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To cite this version:

Christophe Chalons, Frédéric Coquel. Computing material fronts with a Lagrange-Projection approach. 2010. hal-00548938

HAL Id: hal-00548938

https://hal.science/hal-00548938v1

Preprint submitted on 20 Dec 2010

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Computing material fronts with a Lagrange-Projection approach*

Christophe Chalons
CEA-Saclay, DEN/DANS/DM2S/SFME/LETR
F-91191 Gif-sur-Yvette, France.
E-mail: chalons@math.jussieu.fr

Frédéric Coquel
CNRS & Centre de Mathématiques Appliquées, U.M.R. 7641
Ecole Polytechnique, Route de Saclay, 91128 Palaiseau Cedex, France.
E-mail: frederic.coquel@cmap.polytechnique.fr

Abstract

This paper reports investigations on the computation of material fronts in multi-fluid models using a Lagrange-Projection approach. Various forms of the Projection step are considered. Particular attention is paid to minimization of conservation errors.

1 Introduction

It is well-known that standard conservative discretizations of gas dynamics equations in Eulerian coordinates generally develop non physical pressure oscillations near contact discontinuities, and more generally near material fronts in multi-component flows. Several cures based on a local non conservative modification have been proposed. Let us quote for instance the hybrid algorithm derived by Karni in [10] and the Two-Flux method proposed by Abgrall and Karni in [2] for multi-fluid flows. See also [1], [3] and the references therein.
We investigate here a Lagrange-Projection type method to get rid of pressure oscillations. The basic motivation lies in the fact that oscillations do not exist in Lagrangian computations. It is then possible to clearly determine which operation in the projection step sparks off pressure oscillations. As in [10], [2], a non conservative correction is proposed. It is based on a local pressure averaging and a random sampling

*Research of the first author was partially supported by the French Agence Nationale de la Recherche, contract ANR-08-JCJC-0132-01. Research of the authors was partially supported by the Ministère de la Recherche under grant ERTint 1058 entitled *Simulation Avancée du Transport des Hydrocarbures.*

strategy on the mass fraction in order to strictly preserve isolated material fronts and get a statistical conservation property. Numerical results are proposed and compared with the Two-Flux method [2].

2 The model under consideration

We consider a nonlinear partial differential equations model governing the flow of two species Σ_1 and Σ_2 separated by a material interface. For instance, we focus on two perfect gases and we set $p_i(\rho_i, e_i) = (\gamma_i - 1)\rho_i e_i$, $\gamma_i = C_{p,i}/C_{v,i}$ and $T_i(\rho_i, e_i) = e_i/C_{v,i}$ where p_i, ρ_i, e_i, $\gamma_i > 1$, T_i, $C_{p,i} > 0$, $C_{v,i} > 0$ respectively denote the pressure, the density, the internal energy, the adiabatic coefficient, the temperature and the specific heats of Σ_i, $i = 1, 2$. The mixture density is given by $\rho = \rho_1 + \rho_2$ and we adopt a Dalton's law for the mixture pressure $p = p_1(\rho_1, e_1) + p_2(\rho_2, e_2)$. We assume in addition that the two species evolve according to the same velocity u and are at thermal equilibrium, that is $T = T_1(\rho_1, e_1) = T_2(\rho_2, e_2)$. The mixture internal and total energies e and E are defined by $\rho e = \rho_1 e_1 + \rho_2 e_2$ and $\rho E = \frac{1}{2}\rho u^2 + \rho e$. Then, introducing the mass fraction $Y = \rho_1/\rho$, straightforward manipulations yield $\rho e = \rho C_v T$ with $C_v = C_v(Y) = YC_{v,1} + (1-Y)C_{v,2}$ and

$$p = (\gamma - 1)\rho e \quad \text{with} \quad \gamma = \gamma(Y) = \frac{YC_{p,1} + (1-Y)C_{p,2}}{YC_{v,1} + (1-Y)C_{v,2}} > 1.$$

