Numerical approximation of convection-diffusion problems through the PSI method and characteristics method

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Summary. In this work we present some numerical methods for solving evolutive convection-diffusion problems. In order to obtain a physically admissible solution we search for monotone and accurate methods that are also non-linear due to the Godunov's theorem. We will center in Fluctuation Splitting methods, [DSBR93], in particular in PSI scheme, and characteristic type methods, where a new Lagrangian method is proposed. Finally, a numerical test is presented to assess the performance of the numerical methods described in the present work.

Key words: convection-diffusion equation, characteristics method, fluctuation splitting schemes, Galerkin discretization

1 Introduction

In this work we consider the following evolutive convection-diffusion problem:

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + \mathbf{v} \cdot \operatorname{grad} \phi - \nu \Delta \phi = f \text{ in } \Omega \times (0,T), \\ \phi = 0 \qquad\qquad\qquad\qquad \text{on } \Gamma \times (0,T), \\ \phi(x,0) = \phi^0(x) \qquad\qquad \text{in } \Omega, \end{cases} \tag{1}$$

where Ω is a bounded domain of $\mathbb{R}^d$, $d \geq 2$, with boundary Γ and $T > 0$. Also, $\mathbf{v} : \Omega \times (0,T) \longrightarrow \mathbb{R}^d$ is the convection vector field, $f : \Omega \times (0,T) \longrightarrow \mathbb{R}$ is the source term, $\phi^0 : \Omega \longrightarrow \mathbb{R}$ is the initial data and $\nu > 0$ is the diffusion

coefficient. For simplicity we assume the transporting fluid to satisfy the no-slip condition so equivalently, we consider that the velocity field vanishes on the boundary.

Linear convection-diffusion equations model a variety of important problems from different fields of engineering and applied sciences. In many cases the diffusive term is much smaller than the convective one, giving rise to the so-called convection dominated problems. For convection-diffusion problems with dominant convection, methods of characteristics and the Fluctuation Splitting (FS) methods, for convective term discretization, are extensively used (see [P82], [DSBR93], [CGN07]).
Characteristics methods are based on time discretization of the material time derivative. For space discretization, they has been combined with finite differences [DR82], finite elements ([P82], [BPS83], [BD88], [MPS98]), spectral finite elements ([BSW99]), discontinuous finite elements ([BM99]), and so on. When combined with finite elements they are also called Lagrange-Galerkin methods. In particular, when the characteristic methods are formulated in Lagrangian coordinates (respectively, Eulerian coordinates) they are called Lagrangian methods (respectively, semi-Lagrangian methods). In the present work we will consider the combination of Lagrangian and semi-Lagrangian methods with a spatial discretization by using finite elements spaces.

One of the most successful nonlinear Fluctuation Splitting schemes is the PSI method, introduced in [DSBR93]. The PSI method is specifically designed to be exact for linear solutions of the pure transport equation. It is monotone and is particularly accurate in zones of strong gradients or discontinuities of the solution. In the present case, to approximate the equation in (1) we discretize the convection operator by the PSI scheme, the time derivative by a Crank-Nicolson scheme and the diffusion operator by the standard Galerkin method, using linear finite elements. In order to perform the theoretical analysis, the PSI method is formulated as a nonlinear finite element Petrov-Galerkin (see [CGN07]), so the usual techniques are used to develop the existence, convergence and error estimates theory.

After the present section we introduce the PSI method applied to problem (1). In Section 3 a second order full Lagrangian characteristic method is proposed. Finally, to test the proposed methods, a numerical example is presented in Section 4 which has a solution developing a steep layer and a velocity field which is not divergence-free.

2 The PSI method

The PSI method is one of the most advantageous FS schemes. Their main design idea is to split the element convective residual $R^T = \int_T \mathbf{v} \cdot \operatorname{grad} \phi$ be-

tween the nodes of the element that are downstream according to the velocity $\mathbf{v}$. This distribution is made through coefficients β_i^T such that $\beta_i^T R^T$ is the residual contribution of the element T to the node x_i. For consistency these coefficients must satisfy: $0 \leq \beta_i^T \leq 1$ and $\sum_i \beta_i^T = 1$. The way in which these constants are defined is what distinguishes the different FS schemes.
For the particular PSI method these coefficients are determined in order to exactly solve the stationary pure transport equation.

