Stabilization of cell-centered compressible Lagrangian methods using subzonal entropy

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Abstract

This work deals with the stabilization of early stages of Lagrangian calculations of compressible gas dynamics in the context of cell-centered discretization. We describe a totally conservative algorithm based on an entropy analysis of the distortion of a Lagrangian mesh. The resulting scheme is an extension of the cell-centered GLACE scheme [10]. Numerical tests are proposed to assess the accuracy and robustness.

1 Introduction

Lagrangian frame for the kinematical description of hydrodynamic computation is very attractive, because it allows an easy tracking of free surfaces and interfaces between materials. Consequently, material dependent features of the flow (like equation of states for instance) can be handled separately without modeling. Moreover, boundary conditions on moving interfaces, and interfaces peculiar treatments (sliding, surface tension, turbulent mixing, . . .) are much easier to take into account with a lagrangian description of the flow. Unfortunately, Lagrangian hydrodynamics suffers from a severe drawback. Since the mesh follows the flow, it lacks of robustness. If, whatever the reason, the mesh becomes locally pathological (tangling), the whole calculation stops. Less radical but equally problematic, the numerical discrepancies of the numerical Lagrangian algorithm have a direct impact on the quality of the mesh and then can be easily amplified. So the stabilization of Lagrangian computation is a fundamental problem in scientific computing.

Failure of a Lagrangian simulation has two main origins: physical and numerical. First, physics of the flow can induce too large distortions of the mesh (vortex, shear). In this case, switch to an Arbitrary Lagrangian-Eulerian (ALE) frame for describing the flow seems to be the best approach (see for instance references [20, 31]). Algorithms are then used to smooth the mesh so that it prevents the crash of the simulation; such algorithms are somehow close to

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re-meshing algorithms for which the question of having a correct mesh by construction is a fundamental question. This is a very active field of research in the meshing community, see [16, 17, 18, 19, 30]. However, it is highly desirable to delay as much as possible the moment when we apply these techniques near free boundaries or material interfaces, the risk being to lose the benefit of the Lagrangian description. This is why we need to suppress the numerical discrepancies inducing local degeneration of the mesh, which is the second cause of failure of a Lagrangian calculation. In this case, it is mandatory to develop algorithms able to control the spurious modes which are somehow part of any Lagrangian simulations at initial stages. In this direction, a fundamental contribution is [9] where subzonal discretization is analyzed in view of an effective control of hourglass modes (see also [8] for the stabilization of curl-free flows). Stabilization plays also a great role for variational multi-scale formulations of Lagrangian hydrodynamics [25, 26, 27, 28]. The new method, that we describe below, falls in this second class of algorithms. The theoretical development holds in any dimension, but the numerical tests in this paper are only in dimension two.

We focus in this paper on the stabilization of cell-centered Finite Volume numerical methods in the context of Lagrangian gas dynamics [2, 10, 11, 22]. These methods receive increasing interest nowadays. One reason is, they are very easy to couple with re-meshing and projection techniques (but not that easy to optimize), in order to design ALE algorithms, which gives an answer to the first problem mentioned above, and is out of the scope of this paper (see however an illustration in figure 18). However, to our knowledge, no paper addresses the problem of numerical stabilization, in the context of cell-centered Lagrangian schemes. Yet, for reasons mentioned previously, this problem appears crucial for all numerical methods on moving grids [6, 21, 29]. This problem does not show up in dimension one, but is the rule in dimensions two and three. At the theoretical level, this is connected to the weakly hyperbolic structure of non-viscous Lagrangian gas dynamics. In particular, the GLACE scheme used in this work, is very accurate for a wide range of applications, but very sensitive to numerical instabilities, like checkerboard modes.

Our reflection is based on the following basic observation: on simplex meshes, GLACE gives outstanding results (see for instance reference [13]), and does not seem to suffer from spurious numerical features. These pathologies appear only when using non-simplices elements (quadrangle in 2D or hexaedron in 3D for instance). The algorithm described below aims to mimic the stability property of simplex meshes in other type of meshes. A list of the main properties of our algorithm is

- The stabilization procedure is based on an entropy analysis of the mesh distortion. That is subzonal decomposition of the cell is characterized with a convenient concave functional which is added to the physical entropy. Such a general approach provides a way to control meshes of any type, not necessarily made with quadrangles.

- The cell-centered final algorithm is conservative in mass, total momentum
and total energy. It guarantees the correctness of shocks capturing.

- Provided the time step is conveniently adapted, the fully discrete algorithm is as close as needed to the semi-discrete algorithm for which we prove rigorously that the mesh can never become pathological.

- The stabilized algorithm is still consistent: the numerical convergence is always achieved for sequences of finer and finer meshes; it is related to a mimetic property of the method. For a given mesh the amount of dissipation added in practice by the stabilization procedure is low.

The algorithm, based on a modification of the nodal Riemann solver characteristic of cell-centered schemes, is able to stabilize the mesh by construction. This is done with the introduction of what we call a subzonal entropy, i.e., a kind of mixing entropy if one refers to thermodynamics considerations [1,12], but applied to any equation of state (not only perfect gas). This stabilization does not affect the discrete shock structure which is already well captured by the nodal Riemann solvers. We will test two different stabilizations: the first one is based on the decomposition of figure 1 and will be called decomposition I; the second one is based on the decomposition depicted in figure 21 and will be called decomposition II. Our numerical tests show that this procedure effectively eliminates a priori all unphysical pathologies of the Lagrangian mesh. Furthermore, the final algorithm is still consistent with the Euler system.

The organization of this paper is as follows. First, we describe what we call a subzonal entropy. Then we study the compatibility with the geometric conservation by means of some appropriate geometrical vectors. Then we show how to incorporate subzonal entropies in a way compatible with the fundamental principle of thermodynamics. This is done in the context of the cell-centered GLACE scheme, we have introduced and studied in a series of paper [10,14,15]. After giving the formulation of the fully discrete extension of GLACE with subzonal entropy, we focus on the definition of a subzonal entropy adapted to practical calculations. Consistency is briefly discussed. Finally, a series of classical test problems is presented to assess the practical performances of the method.

2 Sub-cell modeling and subzonal entropies

For expository purposes, we detail our main idea about sub-cell decomposition on a simple example. Sub-cell decompositions are considered in the seminal work of Caramana and Shashkov [9], where subzonal pressures are described in the context of staggered discretizations. However, our analysis of the subzonal structure is different since it uses what we call a subzonal entropy. It will appear obvious that the basic ingredient is close to what is called a mixing entropy for perfect gas equation of state in the thermodynamics theory of mixing [1,12].

Let us consider a cell at time step \( t_n \). The volume of the cell is referred to as \( V^n \). The mass in the cell is \( M = V^n \rho^n \). The mass does not depend
upon \( n \) since the scheme is Lagrangian. We denote \( E^n = \sum_n \rho^n c^n \) the total energy and \( \varepsilon^n = c^n - \frac{1}{2} |u^n|^2 \), the specific internal energy (\( u \) stands for the velocity). We will assume a perfect gas pressure law \( p = (\gamma - 1)\rho \varepsilon \): the entropy is \( S = C_v \log (\varepsilon \rho^{-\gamma}) \), \( C_v > 0 \).

Next we split the cell into simplices. For example the quadrangle \( Q \) of figure 1 is split into four triangles \( Q = T_1 \cup T_2 \cup T_3 \cup T_4 \).