In one-space dimension, the model under consideration writes

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0, \\ \partial_t(\rho E) + \partial_x(\rho E + p)u = 0, \\ \partial_t \rho Y + \partial_x(\rho Y u) = 0, \end{cases} \tag{2.1}$$

and for the sake of conciseness, we set

$$\partial_t \mathbf{u}(x,t) + \partial_x \mathbf{f}(\mathbf{u}(x,t)) = 0. \tag{2.2}$$

The flux function $\mathbf{f}$ finds a natural definition with respect to the conservative unknowns $\mathbf{u} = (\rho, \rho u, \rho E, \rho Y)$. Let us mention that (2.2) is hyperbolic with eigenvalues $\lambda_0(\mathbf{u}) = u$ and $\lambda_\pm(\mathbf{u}) = u \pm c(\mathbf{u})$, $c(\mathbf{u}) = \sqrt{\gamma p/\rho}$, provided that $\rho > 0$, $0 \le Y \le 1$ and $p > 0$. The characteristic field associated with λ_0 is linearly degenerate, leading to *contact discontinuities* or *material fronts*. The two extreme fields are genuinely nonlinear.

3 Numerical schemes

This section is devoted to the discretization of (2.2). As already stated, a specific attention must be paid to the contact discontinuities to avoid

pressure oscillations. With this in mind, we first revisit the "Two-Flux Method" proposed by Abgrall and Karni [2] and then present a new numerical procedure based on a Lagrangian approach and a random sampling strategy. Comparisons will be proposed in section 4.
Let us introduce a time step $\Delta t > 0$ and a space step $\Delta x > 0$ that we assume to be constant for simplicity. We set $\lambda = \Delta t/\Delta x$ and define the mesh interfaces $x_{j+1/2} = j\Delta x$ for $j \in \mathbb{Z}$, and the intermediate times $t^n = n\Delta t$ for $n \in \mathbb{N}$. In the sequel, $\mathbf{u}_j^n$ denotes the approximate value of $\mathbf{u}$ at time t^n and on the cell $\mathcal{C}_j = [x_{j-1/2}, x_{j+1/2}[$. For $n = 0$ and $j \in \mathbb{Z}$, we set $\mathbf{u}_j^0 = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{u}_0(x)dx$ where $\mathbf{u}_0(x)$ is the initial condition.

3.1 The Two-Flux method revisited

Aim of this section is to review the Two-Flux method proposed by Abgrall and Karni [2]. Let us first recall that pressure oscillations do not systematically appear in *single-fluid* computations. Abgrall and Karni [2] then propose to replace any conservative *multi-fluid* strategy by a non conservative approach based on the definition of two *single-fluid* numerical fluxes at each interface. We first recall the algorithm in details and then suggest a slight modification in order to lessen the conservation errors. This strategy will be used as a reference to assess the validity of the Lagrangian strategies proposed in the next subsection.

The original algorithm. Let us consider a two-point numerical flux function $\mathbf{g}$ consistent with $\mathbf{f}$. The Two-Flux method proposes to update the sequence $(\mathbf{u}_j^n)_{j\in\mathbb{Z}}$ into two steps, under an usual 1/2 CFL restriction.

First step : evolution of ρ, ρu and p ($t^n \to t^{n+1-}$)
Let us first define $\mathbf{v} = (\rho, \rho u, p, Y)$ and the one-to-one mapping $\mathbf{u} \to \mathbf{v} = \mathbf{v}(\mathbf{u})$ thanks to the thermodynamics closures. Two interfacial numerical fluxes $\mathbf{g}_{j+1/2,L}$ and $\mathbf{g}_{j+1/2,R}$ are then defined by

$$\mathbf{g}_{j+1/2,L} = \mathbf{g}(\mathbf{u}_j^n, \overline{\mathbf{u}}_{j+1,L}^n), \quad \mathbf{g}_{j+1/2,R} = \mathbf{g}(\overline{\mathbf{u}}_{j,R}^n, \mathbf{u}_{j+1}^n), \tag{3.1}$$