We assume Ω to be a polygonal or polyhedral domain and consider a triangulation $\mathcal{T}_h$ of Ω by triangles in 2D and tetrahedra in 3D. We define the finite-dimensional space of piecewise affine finite elements built on $\mathcal{T}_h$:

$$V_h^1 = \left\{ \varphi_h \in C^0(\overline{\Omega}) : \ \varphi_{h|_T} \in P_1(T), \ \forall T \in \mathcal{T}_h, \ v_h = 0 \text{ on } \Gamma \right\}.$$

We use the PSI method just to discretize the convective part. For this aim the test functions corresponding to this term are taken from a new space of piecewise constant functions W_h directly related to the flux distribution coefficients β_i^T. We introduce an interpolation operator Π_{ϕ_h} from V_h^1 onto the space W_h, in particular we have $\Pi_{\phi_h}\varphi_h = \sum_i \varphi_h(x_i)\beta_i^T(\phi_h)$ (see [CGN07] for more details). Notice that it depends on the unknown ϕ_h due to the non-linear nature of the PSI method.

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 $n = 0, 1/2, 1, \ldots, N$. Next, we define the form $a_h^n : V_h^1 \times V_h^1 \longrightarrow \mathbb{R}$ for $0 \leq n \leq N$ as

$$a_h^n(\phi_h, \psi_h) = \int_\Omega (\overline{\mathbf{v}}^n \cdot \operatorname{grad} \phi_h) \Pi_{\phi_h} \psi_h + \nu \int_\Omega \operatorname{grad} \phi_h \cdot \operatorname{grad} \psi_h \tag{2}$$

being $\overline{\mathbf{v}}_{|_T} = \dfrac{1}{|T|} \displaystyle\int_T \mathbf{v}\, dx$, $\forall T \in \mathcal{T}_h$. Here, the time discretization scheme we are going to consider is a Crank-Nicholson-like scheme. It arises from approximating the time derivative at $t = t_{n+\frac{1}{2}}$, for $0 \leq n \leq N-1$, 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, we have the following discrete variational approximation of (1)

$$\begin{cases} \text{Given } \phi_{\Delta t,h}^0 \in V_h^1, \text{ find } \widehat{\phi_{\Delta t,h}} = \{\phi_{\Delta t,h}^n\}_{n=1}^N \in \left[V_h^1\right]^N \text{ such that} \\ \displaystyle\int_\Omega \frac{\phi_{\Delta t,h}^{n+1} - \phi_{\Delta t,h}^n}{\Delta t} \psi_h \, dx + \frac{1}{2}\left(a_h^{n+1}(\phi_{\Delta t,h}^{n+1}, \psi_h) + a_h^n(\phi_{\Delta t,h}^n, \psi_h) \right) \\ = \dfrac{1}{2} \displaystyle\int_\Omega \left(f^{n+1} + f^n \right) \psi_h \, dx, \ \forall \psi_h \in V_h^1, \text{ for } n = 0, \ldots, N-1. \end{cases} \tag{3}$$

In practice, to eliminate the nonlinearity of convective term we use the following approximation

$$\int_\Omega (\overline{\mathbf{v}}^{n+1} \cdot \operatorname{grad} \phi_{\Delta t,h}^{n+1}) \Pi_{\phi_{\Delta t,h}^{n+1}} \psi_h \simeq \int_\Omega (\overline{\mathbf{v}}^{n+1} \cdot \operatorname{grad} \phi_{\Delta t,h}^{n+1}) \Pi_{\phi_{\Delta t,h}^{n}} \psi_h.$$

Notice that due to the use of the PSI method to discretize the convective term, the approximate problem (3) is written under a Petrov-Galerkin formulation. Is just this writting what allows us to develop the theoretical analysis of the discrete problem by using the tools of functional analysis adapted to this kind of formulation.

In [CGN07] the PSI method combined with piecewise linear finite elements is presented and analyzed for steady convection-diffusion equations. The authors perform a convergence, error and maximum principle analysis. In particular, it is proved that the scheme is first-order accurate in H^1 norm and well-balanced up to second order for convection-dominated flows.