![Figure 1: Sub-cell decomposition of a quad into four triangles. It will be referred to as decomposition I. Two other examples of sub-cell decomposition are treated in appendix: the one depicted in figure 21 will be called decomposition II.](image1)

In the remaining of this paper, we consider only the case of quadrangle meshes in dimension two. Extension to other 2D elements is not difficult. Three dimensional extension is more tricky, at least practically.

### 2.1 Link with mixing entropy

We desire to establish a method in order to characterize at the entropy level the nearly pathological evolution from figure 1 to figure 2. First, we decide to analyze the problem from a physical point of view, to establish the link between our method and the work of [1, 12]. We decide arbitrarily that the total mass is split into four equal parts and affected in each triangle \( m_i = \frac{1}{4} M \). Specific
internal energy is an intensive variable, then $\varepsilon_i^n = \varepsilon^n$. The entropy in $T_i$ is $S_i = C_v \log (\varepsilon_i \rho_i^{-\gamma})$. The density in triangle $T_i$ is $\rho_i = \frac{m_i}{|T_i|} = \frac{1}{4} \frac{M}{|T_i|} = \frac{1}{4} f^i$, where $f^i = \frac{|T_i|}{V}$ is the volume fraction. So the entropy in $T_i$ recasts $S_i = \log (\varepsilon_i \rho_i^{-\gamma}) + \gamma C_v \log (4f^i)$. The total entropy in the global cell is assumed to be the average sum of the partial entropies, that is
\[ \mathcal{S} = \frac{S_1 + S_2 + S_3 + S_4}{4} = S + \gamma C_v \sum \log (4f^i). \] (1)

In this very basic example, one sees that sub-cell modeling is equivalent to substitute the entropy $S$ in the cell by a new entropy $\mathcal{S} = S + \phi(f)$, $f = (f_1, \ldots, f_4)$. (2)

In the next subsection, we mimic this construction for our definition of the subzonal entropy.

2.2 Subzonal entropies for stabilization

Analyzing equation (1), we find that the entropy tends to $-\infty$ when $f^i$ tends to zero. As we show below, this definition of subzonal entropy fulfills the requested properties we need to stabilize the scheme. The main idea is: if we are able to construct an entropic scheme for $\mathcal{S}$, and a function $\phi(f)$ which tends to $-\infty$ when $f$ tends to zero, the mesh will never become pathological. Indeed, one volume fraction tending to zero is the signature of a nearly pathological mesh.

That is why we impose the following constraints to the function $\phi(f)$.

**Definition 1.** We say that $\phi$ is a subzonal entropy if it satisfies two conditions:

i) $\phi$ is a concave smooth function.

ii) whatever the volume fraction $f^i$ such that $f^i \to 0^+$, $\phi(f) \to -\infty$.

We see immediately that the function $\phi$ defined by the equation (1) satisfies these properties.

We have assumed a perfect gas pressure law for sake of simplicity. From now we will consider subzonal entropies independently of the entropy law $S$, which may be arbitrary.

In order to stabilize a given Lagrangian computation, the general principle is to introduce a subzonal entropy in the numerical method which can be either staggered [6] or cell-centered in our case [10]. The next proposition explains a fundamental advantage of subzonal entropies.

**Proposition 2.** Consider a Lagrangian scheme which has the property that the entropy in the cell increases from time step $n$ to time step $n + 1$: $S^{n+1} \geq S^n$. Assume that we are able to modify this scheme in order to introduce a subzonal entropy in a way such that $\mathcal{S}^{n+1} \geq \mathcal{S}^n$. (3)

Assume that the subzonal decomposition is the one depicted in figure 1.

Then the mesh is never pathological.
More precisely, tangling never appears in situations like in Figure 2. We argue by contradiction. Starting from a valid mesh, a very small $\Delta t$ guarantees that the mesh at time $(n + 1)\Delta t$ is also correct. Then, if one increases continuously the time step in a thought experiment, continuity with respect to $\Delta t$ imposes the following behavior: a pathological mesh is such that one volume fraction tends to zero, vanishes and then becomes negative. In this case $\varphi^{n+1} \approx -\infty$ and it is in contradiction with the assumption (3). It ends the proof.

The difficulty of proving an inequality such as (3) is greatly reduced by considering the continuous time version of the scheme (that is the semi-discrete scheme). So instead of (3) focus on the semi-discrete version which writes

$$\frac{d}{dt} S \geq 0.$$  \hspace{1cm} (4)

Starting from (3) recasts into $\frac{S^{n+1} - S^n}{\Delta t} \geq 0$ and passing to the limit $\Delta t \to 0$, it is clear that (4) is a necessary condition to have (3) for infinitely small time steps. In practice, we have observed that a convenient control of the time step is sufficient to guarantee that the fully discrete scheme behaves like the semi-discrete one, for instance with an appropriate time step control described in the CFL condition (43). For expository purposes, we will systematically use the semi-discrete scheme.

The natural question arising now is: how to incorporate this new entropy into a scheme, in order to guarantee property (3)? First, we have to link the subzonal entropy $\varphi$ with the descriptors of the mesh (the nodes), which is the subject of the next section. Second, we must incorporate the evolution of $\varphi$, into the evolution of the entropy of the solver, which is the subject of the section 4.

3 Compatibility with the geometric conservation law

In a Lagrangian computation cells move and their volumes change. It has been shown in the literature about Lagrangian discretization, see [4, 5, 10, 22] and references therein, that the compatibility of such an algorithm with the geometric conservation law fundamentally depends on a correct use of some corner vectors that we introduce now.

Let us consider a conforming mesh of a computational domain $\Omega \in \mathbb{R}^d$, cells being indexed by $j$ and vertices by $r$. In practice, the dimension of the problem can be $d = 1, 2$ or $3$. In a Lagrangian computation, the mesh moves with the flow. The volume of a cell with index $j$ at time $t_k = t_{k-1} + \Delta t$ is denoted as $V_j^k$ such that, at each time step $k$: $\sum_j V_j^k = |\Omega^k|$. The vertices of the mesh are $x^k \in \mathbb{R}^d$ and we denote by $x^k = (x_j^k, \cdots, x_r^k, \cdots)$ the collection of all vertices. When timestep is not precised, we implicitly refer to $t_k$.

**Definition 3.** We assume that the volume $V_j$ of a cell $j$ is defined as a function of the vertices of this cell, i.e. $x \mapsto V_j(x)$. We define the gradient of the volume
$V_j$ with respect to the nodal positions $x_r$:

$$C_{jr} = \nabla_{x_r} V_j \in \mathbb{R}^d. \quad (5)$$

We will refer to these vectors as corner vectors.

See [4, 5, 10] for practical formulas for different type of cells. We also need in the following the related unit vectors: $n_{jr} = \frac{C_{jr}}{|C_{jr}|}$. A fundamental relation is the geometric conservation law which writes

$$\frac{d}{dt} V_j = (\nabla_x V_j, x') = \sum_r (C_{jr}, u_r), \quad (6)$$

where $(\cdot, \cdot)$ denotes the scalar product. In other words, the change of volume is due to a discrete divergence. The invariance of the volume with respect to a translation of the vertices implies naturally that

$$\sum_r C_{jr} = 0. \quad (7)$$

A more subtle property [14] is

$$\sum_r C_{jr} \otimes x_r = V_j I. \quad (8)$$

It is shown in [14] that (8) holds true since the formula of volume is compatible with some finite element representation. This is the case for all standard type of cells, triangles and quadrangles in dimension two, tetrahedron and hexahedron in dimension three.