where $\overline{\mathbf{u}}_{j+1,L}^n = \mathbf{u}(\overline{\mathbf{v}}_{j+1,L}^n)$ with $\overline{\mathbf{v}}_{j+1,L}^n = (\rho_{j+1}^n, (\rho u)_{j+1}^n, p_{j+1}^n, Y_j^n)$, and $\overline{\mathbf{u}}_{j,R}^n = \mathbf{u}(\overline{\mathbf{v}}_{j,R}^n)$ with $\overline{\mathbf{v}}_{j,R}^n = (\rho_j^n, (\rho u)_j^n, p_j^n, Y_{j+1}^n)$. In some sense, the mass fraction Y is then assumed to be the same on both side of each interface since $Y = Y_j^n$ is used for the computation of $\mathbf{g}_{j+1/2,L}$ and $Y = Y_{j+1}^n$ for $\mathbf{g}_{j+1/2,R}$. At last, we use $\mathbf{g}_{j+1/2,L}$, respectively $\mathbf{g}_{j+1/2,R}$, to update the conservative unknowns ρ, ρu and ρE on the cell j, resp. $(j+1)$. With clear notations, we get for all $j \in \mathbb{Z}$

$$\begin{aligned}
\rho_j^{n+1-} &= \rho_j^n - \lambda(\mathbf{g}_{j+1/2,L}^{\rho} - \mathbf{g}_{j-1/2,R}^{\rho}),\\
(\rho u)_j^{n+1-} &= (\rho u)_j^n - \lambda(\mathbf{g}_{j+1/2,L}^{\rho u} - \mathbf{g}_{j-1/2,R}^{\rho u}),\\
(\rho E)_j^{n+1-} &= (\rho E)_j^n - \lambda(\mathbf{g}_{j+1/2,L}^{\rho E} - \mathbf{g}_{j-1/2,R}^{\rho E}).
\end{aligned} \tag{3.2}$$

Let us note that $\rho_1 = \rho Y$ is not concerned with (3.2). We simply set $(\rho_1)_j^{n+1-} = \rho_j^{n+1-} \times Y_j^n$ (Y is naturally kept constant in this step) and then $p_j^{n+1-} = p(\mathbf{u}_j^{n+1-})$ with $\mathbf{u}_j^{n+1-} = (\rho, \rho u, \rho E, \rho_1)_j^{n+1-}$.

Second step : evolution of ρ_1 ($t^{n+1-} \to t^{n+1}$)
In this step, ρ_1 is evolved in a conservative way using the numerical flux function g while the values of ρ, ρu and p are kept unchanged. Again with clear notations, the vector $\mathbf{v}_j^{n+1} = (\rho_j^{n+1}, (\rho u)_j^{n+1}, p_j^{n+1}, Y_j^{n+1})$ is then defined $\rho_j^{n+1} = \rho_j^{n+1-}$, $(\rho u)_j^{n+1} = (\rho u)_j^{n+1-}$, $p_j^{n+1} = p_j^{n+1-}$ and $Y_j^{n+1} = (\rho_1)_j^{n+1}/\rho_j^{n+1}$, where

$$(\rho_1)_j^{n+1} = (\rho_1)_j^n - \lambda(\mathbf{g}_{j+1/2}^{\rho Y} - \mathbf{g}_{j-1/2}^{\rho Y}), \tag{3.3}$$

with $\mathbf{g}_{j+1/2} = \mathbf{g}(\mathbf{u}_j^n, \mathbf{u}_{j+1}^n)$. At last, we set $\mathbf{u}_j^{n+1} = \mathbf{u}(\mathbf{v}_j^{n+1})$.

It is worth noticing that the Two-Flux method is not conservative on ρ and ρu since the fluxes $\mathbf{g}_{j+1/2,L}$ and $\mathbf{g}_{j+1/2,R}$ defined at each interface are different as soon as $Y_j^n \neq Y_{j+1}^n$. It is not conservative on ρE either, but by construction the Two-Flux method is conservative on ρ_1.

