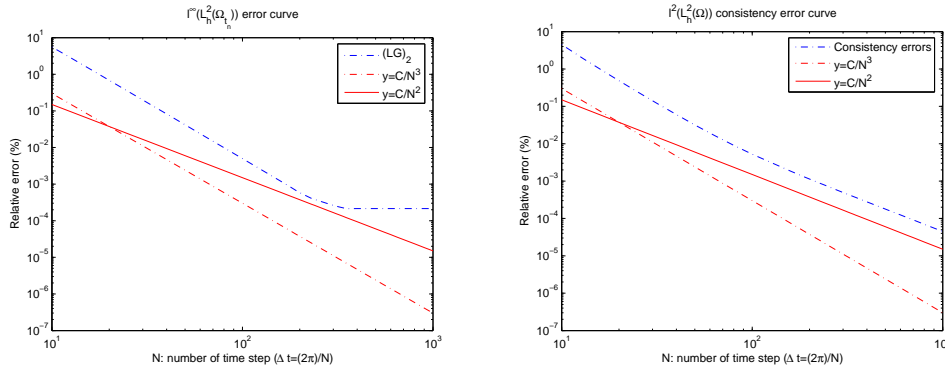


FIG. 5.2. *Example 1: computed  $l^\infty(L_h^2(\Omega_{t_n}))$  errors (left) and  $l^2(L_h^2(\Omega))$  consistency errors (right), in log-log scale, for  $a = 0.001$  versus the number of time steps, for a fixed spatial mesh of  $521 \times 521$  vertices.*

Figure 5.1 we have fixed a uniform spatial mesh of  $133 \times 133$  vertices and shown the  $l^\infty(L_h^2(\Omega_{t_n}))$  and  $l^\infty(H_h^1(\Omega_{t_n}))$  errors versus the number of time steps. Apparently, these results show that schemes  $(\mathcal{LG})_2$  and  $(\mathcal{LG})_3$  possess third-order accuracy in time. However, this behaviour is due to the fact that for “large” time steps the

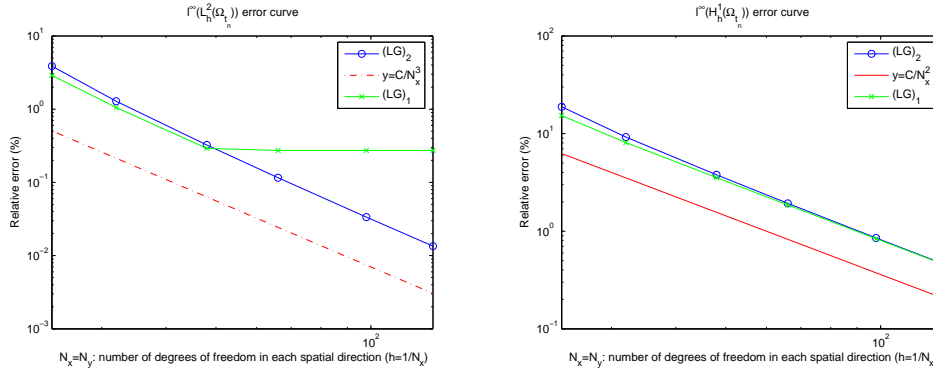


FIG. 5.3. *Example 1: computed  $l^\infty(L_h^2(\Omega_{t_n}))$  (left) and  $l^\infty(H_h^1(\Omega_{t_n}))$  (right) errors, in log-log scale, for  $a = 0.001$  versus  $1/h$ , for  $\Delta t = 2\pi/2000$ .*