We wish to determine what is the generalization of the geometric conservation law for the volume fraction of sub-volume number $i$ in cell number $j$:

$$f^i_j = \frac{V^i_j}{V_j}.$$ 

The conservation law for the sub-volumes will be expressed in the form of a chain rule relation for the volume fractions.

**Definition 4.** We introduce the gradient of $f^i_j$ with respect to $x_r$ and define the vectors

$$Q^i_{jr} = V^i_j \nabla_{x_r} f^i_j. \quad (9)$$

**Remark 5.** By definition the dimension of $Q^i_{jr}$ is the same that the dimension of $C_{jr}$. It helps to get a better interpretation of the final algorithm.

Now, the discrete chain rule takes the form

$$V_j \frac{d}{dt} f^i_j = (V_j \nabla_x f^i_j, x') = \sum_r (Q^i_{jr}, u_r). \quad (10)$$
To be more precise let us consider the example displayed in figure 1 of a quadrangle decomposed into four triangles. We decide arbitrarily that the interior point \( y \) in the current cell is simply the average of the corners of the cell

\[
y = \frac{1}{4} \sum_{r=1}^{4} x_r.
\]  

(11)

In figure 3 we use a local numbering of the vertices. The triangles are: \( T_1 = (y, x_1, x_2), T_2 = (y, x_2, x_3), T_3 = (y, x_3, x_4) \) and \( T_4 = (y, x_4, x_1) \). The sub-volume of triangle \( T_i \) is \( V_i = |T_i| \). Using the definition 4 and the expression of the volume fraction, one has in expanding the derivative of the product:

\[
Q_{jr} = -\frac{V_i}{V_j} C_{jr} + \nabla x_i V_j^i = -f_j C_{jr} + \nabla x_i V_j^i.
\]  

(12)

Consider the first volume fraction, that is \( i = 1 \). Then

\[
dV^1 = d|T_1| = (\nabla y|T_1|, dy) + (\nabla x_1|T_1|, dx_1) + (\nabla x_2|T_1|, dx_2).
\]

The three vectors \( \nabla y|T_1|, \nabla x_1|T_1| \) and \( \nabla x_2|T_1| \) are actually the corner vectors \( C_{jr} \) defined in (5) but for the sub-mesh. One gets the well known formulas [10] where the vectors are colinear to the normal of the opposite edge of the sub-triangle, that is

\[
\nabla x_1|T_1| = \frac{1}{2} \overrightarrow{x_2y_1}, \quad \nabla x_2|T_1| = \frac{1}{2} \overrightarrow{y_2x_1} \quad \text{and} \quad \nabla y|T_1| = \frac{1}{2} \overrightarrow{x_1y_2},
\]

and so on for the three other triangles. Since

\[
dy = \frac{1}{4} (dx_1 + dx_2 + dx_3 + dx_4).
\]

then

\[
d|T_1| = \left( (\nabla x_1|T_1| + \frac{1}{4} \nabla y|T_1|), dx_1 \right) + \left( (\nabla x_2|T_1| + \frac{1}{4} \nabla y|T_1|), dx_2 \right) + \left( (\nabla x_3|T_1| + \frac{1}{4} \nabla y|T_1|), dx_3 \right) + \left( (\nabla y|T_1|), dx_4 \right).
\]  

(13)
Finally, plugging in (12) we find that

\[ Q_{i=1}^{r=1} = -f^1 C_1 + \nabla_{x_1}|T_1| + \frac{1}{4}\nabla_y|T_1| , \]
\[ Q_{i=1}^{r=2} = -f^1 C_2 + \nabla_{x_2}|T_1| + \frac{1}{4}\nabla_y|T_1| , \]
\[ Q_{i=1}^{r=3} = -f^1 C_3 + \frac{1}{4}\nabla_y|T_1| \]

and

\[ Q_{i=1}^{r=4} = -f^1 C_4 + \frac{1}{4}\nabla_y|T_1| . \]

All other vectors are obtained by permutation of the indices.

Some properties of the \( Q_{i,j} \) are given in the next proposition. We will show in the following that the formula (16) has important consequences for the consistency in the mimetic sense of the overall algorithm.

**Remark 6.** In 1D, and also for triangles in 2D and tetrahedrons in 3D, the \( Q_{i,j} \) are zero. Indeed, in these cases, \( f_{i,j}^j = \frac{1}{d+1} \) is a constant, and \( V_j^i = \frac{V_j}{d+1} \).

Then using equation (12) we immediately obtain:

\[ Q_{i,j}^{j,r} = - \frac{1}{d+1} C_{jr} + \frac{\nabla_{x} V_j}{d+1} = 0. \]

**Proposition 7.** Invariance by translation implies that

\[ \sum_r Q_{i,j}^r = 0, \quad \forall j, i. \quad (14) \]

Another property is

\[ \sum_i Q_{i,j}^r = 0, \quad \forall j, r. \quad (15) \]

A consequence of (8) is

\[ \sum_r Q_{i,j}^r \otimes x_r = 0, \quad \forall j, i. \quad (16) \]

If the velocity of all vertices is the same, that is \( u_r = u \), then the volume fraction is unchanged by the fluid motion. Therefore \( 0 = \sum_r (Q_{i,j}^r, u) \) for all \( u \). It proves (14). The formula (15) comes from \( \sum_i Q_{i,j}^r = V_j \sum_i \nabla_{x} f_j^i = V_j \nabla_{x} \left( \sum_i f_j^i \right) = 0 \) since \( \sum_i f_j^i = 1 \) wherever the vertices are.

The next formula needs more work. One has

\[ \sum_r Q_{i,j}^r \otimes x_r = \sum_r (-f_j^i C_{jr} + \nabla_{x} V_j^i) \otimes x_r , \]

\[ = -f_j^i \sum_r C_{jr} \otimes x_r + \sum_r \nabla_{x} V_j^i \otimes x_r . \]
At this point we use the formula (8) so that
\[ \sum_r C_{jr} \otimes x_r = V_j I. \]
So
\[ \sum_r Q_{jr} \otimes x_r = -f_j V_j I + \sum_r \nabla x_r V_j \otimes x_r. \]

To study the remaining term, we consider one more time the example of the triangle \( T_1 \), as it is depicted in figure 3. In this case the vectors \( \nabla x_r V_j \) are provided by the chain rule formula (13), therefore
\[ \sum_r \nabla x_r V_j \otimes x_r = (\nabla x_1 |T_1| \otimes dx_1 + \nabla x_2 |T_1| \otimes dx_2 + \nabla x_3 |T_1| \otimes dx_3 + \nabla y |T_1| \otimes dy) \]
\[ = (\nabla x_1 |T_1| \otimes dx_1 + \nabla x_2 |T_1| \otimes dx_2 + \nabla x_3 |T_1| \otimes dx_3 + \nabla y |T_1| \otimes dy). \]
\[ (17) \]
That means we have recast the equation in function of the vertices of the triangular sub-cell \( T_1 \). Since by construction the partial derivatives of \( |T_1| \) satisfy the relation (8), it means that \( \sum_r \nabla x_r V_j \otimes x_r = |T_1| I = V_j I \). Therefore
\[ \sum_r Q_{jr} \otimes x_r = -f_j V_j I + V_j I = 0 \]
which proves (16). It ends the proof of the proposition.

4 Compatibility with the fundamental principle of thermodynamics

The compatibility with the fundamental principle of the thermodynamics is much easier to study for semi-discrete schemes. It is convenient to recall first how it is insured for a particular Lagrangian scheme, and then to show how to introduce the idea of subzonal entropy. We take the example of the GLACE scheme [10] which is the one used in all the numerical examples. However, we think that this method can be generalized to other cell-centered schemes like [11, 22].