The associated quasi-conservative algorithm. It is actually clear from [10], [2] and the references therein that in standard conservative discretizations of (2.2), only the update formula of the total energy ρE is responsible for the pressure oscillations. We are then tempted to propose a quasi-conservative variant of the Two-Flux method such that only the total energy is treated in a non conservative form. For all $j \in \mathbb{Z}$, we simply replace (3.2) by

$$\begin{aligned} \rho_j^{n+1-} &= \rho_j^n - \lambda(\mathbf{g}_{j+1/2}^{\rho} - \mathbf{g}_{j-1/2}^{\rho}), \\ (\rho u)_j^{n+1-} &= (\rho u)_j^n - \lambda(\mathbf{g}_{j+1/2}^{\rho u} - \mathbf{g}_{j-1/2}^{\rho u}), \\ (\rho E)_j^{n+1-} &= (\rho E)_j^n - \lambda(\mathbf{g}_{j+1/2,L}^{\rho E} - \mathbf{g}_{j-1/2,R}^{\rho E}), \end{aligned} \tag{3.4}$$

where again $\mathbf{g}_{j+1/2} = \mathbf{g}(\mathbf{u}_j^n, \mathbf{u}_{j+1}^n)$. The second step is unchanged.

3.2 The Lagrange-Projection approach with random sampling

In this section, we propose a Lagrangian approach for approximating the solutions of (2.2). The general idea is to first solve this system in Lagrangian coordinates, and then to come back to an Eulerian description of the flow with a projection step. Under its classical conservative form, the Lagrange-Projection method generates spurious oscillations near the material fronts. In order to remove these oscillations, we propose to

adapt the projection step (only). We begin with a description of the Lagrangian step and then recall, for the sake of clarity, the usual conservative projection step (see for instance [8]). Again, an usual 1/2 CFL restriction is used.

The Lagrangian step ($t^n \to t^{n+1-}$)
In this step, (2.2) in written in Lagrangian coordinates and solved by an acoustic scheme (see for instance [7]), which gives

$$\begin{array}{l} \tau_j^{n+1-} = \tau_j^n - \lambda \tau_j^n (u_{j+1/2}^n - u_{j-1/2}^n), \\ u_j^{n+1-} = u_j^n - \lambda \tau_j^n (p_{j+1/2}^n - p_{j-1/2}^n), \\ E_j^{n+1-} = E_j^n - \lambda \tau_j^n \big((pu)_{j+1/2}^n - (pu)_{j-1/2}^n\big), \\ Y_j^{n+1-} = Y_j^n, \end{array} \tag{3.5}$$

where the velocity and the pressure at interfaces are defined by

$$\begin{cases} u_{j+1/2}^n = \dfrac{1}{2}(u_j^n + u_{j+1}^n) + \dfrac{1}{2(\rho c)_{j+1/2}^n}(p_j^n - p_{j+1}^n), \\ p_{j+1/2}^n = \dfrac{1}{2}(p_j^n + p_{j+1}^n) + \dfrac{(\rho c)_{j+1/2}^n}{2}(u_j^n - u_{j+1}^n). \end{cases} \tag{3.6}$$

The proposed local approximation $(\rho c)_{j+1/2}^n$ of the Lagrangian sound speed is $(\rho c)_{j+1/2}^n = \max((\rho c)_j^n, (\rho c)_{j+1}^n)$ but other definitions may be found for instance in [11]. In this step, the grid points $x_{j+1/2}$ move at velocity $u_{j+1/2}^n$ so that $\rho_j^{n+1-} = 1/\tau_j^{n+1-}$, $(\rho u)_j^{n+1-} = \rho_j^{n+1-} \times u_j^{n+1-}$, $(\rho E)_j^{n+1-} = \rho_j^{n+1-} \times E_j^{n+1-}$ and $(\rho_1)_j^{n+1-} = \rho_j^{n+1-} \times Y_j^{n+1-}$ define approximate values of $\mathbf{u}$ on a Lagrangian grid with mesh interfaces $x_{j+1/2}^* = x_{j+1/2} + u_{j+1/2}^n \Delta t$.