$O(\Delta t^3)$  term dominates. This claim has been checked by plotting the errors using a finer mesh with  $521 \times 521$  vertices (Fig. 5.2, left) and also by showing the  $l^2(L_h^2(\Omega))$  consistency errors versus the number of time steps (Fig. 5.2, right). We can observe that for large time steps the term  $O(\Delta t^3)$  dominates. Next, the  $O(\Delta t^2)$  error term is the highest one and finally the spatial error dominates in the interval where the curves are horizontal. In fact, in all the above figures we can observe, for fixed  $h$ , that the error curves become horizontal as the time step decreases below a threshold; this is because the spatial  $O(h^2)$  term dominates the global error. In Figure 5.3 we represent, the computed  $l^\infty(L_h^2(\Omega_{t_n}))$  and  $l^\infty(H_h^1(\Omega_{t_n}))$  errors versus  $1/h$  for a fixed small time step, namely  $\Delta t = 2\pi/2000$ . We can observe that, as predicted by Theorems 4.2 and 4.3, the  $(\mathcal{LG})_2$  scheme possesses second-order accuracy in space in the  $l^\infty(H_h^1(\Omega_{t_n}))$ -norm. Moreover, third-order accuracy in space in the  $l^\infty(L_h^2(\Omega_{t_n}))$ -norm is observed. In Figure 5.4 we represent the errors, obtained with the  $(\mathcal{LG})_2$  scheme for the pure



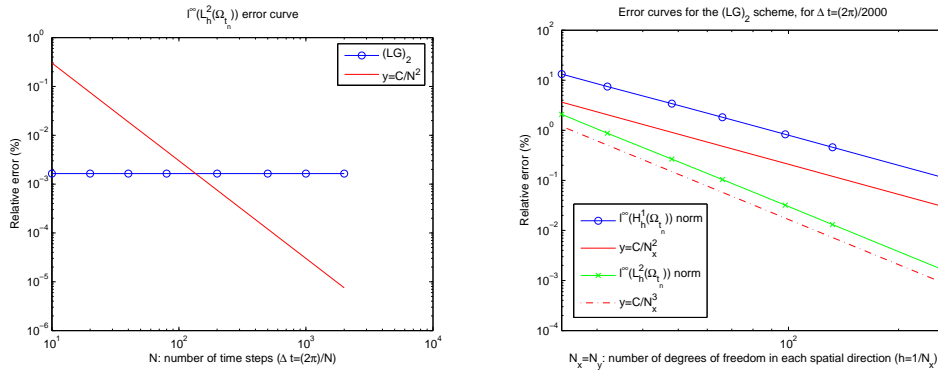


FIG. 5.4. *Example 1: computed errors for the  $(\mathcal{LG})_2$  scheme, in log-log scale, for  $a = 0$ . On the left, the  $l^\infty(L_h^2(\Omega_{t_n}))$  error versus the number of time steps, for a fixed spatial mesh of  $265 \times 265$  vertices. On the right, the  $l^\infty(L_h^2(\Omega_{t_n}))$  and  $l^\infty(H_h^1(\Omega_{t_n}))$  errors versus  $1/h$ , for  $\Delta t = 2\pi/2000$ .*

convection problem ( $a = 0$ ). On the left, we fix a uniform spatial mesh of  $265 \times 265$  vertices, and show the  $l^\infty(L_h^2(\Omega_{t_n}))$  errors versus the number of time steps. On the right, we represent the computed  $l^\infty(L_h^2(\Omega_{t_n}))$  and  $l^\infty(H_h^1(\Omega_{t_n}))$  errors versus  $1/h$  for fixed small time step  $\Delta t = 2\pi/2000$ . Notice that, for the pure convection problem, the spatial error is dominant in the total error. These results show that, as predicted in Remark 4.2, the  $(\mathcal{LG})_2$  scheme possesses third-order accuracy in space, in the  $l^\infty(L_h^2(\Omega_{t_n}))$ -norm. Moreover, it is remarkable that even for the pure convection problem, second-order accuracy in space is observed in the  $l^\infty(H_h^1(\Omega_{t_n}))$ -norm. In