4.1 The semi-discrete GLACE scheme

We first recall the entropic property of the GLACE scheme, to facilitate understanding of the construction of the stabilized scheme. The GLACE scheme admits the compact semi-discrete form
\[ \begin{align*}
M_j r_j'(t) &= \sum_r (C_{jr}, u_r), \\
M_j u_j'(t) &= -\sum_r C_{jr} p_{jr}, \\
M_j c_j'(t) &= -\sum_r (C_{jr}, u_r) p_{jr}.
\end{align*} \]
\[ (18) \]
The first equation is the discretization of the mass conservation relation, and reflects the compatibility of the method with the geometric conservation law.
The last two equations are the semi-discrete versions of the momentum and total energy equations. The system (18) is completed by the definition of the corner velocities $u_r$ and corner pressures $p_{jr}$. It is shown in [10] that an efficient procedure is to consider the linear system

$$\begin{aligned}
\{ p_{jr} - p_j + \rho_j c_j (u_r - u_j, n_{jr}) = 0, \\
\sum_j C_{jr} p_{jr} = 0,
\end{aligned}$$

(19)

where $c_j$ denotes the speed of sound. The solution is provided by the reduced linear system $A_r u_r = b_r$ obtained from the elimination of the pressure $p_{jr}$, where the matrix is $A_r = \sum_j \rho_j c_j C_{jr} \in \mathbb{R}^{d \times d}$. By construction $A_r = A_t r$ and is non negative. If the mesh is non degenerate then $A_r > 0$. The right hand side is $b_r = \sum_j C_{jr} p_{jr} + \sum_j \rho_j c_j C_{jr} u_j$. The solution of the reduced linear system is $u_r = A_r^{-1} b_r$. Once the nodal velocities $u_r$ have been calculated, one computes the nodal pressures $p_{jr}$ explicitly with $p_{jr} = p_j + \rho_j c_j (u_r - u_j, n_{jr})$. 

**Proposition 8.** The semi-discrete scheme (18) with the nodal solver (19) is compatible with the second principle of thermodynamics, that is $\frac{d}{dt} S_j \geq 0$.

The proof is elementary [10]. One has $T dS = d(e + p\tau) = d(e - (u, du) + p\tau)$, so

$$M_j T_j \frac{d}{dt} S_j = M_j c'_j(t) - (u_j, u'_j(t)) + p_j \tau'_j(t),$$

$$= - \sum_r (C_{jr}, u_r) p_{jr} + (u_j, \sum_r C_{jr} p_{jr}) + p_j \sum_r (C_{jr}, u_r).$$

Since (7) holds true, one can subtract $\sum_r (C_{jr}, u_j) p_j = 0$ and reorganize the sum to get

$$M_j T_j \frac{d}{dt} S_j = \sum_r |C_{jr}| (p_j - p_{jr}) (u_r - u_j, n_{jr}),$$

(20)

$$= \rho_j c_j \sum_r |C_{jr}| (u_r - u_j, n_{jr})^2 \geq 0,$$

due the first equation of the nodal system (19).

**4.2 Generalization to subzonal entropies**

We now focus on the generalization of (18)-(19) to the new entropy $S = S + \varphi(f)$, see equation (2). Consider first the unmodified scheme (18), and analyze the consequences on the new entropy $S$.

**4.2.1 Entropy analysis of the unmodified scheme**

Assume we make the lazy choice to keep unchanged the system (18), and let us evaluate the consequences. The second principle of thermodynamics for $S$ writes

$$T dS = T dS + T d\varphi = T dS + \sum_i \left( T \frac{\partial \varphi}{\partial f^i} \right) df^i.$$
The discrete version of this principle writes, for the cell $j$,
\[
M_j T_j \frac{d}{dt} S_j = M_j T_j \frac{d}{dt} S_j + \sum_i \left( \rho_j T_j \frac{\partial \varphi}{\partial f_i^j} \right) V_j \frac{d}{dt} f_i^j.
\]

**Definition 9.** For our purposes we introduce the coefficient
\[
q_i^j = \rho_j T_j \frac{\partial \varphi}{\partial f_i^j}.
\]  
(21)

Since $\varphi$ has the dimension of an entropy, the coefficient $q_i^j$ has the dimension of a pressure.

The derivative of the cell based entropy $S_j$ is the sum of (20) and of the new terms that come from
\[
V_j \frac{d}{dt} f_i^j(t) = \sum_r (Q_i^j r, u_r), \quad \forall i.
\]

One gets
\[
M_j T_j \frac{d}{dt} S_j = \rho_j c_j \sum_r |C_{jr}| (u_r - u_j, n_{jr})^2 + \sum_i \sum_r q_i^j (Q_i^j r, u_r).
\]

The last contribution is not positive in general, so nothing guarantees the non negativity of the increase of entropy. In other words, the system (18) is not compatible with the second principle of thermodynamics for the entropy $S$.

### 4.2.2 Building an entropic scheme for $\bar{S}$

The previous analysis showed that the chain rule relation for the variation in time of $f_i^j$ adds new terms in the entropy deposit. So, it is worthwhile to incorporate this chain rule relation directly into the semi-discrete system (22). Considering the symmetry of the first two equations in (22), a natural idea is to try to preserve this symmetry also for the last two equations. We obtain the semi-discrete scheme

\[
\begin{align*}
M_j \tau_i^j(t) &= \sum_r (C_{jr}, u_r), \\
V_j \frac{d}{dt} f_i^j(t) &= \sum_r (Q_i^j r, u_r), \\
M_j u_i^j(t) &= -\sum_r C_{jr} p_{jr} - \sum_i \sum_r Q_i^j r q_i^j r, \\
M_j e_i^j(t) &= -\sum_r (C_{jr}, u_r) p_{jr} - \sum_i \sum_r (Q_i^j r, u_r) q_i^j r.
\end{align*}
\]  
(22)

**Proposition 10.** The entropy production of (22) is
\[
M_j T_j \frac{d}{dt} S_j = \rho_j c_j \sum_r |C_{jr}| (u_r - u_j, n_{jr})^2 + \sum_i \sum_r (q_i^j - q_i^j r)(Q_i^j r, (u_r - u_j)).
\]  
(23)
One has

\[ M_j T_j \frac{d}{dt} S_j = M_j \eta_j^t - (u_j, M_j \eta_j^t(t)) + p_j M_j \eta_j^t(t) + \sum_i q_j^i V_j \frac{d}{dt} f_j^i, \]

\[ = p_j \sum_r (C_{jr}, u_r) + \sum_j q_j^i \sum_r (Q_{jr}^i, u_r) \]

\[ + (u_j, \sum_r C_{jr} p_{jr} + \sum_i \sum_r Q_{jr}^i q_{jr}^i) \]

\[ - \sum_r (C_{jr}, u_r) p_{jr} - \sum_i \sum_r (Q_{jr}^i, u_r) q_{jr}^i, \]

Since (7) and (14) hold true, one can substract

\[ \sum_r (C_{jr}, u_j) p_j + \sum_i \sum_r (Q_{jr}^i, u_j) q_j^i = 0. \]

One gets after rearrangements

\[ M_j T_j \frac{d}{dt} S_j = \sum_r |C_{jr}| (p_j - p_{jr}) (u_r - u_j, n_{jr}) \]

\[ + \sum_r \sum_i |Q_{jr}^i| (q_j^i - q_{jr}^i) (u_r - u_j, m_{jr}), \]

where \( m_{jr} = \frac{Q_{jr}^i}{|Q_{jr}^i|} \) and \( n_{jr} = \frac{C_{jr}}{|C_{jr}|} \). So to get the non negativity of the entropy production, it is natural to postulate a proportional relation between the terms arising in the products. In order words, we assume that

\[ \left\{ \begin{array}{l} p_{jr} - p_j + \rho_j c_j (u_r - u_j, n_{jr}) = 0, \\
q_{jr}^i - q_j^i + \rho_j a_j^i (u_r - u_j, m_{jr}) = 0, \forall i, \end{array} \right. \]

where \( a_j^i \geq 0 \) is to be defined. This term has the dimension of a velocity, like \( c_j \).