The usual projection step ($t^{n+1-} \to t^{n+1}$)
Aim of this step is to project the solution obtained at the end of the first step on the Eulerian grid defined by the mesh interfaces $x_{j+1/2}$. *Usually*, the choice is made to project the conservative vector $\mathbf{u}$ in order to obtain a conservative Lagrange-Projection scheme (see again [8]). More precisely, such a choice writes

$$\varphi_j^{n+1} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \varphi^{n+1-}(x) dx \quad \text{with} \quad \varphi = \rho, \rho u, \rho E, \rho_1 = \rho Y, \tag{3.7}$$

or, with $\Delta x_j^* = x_{j+1/2}^* - x_{j-1/2}^*$ and $\varepsilon(j,n) = \begin{cases} -1/2 \text{ if } u_{j+1/2}^n > 0, \\ 1/2 \text{ if } u_{j+1/2}^n < 0, \end{cases}$,

$$\varphi_j^{n+1} = \frac{1}{\Delta x}\{\Delta x_j^* \varphi_j^{n+1-} - \Delta t (u_{j+1/2}^n \varphi_{j+1/2+\varepsilon(j,n)}^{n+1-} - u_{j-1/2}^n \varphi_{j-1/2+\varepsilon(j-1,n)}^{n+1-})\}.$$

What is wrong with this scheme ? The Lagrange-Projection approach allows to precisely reveal the operation that makes the material fronts necessarily damaged by pressure oscillations. Let us indeed consider an isolated material front with uniform velocity and pressure profiles : $u(x,0) = u^0 > 0$ and $p(x,0) = p^0$, while $Y(x,0) = 1$ if $x < 0$ and $Y(x,0) = 0$ if $x > 0$. The density is also set to be uniform for simplicity : $\rho(x,0) = \rho^0$. We first observe that this profile is clearly preserved in the Lagrangian step since by (3.6) we have $u^0_{j+1/2} = u^0$ and $p^0_{j+1/2} = p^0$ by (3.6). Then, the projection procedure (3.7) gives $\rho^1_j = \rho^0$ and $(\rho u)^1_j = \rho^0 u^0$ so that $u^1_j = (\rho u)^1_j/\rho^1_j = u^0$. After the first time iteration, the velocity profile is then still free of spurious oscillations. At last, using the property that this velocity is constant and positive, and focusing for instance on the cell of index $j = 1$, (3.7) gives for $\varphi = \rho E, \rho_1$

$$(\rho E)^1_1 = (\rho E)^0_1 - u^0\lambda\big((\rho E)^0_1 - (\rho E)^0_0\big) \quad \text{and} \quad Y^1_1 = u^0\lambda.$$

The pressure is then given after easy calculations by

$$p^1_1 = p^0 \times \big(\gamma(Y^1_1) - 1\big) \times \big(\frac{1}{\gamma_2 - 1}(1 - u^0\lambda) + u^0\lambda\frac{1}{\gamma_1 - 1}\big).$$

At this stage, there is no reason for p^1_1 to equal p^0 From the very first time iteration, a pressure oscillation is then created. As an immediate consequence, the velocity profile will not remain uniform in the next time iteration and the numerical solution is damaged for good.

It is then clear that the way the pressure is updated in the projection step (only) is responsible for the spurious oscillations in an usual conservative Lagrange-Projection scheme. We propose to modify this step. As for the Two-Flux method, the idea is to give up the conservation property in order to maintain uniform the pressure p across material fronts. Let us emphasize that the Lagrangian step is unchanged.