3 Characteristics method

In this section we consider a second order characteristics scheme combined with quadratic finite elements for discretization of (1). We denote by X_e the motion corresponding to the velocity $\mathbf{v}$ and P its reference map, and define the material description Ψ_m of a spatial field Ψ by

$$\Psi_m(p,t) = \Psi(X_e(p,t),t). \tag{4}$$

We recall that, according to the standard formalism of continuum mechanics, $x = X(p,t)$ is the position at time t of the material point p, while the reference map $P(x,t)$ yields the material point located at position x at time t. We assume that $X_e(p,0) = p$, $\forall p \in \overline{\Omega}$. We are going to write the problem (1) in Lagrangian coordinates p. For this, we introduce the change of variable $x = X_e(p,t)$ and use the chain rule, obtaining (see [Ben09])

$$\begin{cases} \dot{\phi}_m \det F - \nu \,\mathrm{Div}\left[F^{-1}F^{-T}\nabla\phi_m \det F\right] = f_m \det F \text{ in } \Omega\times(0,T), \\ \phi_m = 0 \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{on } \Gamma\times(0,T), \\ \phi_m(p,0) = \phi^0(p) \qquad\qquad\qquad\qquad\qquad\qquad \text{in } \Omega, \end{cases} \tag{5}$$

being $F(\cdot,t)$ the Jacobian matrix of the deformation $X_e(\cdot,t)$. The time discretization scheme we are going to consider 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 $t = t_{n+\frac{1}{2}}$.

Regarding the space discretization we use the piecewise quadratic finite elements space. We consider the finite-dimensional spaces of piecewise quadratic finite elements built on $\mathcal{T}_h$:

$$V_h^2 = \left\{\varphi_h \in C^0(\overline{\Omega}) :\ \varphi_{h|_T} \in P_2(T),\ \ \forall T \in \mathcal{T}_h,\ \varphi_h = 0 \text{ on } \Gamma\right\}.$$

Thus, we have the following discrete variational approximation of (5)

$$\begin{cases} \text{Given } \phi^0_{m,\Delta t,h} \in V_h^2, \text{ find } \widehat{\phi_{m,\Delta t,h}} = \{\phi^n_{m,\Delta t,h}\}_{n=1}^N \in \left[V_h^2\right]^N \text{ such that} \\ \dfrac{1}{2}\displaystyle\int_\Omega \left(\det F^{n+1} + \det F^n\right) \dfrac{\phi^{n+1}_{m,\Delta t,h} - \phi^n_{m,\Delta t,h}}{\Delta t}\psi_h \\ +\dfrac{\nu}{4}\displaystyle\int_\Omega ([F^{-1}F^{-T}\det F]^{n+1} + [F^{-1}F^{-T}\det F]^n) \\ \qquad (\nabla\phi^{n+1}_{m,\Delta t,h} + \nabla\phi^n_{m,\Delta t,h})\cdot\nabla\psi_h \\ = \displaystyle\int_\Omega \dfrac{\det F^{n+1}f^{n+1}_m + \det F^n f^n_m}{2}\psi_h, \ \forall\psi_h \in V_h^2, \text{ for } n = 0,\dots,N-1. \end{cases} \tag{6}$$

Since usually the characteristic curves cannot be exactly computed, in practice, we replace in (6) the exact characteristic curves and gradient tensors by accurate enough approximations. More precisely, we use a second order Runge-Kutta approximation of X_e. Moreover, in order to obtain an approximate solution of ϕ^n in Eulerian coordinates, we are going to calculate the spatial description of material field $\phi^n_{m,\Delta t,h}$. More precisely, we calculate $\widehat{\phi_{\Delta t,h}} \sim \widehat{\phi}$ as follows

$$\phi^n_{\Delta t,h}(x) := \phi^n_{m,\Delta t,h}(P^n_{RK}(x)) \quad \forall x \in \overline{\Omega},\ 0 \le n \le N, \tag{7}$$

being P^n_{RK} the second order Kunge-Kutta approximation of P^n.

Thus, we shall denote this Lagrangian method by $(\mathcal{LG})_2$. Furthermore, we shall 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 [Ben09] for more details).