**Proposition 11.** The semi-discrete scheme (22) with the nodal solver (25) is compatible with the second principle of thermodynamics, that is \( \frac{d}{dt} S_j \geq 0 \).

The identity (24) recasts

\[ M_j T_j \frac{d}{dt} S_j = \rho_j c_j \sum_r |C_{jr}| (u_r - u_j, n_{jr})^2 \]

\[ + \rho_j \sum_i a_j^i \sum_r |Q_{jr}^i| (u_r - u_j, n_{jr})^2 \geq 0. \]

The right hand side in the impulse equation in (22) may be interpreted as the sum of some forces which are defined at the vertices. The total impulse conservation requires also that the total sum of the forces is zero. This is the case if the sum of forces vanishes at all vertices independently, that is

\[ \sum_j C_{jr} p_{jr} + \sum_i \sum_j Q_{jr}^i q_{jr}^i = 0. \]
The linear system constituted by (25-27) is obviously non-singular. Indeed, its solution is obtained by the elimination of the $p_{jr}$'s and the $q_{jr}^i$'s in (27). One gets formally the same linear system

$$A_r u_r = b_r$$

but the matrix is now

$$A_r = \sum_j \rho_j c_j \frac{C_{jr} \otimes C_{jr}}{|C_{jr}|} + \sum_i \sum_j \rho_j a_j^i q_{jr}^i \frac{Q_{jr}^i \otimes Q_{jr}^i}{|Q_{jr}|},$$

(28)

and the right hand side is

$$b_r = \sum_j \left( C_{jr} p_j + \rho_j c_j \frac{C_{jr} \otimes C_{jr}}{|C_{jr}|} u_j \right) + \sum_i \sum_j \left( Q_{jr}^i q_j^i + \rho_j a_j^i \frac{Q_{jr}^i \otimes Q_{jr}^i}{|Q_{jr}|} u_j \right).$$

(29)

Once the velocity is computed, it is immediate to calculate $p_{jr}$ and $q_{jr}^i$ with (25).

Finally the semi-discrete scheme with a subzonal entropy is defined by (22) with the nodal solver defined by (25-27).

**Remark 12.** Due to the remark 6, the stabilization has no effect in 1D and on simplex meshes.

5 GLACE scheme with subzonal entropy

The fully discrete GLACE scheme with a subzonal entropy is obtained by replacing the two continuous in time equations of the system (22) by their fully discrete equivalent. The idea is that if the control of the time step is appropriate, the fully discrete algorithm behaves like the semi-discrete one. One obtains the following loop in time. From now on, the index $k$ will indicate the time step ($t_k = k \Delta t$).

1) At the beginning of the time step $t_k = k \Delta t$, one computes the geometrical vectors $C_{jr}^k$ and $Q_{jr}^k$ for all $j, r, i$, as a function of the vertices $x_r^k$.

2) Then one determines the nodal velocities $u_r^k$, the nodal pressures $p_{jr}^k$ and the new terms $q_{jr}^i$ using the nodal solver (25-27).

3) It is enough to update the total momentum and the total energy. For the momentum one uses

$$M_j \frac{u_{jr}^{k+1} - u_{jr}^k}{\Delta t} = - \sum_r C_{jr}^k p_{jr}^k - \sum_i \sum_r Q_{jr}^i q_{jr}^i.$$  

(30)

The total energy is updated with

$$M_j \frac{e_{jr}^{k+1} - e_{jr}^k}{\Delta t} = - \sum_r (C_{jr}^k, u_r^k) p_{jr}^k - \sum_i \sum_r (Q_{jr}^i, u_r^i) q_{jr}^i.$$  

(31)
4) Then the vertices are moved

\[ x_k^{k+1} = x_k^k + \Delta t \, u_k^k. \] (32)

One computes the new volume \( V_{j+1} \) and the new sub-volumes, which gives the new volume fractions \( f_{j+1}^k \).

5) Finally the new density in the cell is computed

\[ \rho_{j+1} = \frac{M_j}{V_{j+1}}. \] (33)

For the algorithm to be fully defined, it remains to precise the time step restriction (CFL condition) and the optimal choice of the constants \( a_{ij} \) which are ultimately related to the choice of an optimal subzonal entropy. Some properties are however independent of these considerations.

**Proposition 13.** By construction, the GLACE scheme with subzonal entropy is locally conservative in total mass, total momentum and total energy.

By construction the scheme is conservative for the mass of each cell, so the total mass is also preserved. Concerning the total momentum one has

\[ \sum_j M_j \frac{u_{j+1}^k - u_j^k}{\Delta t} = - \sum_j \sum_r C_{j,r}^k p_{j,r}^k - \sum_j \sum_i \sum_r Q_{i,jr}^k q_{j,r}^k, \]

\[ = - \sum_r \left( \sum_j C_{j,r}^k p_{j,r}^k + \sum_j \sum_i Q_{i,jr}^k q_{j,r}^k \right) = 0, \]

due to the nodal equation (27). Therefore the total momentum is indeed preserved. A similar algebra shows that

\[ \sum_j M_j \frac{e_{j+1}^k - e_j^k}{\Delta t} = - \sum_r \left( \sum_j C_{j,r}^k p_{j,r}^k + \sum_j \sum_i Q_{i,jr}^k q_{j,r}^k \right), u_r^k \right) = 0 \]

for the same reason. Therefore the total energy is preserved.

6 Design of a particular subzonal entropy

In this section we focus on the effective construction of a subzonal entropy which is the one used for the numerical tests.
6.1 The rest property

It is now clear, considering the momentum equation (30), that \( \sum_i \sum_j Q_{jr}^i q_{jr}^i \) is some kind of numerical force stabilizing the calculation. A natural requirement is that this force vanishes if the flow is at rest, that is if the physical force vanishes \( \sum_j C_{jr} p_{jr} = 0 \). That is why we propose to add a new constraint on \( \varphi \), which is highly desirable at least at the initial time: the rest property. It means that if the pressure is locally constant, \( p_j = p \) for all \( j \), and the velocity is locally constant, \( u_j = u \) for all \( j \), then the solution of the linear solver must be such that \( p^r_{jr} = p \) and \( u^r_j = u \) for all \( r \) and all \( j \).