The quasi-conservative p-projection step ($t^{n+1-} \to t^{n+1}$)
First of all, ρ, ρu and ρ_1 still evolve according to (3.7) so that the algorithm remains conservative on these variables. We will keep on using (3.7) for $\varphi = \rho E$ only for j not in a subset $\mathbb{Z}^\varepsilon_p$ of $\mathbb{Z}$ defined below. On the contrary, the pressure p (instead of ρE) is averaged for $j \in \mathbb{Z}^\varepsilon_p$:

$$p^{n+1}_j = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} p^{n+1-}(x)dx. \tag{3.8}$$

For $j \in \mathbb{Z}^\varepsilon_p$, we then set $\mathbf{v}^{n+1}_j = (\rho^{n+1}_j, (\rho u)^{n+1}_j, p^{n+1}_j, Y^{n+1}_j)$ with $Y^{n+1}_j = (\rho_1)^{n+1}_j/\rho^{n+1}_j$, and $\mathbf{u}^{n+1}_j = \mathbf{u}(\mathbf{v}^{n+1}_j)$.

Definition of $\mathbb{Z}_p^\varepsilon$. Up to our knowledge, the idea of averaging the pressure p in a Lagrange-Projection strategy first appeared in [3]. This way to proceed is clearly sufficient to remove the pressure oscillations near the material fronts if $\mathbb{Z}_p^\varepsilon = \mathbb{Z}$. However, averaging the pressure p instead of the total energy ρE for all $j \in \mathbb{Z}$ gives a non conservative scheme that is expected to provide discontinuous solutions violating the Rankine-Hugoniot conditions, see for instance Hou and LeFloch [9] (note however that here, the Lagrangian system associated with (2.1) is actually treated in a *conservative* form, while the pressure averaging takes place in the projection step only). This was confirmed in practice when considering solutions involving shocks with large amplitude. Then, in order to lessen the conservation errors, we propose to localize the non conservative treatment around the contact discontinuities setting $\mathbb{Z}_p^\varepsilon = \{j \in \mathbb{Z}, \max(|Y_j^n - Y_{j-1}^n|, |Y_{j+1}^n - Y_j^n|) > \epsilon\}$ for a given $\epsilon > 0$. Following Karni [10], we will use $\epsilon = 0.05$ in practice.

The quasi-conservative p-projection step with sampling ($t^{n+1-} \to t^{n+1}$) The quasi-conservative p-projection step will be seen in the next section to properly compute large amplitude shock propagations. Localizing the averaging process of p nevertheless prevents the method from keeping strictly uniform the velocity and pressure profiles of an isolated material front, see **Test A** below. Indeed, note that since $\mathbb{Z}_p^\varepsilon$ is generally a *strict* subset of $\mathbb{Z}$ due to the numerical diffusion on Y (*i.e.* $\mathbb{Z}_p^\varepsilon \subsetneq \mathbb{Z}$), an usual conservative treatment is still used on ρE as soon as j not in $\mathbb{Z}_p^\varepsilon$. This is sufficient to create pressure oscillations. In order to cure this problem, we propose to get rid of the numerical diffusion on Y so as to enforce the non conservative treatment (3.8) across an isolated material front. This objective is achieved when replacing the conservative updating formula (3.7) for ρ_1 with random sampling strategy applied to Y (see also [4] and [5] for similar ideas). More precisely, we consider an equidistributed random sequence (a_n) in $(0,1)$ (following Collela [6], we take in practice the celebrated van der Corput sequence), define $x_j^* = x_{j-1/2} + a_{n+1}\Delta t$ for all $j \in \mathbb{Z}$ and set

$$\begin{cases} Y_j^{n+1} = Y_{j-1}^{n+1-} \text{ if } x_j^* \leq x_{j-1/2}^*, \\ Y_j^{n+1} = Y_j^{n+1-} \text{ if } x_{j-1/2}^* \leq x_j^* \leq x_{j+1/2}^*, \\ Y_j^{n+1} = Y_{j+1}^{n+1-} \text{ if } x_j^* \geq x_{j+1/2}^*. \end{cases}$$

Then, we set $(\rho_1)_j^{n+1} = \rho_j^{n+1} Y_j^{n+1}$ so that the conservation of ρ_1 now holds only statistically.