In [Ben09] the Lagrange Galerkin method (6) with a second order Runge-Kutta approximation of X_e is analyzed for a more general problem. A $l^\infty(L^2)$ stability inequality is stated and $l^\infty(L^2)$ error estimates of order $O(\Delta t^2) + O(h^2)$ are obtained; these estimates are uniform in the hyperbolic limit. More precisely, for Δt small enough, the following estimate is obtained:

$$\left|\left|\phi_m - \widehat{\phi_{m,\Delta t,h}}\right|\right|_{l^\infty(L^2(\Omega))} + \sqrt{\nu}\left|\left|\mathcal{S}[\nabla\phi_m - \widehat{\nabla\phi}_{m,\Delta t,h}]\right|\right|_{l^2(\mathbf{L}^2(\Omega))} \le J_1(\Delta t^2 + h^2), \tag{8}$$

where $\widehat{\mathcal{S}[\psi]} := \{\psi^{n+1} + \psi^n\}_{n=0}^{N-1}$ for a sequence $\widehat{\psi} = \{\psi\}_{n=0}^N$. Here, J_1 is bounded in the hyperbolic limit. In particular, this result is also valid when $\nu = 0$. Furthermore, stability and error estimates of order $O(\Delta t^2) + O(h^2)$ are proved in the $l^\infty(H^1)$-norm. More precisely, the following estimate is obtained:

$$\left|\left|\mathcal{R}_{\Delta t}[\phi_m - \widehat{\phi}_{m,\Delta t,h}]\right|\right|_{l^2(L^2(\Omega))} + \sqrt{\nu}\left|\left|\nabla\phi_m - \widehat{\nabla\phi}_{m,\Delta t,h}\right|\right|_{l^\infty(\mathbf{L}^2(\Omega))} \le J_2(\Delta t^2 + h^2), \tag{9}$$

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_2 does not depend on ν. From these estimates and by using appropiate changes of variable, analogous estimates in Eulerian coordinates are deduced.

4 Numerical results

We consider the following example to compare the numerical results obtained with semi-Lagrangian, (full) Lagrangian methods and the PSI method.
The spatial domain is $\Omega = (0,1)\times(0,1)$, $T = 1$, and $\mathbf{v} = \nabla\psi, \quad \nu = \sigma_1, \quad f = 0$, being $\psi = (1 - cos(2\pi x_1))(1 - cos(2\pi x_2))$ and $\sigma_1 = 0.001$. The initial data varies between $\phi^0(0,0) = 0$ and $\phi^0(1,1) = 1$ according to the following expression:

$$\phi^0(x_1,x_2) = \begin{cases} 0 & \text{if } \xi < 0, \\ \frac{1}{2}(1 - cos(\pi\xi)) & \text{if } 0 \le \xi \le 1, \\ 1 & \text{if } 1 < \xi, \end{cases} \tag{10}$$

where $\xi = x_1 + x_2 - 1/2$. We impose Dirichlet boundary conditions given by the initial data. In Figure 1 we plot the velocity field and the initial data. This example has been solved in [CW08] with a semi-Lagrangian method combined with a discontinuous Galerkin discretization, and also with a standard Galerkin scheme. The Gibbs phenomena is observed for both methods. The oscillations produced by the standard Galerkin scheme are observed even far from the transition layer.

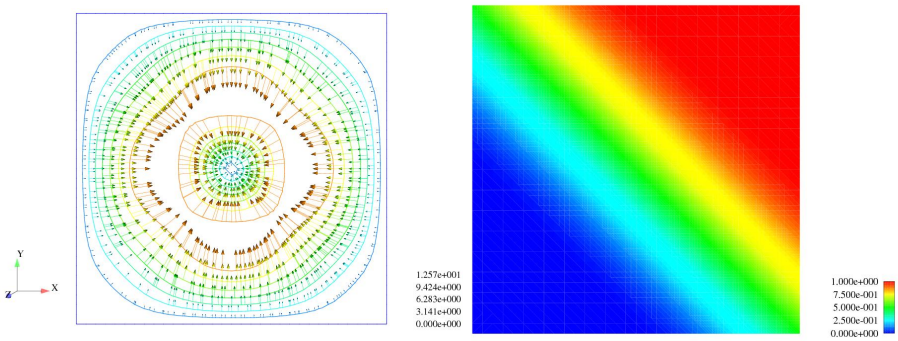

Fig. 1. Velocity field (left) and initial date (right).

Here we solve this problem with the Lagrangian method $(\mathcal{LG})_2$, the semi-Lagrangian scheme $(\mathcal{SLG})_2^1$ and with the PSI scheme given by (3).

In Fig. 2, 3 and 4 we represent the numerical solution contours at final time $T = 1$ and the section $x_1 \longrightarrow \phi^N_{\Delta t,h}(x_1, 1/2)$, computed by using the $(\mathcal{SLG})_2^1$, $(\mathcal{LG})_2$ and PSI methods, respectively. The semi-Lagrangian method presents oscillations near the transition layer, so Gibbs phenomena is observed, while the Lagrangian method and the PSI scheme are accurate even in the steep layer around the diagonal. These features can be observed on the plots of the sections.