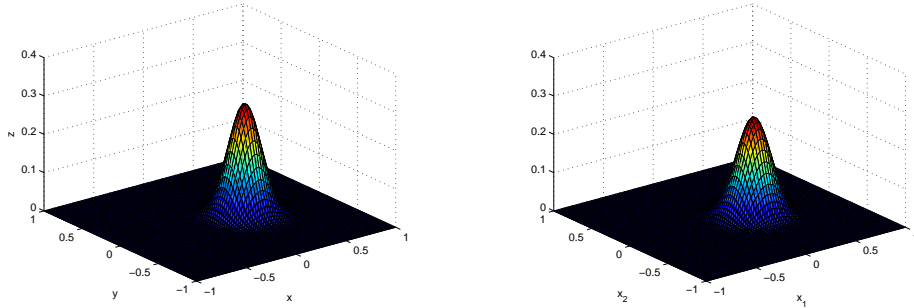


FIG. 5.5. *Exact (left) and computed (right) solution of **Example 1** with  $a = 0.001$  at time  $T = 2\pi$ , with the classical first order scheme and mesh parameter  $h = 1/132$  and  $\Delta t = 2\pi/400$ .*

Figure 5.5 we can see the exact solution compared with the solution computed by using the classical first order characteristics method combined with piecewise linear finite elements. In Figure 5.6 the exact solution is compared with the numerical solution obtained by using the second order method  $(\mathcal{LG})_2$  proposed in the present paper. In both cases a uniform spatial mesh of  $133 \times 133$  vertices has been used and we have chosen the number of time step minimizing the  $l^\infty(L^2(\Omega_{t_n}))$  error. Clearly,  $(\mathcal{LG})_2$  achieves better results than the corresponding classical first order method.

Notice that, for this example, the exact characteristics can be easily determined.

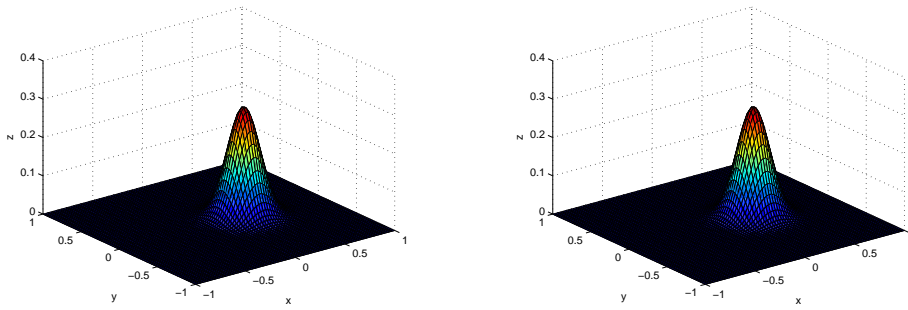


FIG. 5.6. *Exact (left) and computed (right) solution of Example 1 with  $a = 0.001$  at time  $T = 2\pi$ , with the second order scheme  $(\mathcal{LG})_2$ , mesh parameter  $h = 1/132$  and  $\Delta t = 2\pi/100$ .*

In other words, the analytical expression for  $X_e$  is known:

$$X_e(p, t) = \begin{pmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}.$$

### Example 2

We consider a second example to compare the numerical results obtained with semi-Lagrangian and pure Lagrangian methods. It has a solution developing a steep layer and a velocity field which is not divergence-free. This example has been solved in [17]. The spatial domain is  $\Omega = (0, 1) \times (0, 1)$ ,  $T = 1$ , and

$$\mathbf{v} = \nabla\psi, \quad A = aI, \quad f = 0, \quad \rho = 1,$$

being

$$\psi(x_1, x_2) = (1 - \cos(2\pi x_1))(1 - \cos(2\pi x_2)), \quad a = 0.001.$$

The initial data varies between  $\phi^0(0, 0) = 0$  and  $\phi^0(1, 1) = 1$  according to the following expression:

$$(5.2) \quad \phi^0(x_1, x_2) = \begin{cases} 0 & \text{si } \xi < 0, \\ \frac{1}{2}(1 - \cos(\pi\xi)) & \text{si } 0 \leq \xi \leq 1, \\ 1 & \text{si } 1 < \xi, \end{cases}$$