4 Numerical results

We propose two numerical experiments with $\gamma_1 = 1.4$ and $\gamma_2 = 1.6$ associated with a Riemann initial data. The left and right vectors $\mathbf{v}$ are denoted $\mathbf{v}_L$ and $\mathbf{v}_R$ and the initial discontinuity is at $x = 0.5$. In the first simulation (**Test A**), we consider the propagation of an isolated material interface with $\mathbf{v}_L = (1, 1, 1, 1)$ and $\mathbf{v}_R = (0.1, 0.1, 1, 0)$. We take $\Delta x = 0.005$ and plot the solutions at time $t = 0.15$. The second simulation (**Test B**) develops a strong shock due to a large initial pressure ratio. More precisely, we choose $\mathbf{v}_L = (1, 0, 500, 1)$ and $\mathbf{v}_R = (1, 0, 0.2, 0)$. We take $\Delta x = 0.00125$ and plot the solutions at time $t = 0.008$.
We observe that the Two-Flux method and the Lagrangian methods are in agreement with the exact solutions and give similar results. As expected, note that the Lagrangian approach without sampling does not strictly maintain uniform the pressure profile for **Test A**. Note also that the mass fraction Y is sharp when a random sampling is used. At last, the relative conservation error on ρE (see for instance [5] for more details) for the Lagrangian approach with random sampling is actually less important and swings around 0.2% only.

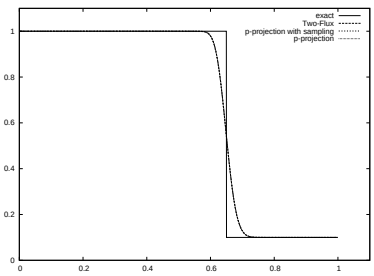

Figure 4.1: ρ (**Test A**)

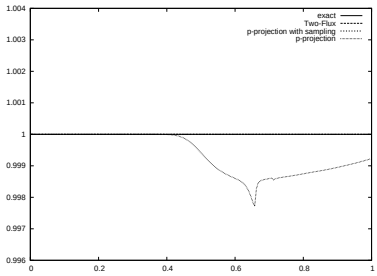

Figure 4.2: p (**Test A**)

5 Concluding remarks

We have investigated a Lagrange-Projection approach for computing material fronts in multi-fluid models. We get similar results to the Two-Flux method [2] with less important conservation errors on ρE. Let us mention that other strategies, like for instance the one consisting in a local random sampling of $\mathbf{u}$ (instead of Y only) in the Lagrangian step, have been investigated. The results are not reported here.

Acknowledgements. The authors are grateful for helpful discussions

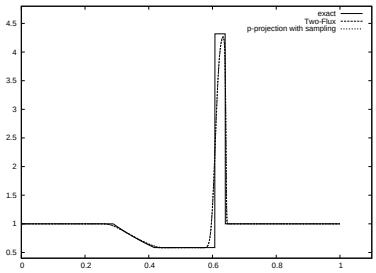

Figure 4.3: ρ (**Test B**)

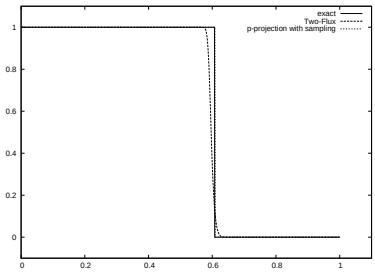

Figure 4.4: Y (**Test B**)

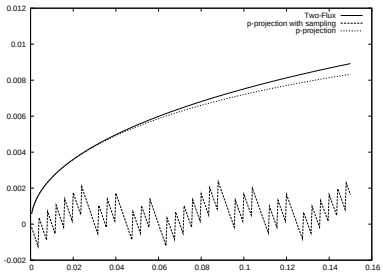

Figure 4.5: Conservation errors (**A**)

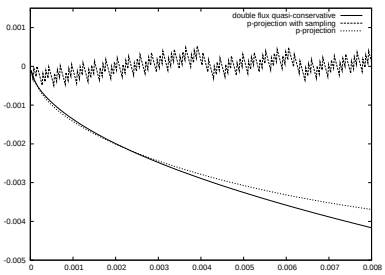

Figure 4.6: Conservation errors (**B**)

and exchanges with P. Helluy and F. Lagoutière.

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