So we can conclude that for obtaining a physically acceptable solution, both $(\mathcal{LG})_2$ and PSI can be used. In order to compare them, we can say that

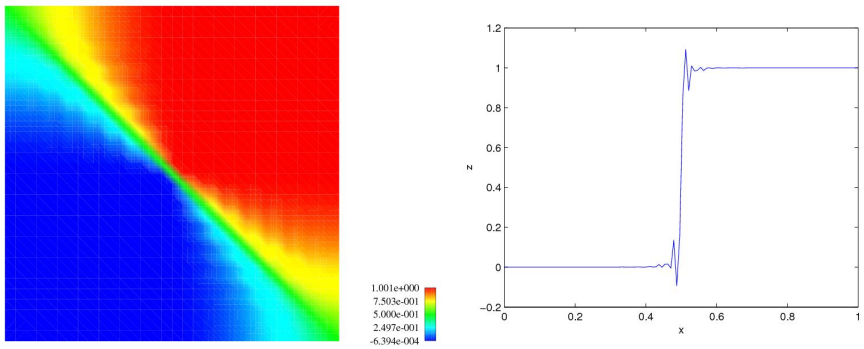

Fig. 2. Numerical solution contours at $T = 1$ (left) and the section $x_1 \longrightarrow \phi^N_{\Delta t,h}(x_1, 1/2)$ (right) for the $(\mathcal{SLG})^1_2$ scheme, $h = 1/16$, $\Delta t = 1/60$.

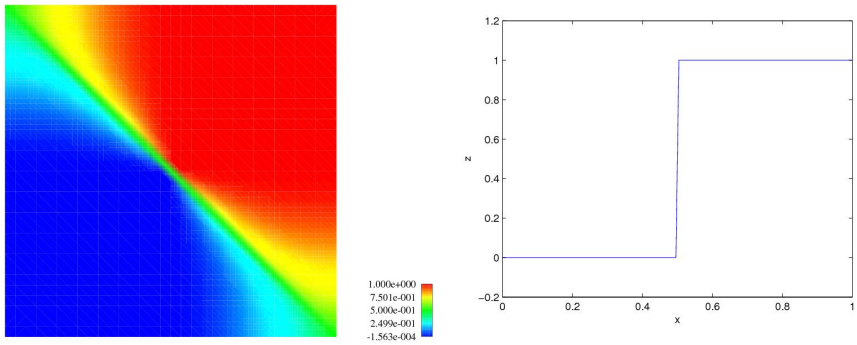

Fig. 3. Numerical solution contours at $T = 1$ (left) and the section $x_1 \longrightarrow \phi^N_{\Delta t,h}(x_1, 1/2)$ (right) for the $(\mathcal{LG})_2$ scheme, $h = 1/16$, $\Delta t = 1/60$.

although $(\mathcal{LG})_2$ is less diffusive than PSI, it is also computationally more expensive (see [Ben09]).

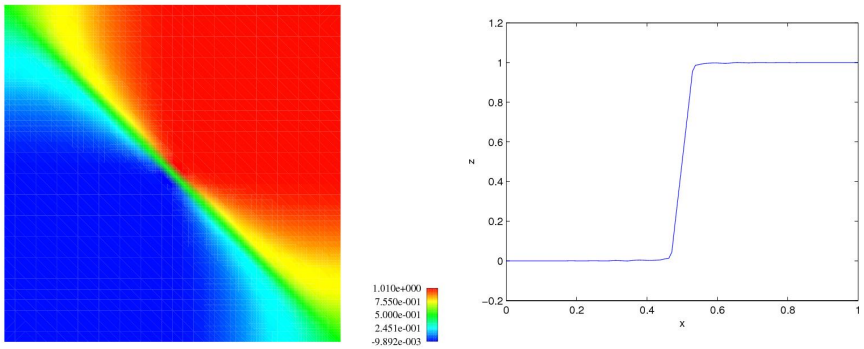

Fig. 4. Numerical solution contours at $T = 1$ (left) and the section $x_1 \longrightarrow \phi^N_{\Delta t,h}(x_1, 1/2)$ (right) for the $(\mathcal{PSI})$ scheme, $h = 1/32$, $\Delta t = 1/60$.

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