where  $\xi = x_1 + x_2 - 1/2$ . Notice that the velocity field is null on the boundary so  $\Omega_t = \Omega \forall t \in [0, 1]$ . We impose Dirichlet boundary conditions given by the initial data, that is  $\phi_D = \phi^0|_{\Gamma}$ . In Figure 5.7 we plot the velocity field and the initial data. We solve this problem with the pure Lagrangian methods  $(\mathcal{LG})_1$  and  $(\mathcal{LG})_2$  and with two second order semi-Lagrangian methods. More precisely, we denote by  $(\mathcal{SLG})_2^1$  the semi-Lagrangian scheme analogous to  $(\mathcal{LG})_2$ , but re-initializing the transformation to the identity at the beginning of each time step (see [8] for more details), and by  $(\mathcal{SLG})_2^2$  a two-step second order semi-Lagrangian method. The latter has been proposed and analyzed for one-dimensional convection-diffusion equations in [20], and for the incompressible Navier-Stokes equations in [14]. In all cases we have chosen piecewise quadratic finite elements for space discretization. Moreover, as in the previous example, an exact quadrature formula for polynomials of degree

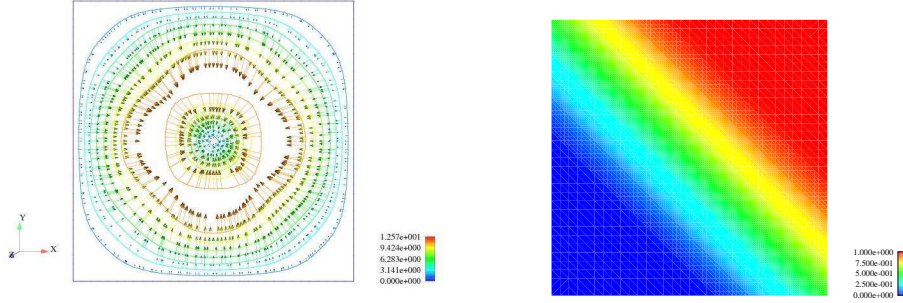


FIG. 5.7. *Example 2: velocity field (left) and initial data (right).*

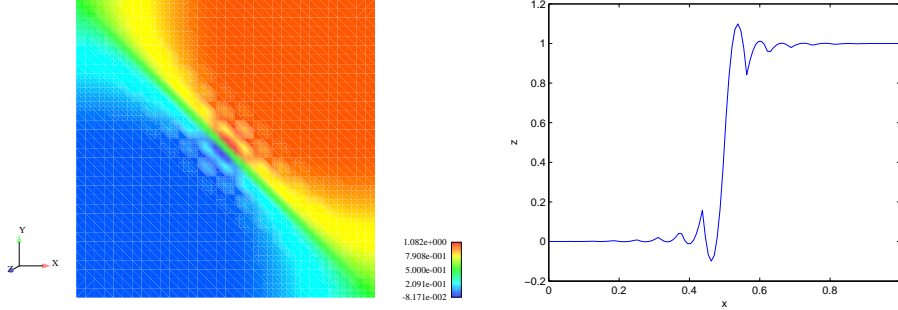


FIG. 5.8. *Example 2: numerical solution contours at  $T = 1$  (left) and the section  $x_1 \rightarrow \phi_{\Delta t, h}^N(x_1, 1/2)$  (right) for  $(\mathcal{SLG})_2^2$  semi-Lagrangian scheme,  $h = 1/16$ ,  $\Delta t = 1/60$ .*