It is quite easy to determine a sufficient condition so that the rest property holds. Let assume the hypothesis of the definition is verified. Then the right hand side of the linear system (29) recasts

\[
\mathbf{b}_r = \mathbf{A}_r \mathbf{u} + \sum_i \sum_j Q_{jr}^i q_{jr}^i, \tag{34}
\]

since \( \sum_j C_{jr} = 0 \) and using the definition of \( \mathbf{A}_r \) (28). On the other hand, the right hand side of the impulse equation (31) is

\[
\text{RHS} = -\sum_j C_{jr} p_{jr} - \sum_i \sum_r Q_{jr}^i q_{jr}^i. \tag{35}
\]

We find that assuming

\[
\sum_i \sum_j Q_{jr}^i q_{jr}^j = 0, \tag{36}
\]

the equations (34) gives us \( \mathbf{u}_r = \mathbf{u} \) since \( \mathbf{A}_r \mathbf{u}_r = \mathbf{b}_r \). Therefore, equation (25) give us necessarily \( p_{jr} = p_j = p \) and \( q_{jr}^i = q_j^i \). Substituting these terms into the equation (35) gives us

\[
\text{RHS} = -\sum_i \sum_r Q_{jr}^i q_{jr}^i. \tag{37}
\]

If we now also assume

\[
\sum_i \sum_r Q_{jr}^i q_{jr}^i = 0, \tag{37}
\]

the rest property is fulfilled.

Considering (36-37) and (15), a sufficient condition to have the rest property is \( q_j^i = q_j \) independently of the sub-volume index \( i \), at least at initial stages of the computation. If this \( q_j \) is also independent of the time step, it means that, up to the redefinition of the concave function \( \varphi \), it is possible to set \( q_j \) to zero. That is why we will consider for simplicity the case

\[
q_j^i = 0, \quad \forall i. \tag{38}
\]

Considering the definition (21) and the fact that \( \varphi \) is concave, it means that \( \varphi \) reaches its maximum.
Definition 14. Assume a perfect gas pressure law with coefficient $C_v$. Let $0 < \mu \leq 1$ be a scaling coefficient. The following family of subzonal entropies satisfy the rest property at initial time

$$\varphi(f) = \mu C_v \sum \left( \log f^i_j - \frac{f^i_j}{f^i_{j,0}} \right),$$

(39)

where $f^i_{j,0}$ is the initial value of the volume fraction $i$ in cell $j$.

The function $\varphi$ is clearly concave and equal to $-\infty$ if one volume fraction vanishes. One has

$$\frac{\partial \varphi}{\partial f^i_j} = \mu C_v \left( \frac{1}{f^i_j} - \frac{1}{f^i_{j,0}} \right),$$

(40)

so $q^i_j = 0$ at initial time $t = 0$. Therefore the rest property is satisfied at initial time.

Remark 15. It is worthwhile to note that this subzonal entropy has nothing physical. It cannot be derived from a physically relevant entropy. For a general pressure law we use in practice the same subzonal entropy with $C_v = \partial T/\partial \varepsilon$.

Remark 16. The expression (40) shows that a kind of force tries to restore $f^i_j \approx f^i_{j,0}$ during the computation. It has at least two important consequences. Firstly it controls the appearance of hourglass modes: in our context a hourglass mode [9] corresponds to a strong deviation from $f^i_j \approx f^i_{j,0} \approx \frac{1}{4}$; subzonal entropies control this phenomenon as shown in figure 8. Secondly this restoring force is larger and larger if $f^i_j \approx 0$ which is characteristic of an almost tangling situation; at the limit the restoring is infinite which prevents tangling. We will show in the next section that this restoring force is nevertheless consistent, that is the limit solution for small cells is the correct one.

6.2 The parameter $a^i_j$

Finally we precise the choice of the constant $a^i_j$ which appears in (25). This coefficient is a kind of speed of sound, but for the subzonal entropy. It is possible in principle to use $a^i_j = c_j$, but we propose another choice. In our computations we mostly use the formula

$$a^i_j = \sqrt{-T_j \frac{\partial^2 \varphi}{(\partial f^i_j)^2}}.$$  

(41)

We have derived this formula by analogy with the classical formula for the speed of sound $c$

$$\rho c = \sqrt{\frac{\partial p}{\partial \tau}} = \sqrt{- \frac{\partial}{\partial \tau} \left( T \frac{\partial S}{\partial \tau} \right)}.$$  

Since $\varphi$ has the dimension of an entropy, it shows that (41) is correct from that point of view. The advantage of (41) is that $a^i_j$ may be kept as small as desired.
just by lessening the parameter \( \mu \) in (39). At the limit \( \mu \to 0 \) one recovers the original algorithm without subzonal entropy.

If one uses the subzonal entropy (39) and a perfect gas law such that \( \varepsilon = C_v T \) and \( c^2 = \gamma(\gamma - 1)\varepsilon \), one obtains

\[
a^j_i = \sqrt{\frac{\mu C_v T_j}{(f_j)^{3/2}}} = \sqrt{\frac{\mu C_v T_j}{f_j^3}} = \sqrt{\frac{\mu}{\gamma(\gamma - 1)}} \times f_j^1. \tag{42}
\]

It shows that the speed of sound \( c_j \) is multiplied by a constant factor \( \sqrt{\frac{\mu}{\gamma(\gamma - 1)}} \) which can be made as small or as large as desired just by changing \( \mu \). But probably much more important, one sees that if the volume fraction becomes close to zero, which is the indication of a nearly pathological mesh, then the coefficient \( a^j_i \) becomes very large. This is a kind of non linear feedback of the subzonal entropy.

6.3 Time step restriction

The CFL restriction on the time step must of course be of the same nature that the one used in standard Lagrangian computations, that is

\[
\max_j \left( \frac{c_j}{\Delta x_j} \right) \Delta t \leq \text{CFL}_1 \leq 1,
\]

where \( c_j \) is the speed of sound in the cell, \( \Delta x_j \) is the local length of the cell and \( \text{CFL}_1 \leq 1 \) is a security coefficient. We refer to \([10]\) for a more precise description in the context of the GLACE scheme. Usually an additional constraint on the variation of the volume of cell

\[
\max_j \left| \frac{V^k_j - V^{k-1}_j}{V^k_j} \right| \leq \text{CFL}_2 \leq 1,
\]

is considered in order to enhance the stability. We have made various tests in order to determine an optimal time step restriction for the new algorithm. We propose to consider

\[
\max_{ij} \left( \frac{c_j + a^j_i}{\Delta x_j} \right) \Delta t \leq \text{CFL}_4. \tag{43}
\]

It has the advantage of lessening the time step when one volume fraction is close to zero, because in this case \( a^j_i \) becomes large, see (42). The discrete algorithm (30-33) is then closer to the semi-discrete algorithm described in (22) for which stability holds due to the general entropy inequality

\[
\frac{d}{dt} S_j \geq 0
\]

with a subzonal entropy.

7 Consistency

The introduction of the subzonal entropy has been done in a way compatible with some fundamental principles which are conservativity, the satisfaction of
various chain rule relations and the entropy principle. In doing this, we have deeply modified the original algorithm: one may consider as well that we have modified the model itself. It raises the natural question of how much the new terms are consistent or not. We propose three different arguments which explain why the stabilized GLACE scheme with subzonal entropies is still consistent.

Our first argument is more at the philosophical level. Indeed, the notion of a subzonal entropy is derived from some geometric decomposition of a quadrangular cell into triangular sub-cells. Numerous test cases have shown that Lagrangian computations with either quadrangular or triangular cells give the same quasi-converged solution, for very small mesh length. It is an indication that the consistency of the method is somehow independent of the mesh structure. We also remark, our subzone entropy is very close to the mixing subzone entropy described in the subsection 2.1.

Second we analyze in the appendix the consistency in the mimetic sense of the subzonal entropy contribution to the discrete gradient operator. This analysis gives an indication of why the method used in [14] should work to prove the weak consistency of the algorithm proposed in this work. The notion of a mimetic discretization has been introduced in a series of papers by Shashkov and coworkers. It consists in checking whether a given discrete first-order partial differential operator is exact for linear profiles, or not. Actually in the mentioned works it is more a design principle for the construction of new numerical methods. In our case, it is an a posteriori analysis. This mimetic interpretation may be viewed as a sanity check test of consistency.

Third we propose in the numerical section a series of numerical tests which indeed show the convergence of the procedure independently of the subzonal entropy. It shows that the limit solution for small mesh size is the correct one: this approach is of course restricted to problems for which a reference analytical solution is available.

8 Numerical examples

In this section we present the results of a selection of standard test problems in the context of Lagrangian algorithms for 2D compressible gas dynamics equations (see for example [10, 22, 9, 25] and many other related works). In most of these computations we use the decomposition described in figure 1. For Noh and Sedov problems we also present some results computed with the decomposition depicted in figure 21. To simplify the presentation, the decomposition of figure 1 (resp. figure 21) will be called decomposition I (resp. decomposition II). The time step restriction is $CFL_1 \approx 0.4$ and $CFL_2 \approx 0.1$. For all these problems, we use a second-order extension of the GLACE scheme described in [10], except for the shell problem, computed using the first-order scheme. By second-order we mean that pressures and velocities used in the nodal Riemann solvers are enhanced with a standard second-order MUSCL reconstruction. The stabilized quantities are used first-order.
8.1 Sod problem

First numerical experiment is dedicated to the well-known Sod problem. It is a Riemann shock tube, with a mild discontinuity. The solution consists in an expanding rarefaction at the left, a contact discontinuity, and a shock moving to the right. We use a computational domain of size $1 \times 0.1$ in the $x$ and $y$ directions. The contact discontinuity is initially at $x = 0.5$. The domain is filled with an ideal gas with $\gamma = 1.4$. In the left part of the domain, $p = 1$ and $\rho = 1$ initially, while in the right part $p = 0.1$ and $\rho = 0.125$. We perform a convergence study on this case. For our coarsest simulation, we use $N_x = 20$ and $N_y = 6$ cells respectively in the $x$ and $y$ direction. We refine the mesh by a factor 2 in each direction until a resolution of $N_x = 640$ and $N_y = 96$. The $L^1$ error norm $e$ is simply computed by:

$$ e = \frac{\sum_j |\rho_j - \rho_{\text{analytic}}(x_j)| V_j}{\sum_j M_j} $$

(44)

where $\rho_{\text{analytic}}(x_j)$ accounts for the analytical value of the density at the center of the cell $j$. Since $\rho$ is discontinuous at the contact discontinuity and at the shock, this formula is only order 1 accurate, but it is sufficient because we expect a convergence rate lower than 1.

We run first the simulation on a classical regular planar mesh: we will say that this mesh corresponds to a 0% perturbation. Nevertheless we use a subzonal entropy. Since the mesh is kept regular planar during the computation it means that $f^i_j = \frac{1}{4}$ for all cells and at each time steps. Therefore the limiting force (40) vanishes and the only effect of stabilization is a very slight increase of the magnitude of $A_r$ (28) and $b_r$ (29). We observe that the results are as good as without stabilization. At least the numerical results converge to the correct solution when $h \to 0^+$ whatever $\mu$ is, as shown is the last line of table 1. Now we impose a perturbation to the initial mesh, consisting in randomly moving the initially regularly spaced position of the nodes. The maximal random displacement is chosen to be of 30% and 50% of the regular spacing of the nodes, giving an almost singular initial mesh for the last case. Several values of the
Figure 5: Zoom on mesh structures of the Sod shock tube problem with a perturbed initial mesh.

coefficient $\mu$ are probed from 0 (original GLACE scheme) to 1 (strong stabilization). Results, all obtained with decomposition $I$, are given in tables 1 to 3. Values in red correspond to tangled mesh and failed simulations.

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>20</th>
<th>40</th>
<th>80</th>
<th>160</th>
<th>320</th>
<th>640</th>
<th>Order</th>
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<td>0.61</td>
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Table 1: Relative $L^1$-error and convergence order for a regular mesh

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>20</th>
<th>40</th>
<th>80</th>
<th>160</th>
<th>320</th>
<th>640</th>
<th>Order</th>
</tr>
</thead>
<tbody>
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<td>2.14e-2</td>
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<td>failed</td>
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</tr>
</tbody>
</table>

Table 2: Relative $L^1$-error for a random displacement of 30%

General considerations about these tables are the following:
Table 3: Relative $L^1$-error for a random displacement of 50%

<table>
<thead>
<tr>
<th>$\mu$</th>
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<th>40</th>
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<th>160</th>
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<td>2.319e-2</td>
<td>3.163</td>
<td>failed</td>
<td>failed</td>
<td></td>
</tr>
</tbody>
</table>

- All calculations using the stabilization succeed to give correct results, while original GLACE scheme does not succeed to simulate the problem for perturbed fine meshes.
- Order of convergence is between 0.6 to 0.82, whatever the level of stabilization, which is comparable with the order of convergence of the non stabilized GLACE scheme (0.61).
- Errors are significantly higher for $\mu = 1$, but for lower values of $\mu$ there are of the same order of magnitude than for the non stabilized scheme.

This convergence test makes us confident in the consistency of the global scheme (GLACE+stabilization) whatever the choice of $\mu$.

### 8.2 Saltzman problem

The Saltzmann test problem is a severe shock tube problem computed on a distorted mesh. The data are described in [7]. At $t = 0$, the density is $\rho = 1$, the pressure is $\approx 0$ ($10^{-6}$ in practice), the velocity is 0. The piston’s velocity is 1. Since the initial length is $L = 1$, it is not possible to run the problem after $T = 1$. Cell-centered methods give already very reasonable results in term of accuracy and robustness [10, 22]. Here we consider a final time of $t = 1 - 10^{-2}$ which is very close to the final time. At this time the very high compression of the flow induces a severe tangling of the mesh: see the result on the left of figure 6 which is computed without stabilization. On the contrary the entropy stabilization effectively eliminates this unphysical pathology of the mesh: the right plot in figure 6 uses $\mu = 10^{-1}$; the plot in the center uses $\mu = 10^{-3}$.

### 8.3 Shell problem

This quasi-incompressible problem is described in [10] and is very sensitive to the intrinsic dissipation of the cell-centered numerical method in use. Initial mesh is characteristic of a shell $R^- = 0.95 \leq r \leq 1 = R^+$. Initial values are: $\rho = 1$, $p = 2$, and the velocity is directed towards the center $u = -\frac{1}{2}r$. Initial velocity is divergence free. We take $\gamma = 2$: other values are possible without major changes. The boundary conditions are the following: sliding
Figure 6: Plot of the Saltzmann test problem for $t = 0.99$. Without stabilization, the mesh tangles on the left because some nodes that should be internal are now out of the physical domain of simulation. With entropy stabilization (based on decomposition I in this test), the mesh is always correct since the volumes are kept positive. The coefficient is $\mu = 0$ on the left, $\mu = 10^{-3}$ in between and $\mu = 10^{-1}$ on the right.

walls on the planes, and a given pressure $p_{\text{ext}} = 2$ on the internal and external boundaries. This problem is computed with a reasonable mesh 40 layers and 20 sectors. We plot in figures (7) the radial density profile versus the radius $r$. We use the decomposition I. It shows that overall viscosity added by the stabilization procedure is low. Therefore it still allows to compute an accurate solution for this stringent quasi-incompressible problem. In every cases, results are one order of magnitude better than result of the same problem computed with a more viscous first-order scheme like [22] (note that second order extension enhances greatly this result). We refer to [10] for a detailed analysis of the viscous structure of the basic GLACE scheme and for more comparisons.