2 is used to approximate all the integrals. For the  $(\mathcal{SLG})_2^2$  scheme, we use a first-order semi-Lagrangian method to calculate the numerical solution at the first time step. In Figures 5.8, 5.9, 5.10 and 5.11 we represent the numerical solution contours at final time  $T = 1$  and the section  $x_1 \rightarrow \phi_{\Delta t, h}^N(x_1, 1/2)$ , computed by using the  $(\mathcal{SLG})_2^2$ ,  $(\mathcal{SLG})_2^1$ ,  $(\mathcal{LG})_1$  and  $(\mathcal{LG})_2$  methods, respectively, and  $h = 1/16$ . The semi-Lagrangian methods present oscillations near the transition layer, so Gibbs phenomena is observed, while the pure Lagrangian methods are accurate even in the steep layer around the diagonal. These features can be observed on the plots of the sections. Maybe these oscillations could be removed by using limiters (see [24]) but this issue is beyond the scope of this paper. This problem has been also solved in [17] with a semi-Lagrangian method combined with a discontinuous Galerkin discretization, and also with a standard Galerkin one. The Gibbs phenomena is also observed for both methods even for very fine meshes, with  $h = 1/32$ . The oscillations produced by the standard Galerkin scheme are observed even far from the transition layer.

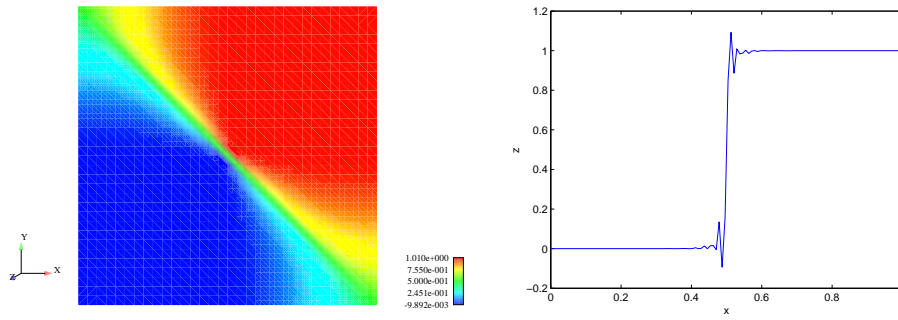


FIG. 5.9. *Example 2: numerical solution contours at  $T = 1$  (left) and the section  $x_1 \rightarrow \phi_{\Delta t, h}^N(x_1, 1/2)$  (right) for the  $(\mathcal{SLG})_2^1$  scheme,  $h = 1/16$ ,  $\Delta t = 1/60$ .*

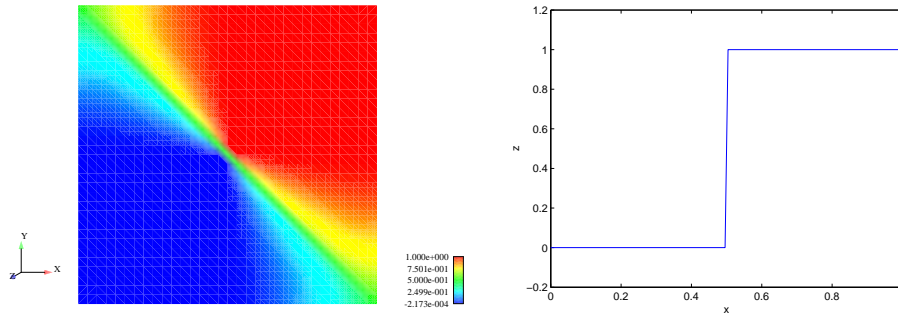


FIG. 5.10. *Example 2: numerical solution contours at  $T = 1$  (left) and the section  $x_1 \rightarrow \phi_{\Delta t, h}^N(x_1, 1/2)$  (right) for the  $(\mathcal{LG})_1$  scheme,  $h = 1/16$ ,  $\Delta t = 1/60$ .*

**6. Conclusions.** We have performed the numerical analysis of a second-order pure Lagrange-Galerkin 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. In a previous paper the proposed second order pure Lagrangian time discretization scheme has been rigorously introduced and analyzed for the same problem. Although our analysis considers any velocity field and use approximate characteristic curves, error estimates of order  $O(\Delta t^2) + O(h^k)$  have been obtained when data and solutions are smooth enough. These results have been proved by using some properties obtained in the previous paper [8]. Numerical tests have been presented to confirm the predicted behavior.

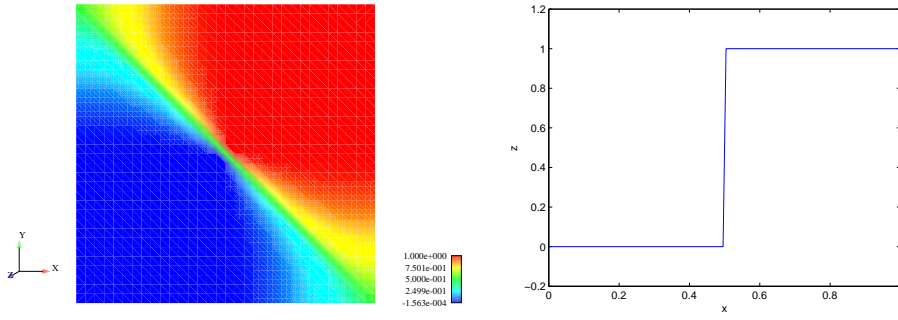


FIG. 5.11. *Example 2: numerical solution contours at  $T = 1$  (left) and the section  $x_1 \rightarrow \phi_{\Delta t, h}^N(x_1, 1/2)$  (right) for the  $(\mathcal{LG})_2$  scheme,  $h = 1/16$ ,  $\Delta t = 1/60$ .*

$\Omega$ : bounded domain

$\Omega_t := X_e(\Omega, t)$

$\mathcal{O} := \bigcup_{t \in [0, T]} \bar{\Omega}_t$

$P$ : reference map of  $X_e$

$L := \text{grad } \mathbf{v}$

$A = \begin{pmatrix} A_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$ : diffusion tensor field

$\mathbf{m}$ : the outward unit normal vector to  $\Gamma := \partial\Omega$

$X_{RK}^n$ : second order Runge-Kutta approximation of  $X_e^n$

$\Omega_t^\delta := \bigcup_{x \in \bar{\Omega}_t} B(x, \delta)$

$\rho$ : density

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

$\tilde{A}_{RK}^n := (F_{RK}^n)^{-1} A \circ X_{RK}^n (F_{RK}^n)^{-T} \det F_{RK}^n$

$C = \sqrt{A}$

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

$B = \begin{pmatrix} I_{n_1} & \Theta \\ \Theta & \Theta \end{pmatrix}$ ,  $I_{n_1}$  is the  $n_1 \times n_1$  identity matrix

$\widehat{\mathcal{S}}[\psi] := \{\psi^{n+1} + \psi^n\}_{n=0}^{N-1}$

$X_e$ : motion

$\mathcal{T}$ : trajectory of the motion

$F = \nabla X_e$ : Jacobian matrix of the deformation

$\mathbf{v}$ : spatial description of the velocity

$\Psi_m$ : material description of a spatial field  $\Psi$

$\tilde{A}_m(p, t) := F^{-1}(p, t) A_m(p, t) F^{-T}(p, t) \det F(p, t)$

$\tilde{m}(p, t) := |F^{-T}(p, t) \mathbf{m}(p)| \det F(p, t)$

$F_{RK}^n := \nabla X_{RK}^n$

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

$\gamma$ : lower bound for  $\rho$

$\Lambda$ : lower bound for the eigenvalues of  $A_{n_1}$

$\tilde{m}_{RK}^n = |(F_{RK}^n)^{-T} \mathbf{m}| \det F_{RK}^n$

$c_A = \max\{\|G\|_{\infty, \mathcal{O}^\delta}^2, \|C\|_{\infty, \mathcal{O}^\delta}^2\}$ ,  $G_{ij} = |\text{grad } C_{ij}|$

$\tilde{C}_{RK}^n := C \circ X_{RK}^n (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n}$

$\tilde{B}_{RK}^n = B (F_{RK}^n)^{-T} \sqrt{\det F_{RK}^n}$

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

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