8.4 Noh problem

The Noh problem is known to be a severe one for many Lagrangian schemes, and particularly for the basic GLACE scheme [10]. The results displayed below show that the stabilization procedure effectively controls all the previous unphysical features. The final time is $t = 0.6$ and the exact shock position is at $r = 0.2$. Analytical value of the density in the plateau is $\rho = 16$.

8.4.1 Polar mesh

The Noh problem on a polar mesh may induces spurious modes near the center because of the infinite strength of the shock. This is particularly the case for
calculation with the GLACE scheme.

We run this problem without stabilization, and compare with the stabilization based on decomposition I. We observe as usual spurious modes without stabilization. On the other hand, the stabilization is able to completely control appearance of spurious modes, whereas we use here a low value of the parameter \( \mu = 10^{-3} \). Symmetries discrepancy in the mesh is between the machine accuracy \( \approx 10^{-16} \) at time \( t = 0 \) and \( \approx 10^{-14} \) at final time \( t = 0.6 \).

It shows that stabilization fulfills its role of controlling spurious numerical modes of the calculation, even if the mesh is far to be pathological.

8.4.2 Cartesian mesh

This is a challenging test problem for most Lagrangian schemes because of tangling. Without stabilization we observe spurious modes and the computation fails. With stabilization the mesh never tangles since \( \mu > 0 \). The quality of the results depends however of the parameter \( \mu \). For small \( \mu \) the mesh is of course close to a pathological mesh.

In figure 10 we compare the result computed with the standard decomposition I with the one computed with decomposition II which guarantees that all cells remain convex. This is indeed what we observe. It also enhances the global quality of the mesh.

In figure 11 we plot four different results computed with three mesh sizes \( \Delta x = \frac{1}{40} \), \( \Delta x = \frac{1}{80} \) and \( \Delta x = \frac{1}{160} \). It illustrates the numerical convergence of the discrete density plateau to the analytical value \( \rho = 16 \). The shock position is accurate. We also plot a fourth result obtained with the decomposition II: it shows that forcing convex cells enhances the quality of the numerical result.

In the last figure of this series we plot the history of the integrated Riemann entropy production which is the first contribution in the right hand side of the entropy identity of (26) (for convenience, time index is omitted in the following
Figure 8: Noh problem without stabilization on the right and with stabilization on the left. On the right part spurious modes spoil the calculation. In this test these spurious modes seem to be the sum of short range hourglass modes and of a long range spurious mode. The total deformation is much more pronounced near the boundaries. We observe that stabilization inhibits all these spurious modes.

Figure 9: Density plot of the Noh problem on a polar mesh, $t = 0.6$. The shock locus at $r = 0.2$ is perfect for all tested parameters $\mu = 0.1$ and $\mu = 0.001$. The default of symmetry of the mesh is between the machine accuracy $\approx 10^{-16}$ at $t = 0$ and $\approx 10^{-14}$ at the final time $t = 0.6$. The density plateau is very close to the analytical value which is $\rho = 16$. One observes that stronger stabilization gives a slightly better control of the oscillations due to wall heating at origin.

Formulas

$$E_{\text{Riemann}} = \sum_j \rho_j c_j \sum_r |C_{jr}| (u_r - u_j, n_{jr})^2$$

and of the integrated sub-cell entropy production which is the second contribu-
tion in (26)

\[ E_{\text{Sub-cell}} = \sum_j \rho_j \sum_i a_i^j \sum_r |Q_{jr}^r| (\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr})^2. \]

The sum is the total entropy production

\[ E_{\text{Total}} = E_{\text{Riemann}} + E_{\text{Sub-cell}}. \]

We plot the history of these quantities, that is \( t \mapsto E_{\text{Riemann}}(t) \) and so on, in figure 12. We see that the entropy productions are linear with respect to \( t \) which is easy to explain since the length of shock line is also a linear function of \( t \) and the shock strength is constant. What is particularly interesting in this case is the fact that \( E_{\text{Sub-cell}} \) > \( E_{\text{Riemann}} \) but is also of the same order of magnitude. It shows the stabilization terms provide an important contribution to the entropy production required to stabilize the mesh. We also note on the same figure that the entropy production indicators are somehow independent of the mesh size.

Figure 10: Noh problem on a Cartesian mesh. We use the stabilization with decomposition I on the right, \( \mu = 10^{-1} \). The left part (\( \mu = 10^{-2} \)) of the figure has been computed with decomposition II explained in the appendix: by construction this stabilization prevents from non-convex cells; we observe that the mesh is indeed more regular on the left.

8.5 Sedov problem on a square mesh

Even if the physics of the Sedov problem is different from the Noh problem, our conclusions about the interest of the stabilization are somewhat identical.

In figure 13 we plot the result of four different calculations which show that the mesh never tangles, but also that the best results are obtained with, either
Figure 11: Density plot of the Noh problem on Cartesian meshes. Top left 40 × 40 cells, top right 80 × 80 cells, bottom left 160 × 160. The dispersion of the results is characteristics of Cartesian meshes. These three results have been computed with $\mu = 0.1$ and show the convergence to the exact solution. Bottom right 160 × 160 cells with $\mu = 0.01$ and the decomposition II: the use of a decomposition that guarantees convex cells enhances the quality of the discrete solution near the origin with respect to the result on its left.

$\mu = 10^{-2}$ and the convex decomposition II, or $\mu = 10^{-1}$ and the standard decomposition I.

The dispersion of the density computed with these two best choices of the parameters is displayed in figure 16. The shock is sharp at the correct position $x = 1$ and with the correct intensity $\rho = 6$.

We plot in figure 15 entropy productions, that are $E_{\text{Riemann}}$, $E_{\text{Sub-cell}}$ and $E_{\text{Total}} = E_{\text{Riemann}} + E_{\text{Sub-cell}}$. In all cases Riemann entropy production and sub-cell entropy production are of the same order of magnitude. We see that the two best results of figure 13 corresponds to a sub-cell entropy production greater than the Riemann entropy production.

8.6 Resistance to axis impact

This problem is a severe test of intrinsic stability of the underlying Lagrangian scheme. A polar mesh is initially at rest. The pressure at boundary is equal to the pressure inside the domain $p_0 = 1$. The velocity at boundary is zero, equal to the initial velocity inside the domain $u_0 = 0$, except at the two exterior corners of the mesh. At these two points the inward velocity is set to 1, that is $|u_{\text{impact}}| = 1$. There is no analytical or reference solution to such a problem which is not physical. The result displayed on the left of figure 16 is highly representative of the fundamental stability property of the algorithm described.
Figure 12: Entropy production for the Noh problem with $\mu = 10^{-1}$. Top left we use a $40 \times 40$ cells mesh and top right a $80 \times 80$ cells mesh, both with the standard decomposition I. Bottom results are computed with the $160 \times 160$ cells mesh: on the left with the standard decomposition I, on the right with decomposition II. The total entropy production is linear with respect to $t$. We observe that the entropy production indicators are somehow independent of the mesh size; it indicates that these indicators are correlated to the physics of the problem and that they are a good measurement of the ratio between the dissipation needed to propagate the shock and the dissipation needed to control the mesh. It is an indication that the sub-cell entropy production is essential to compensate for a too weak Riemann entropy production. The sub-cell entropy production is slightly greater with the last result computed with decomposition II.

in this paper. As far as we know, no other Lagrangian method is able to resist to the corner forces without tangling.

8.7 Perspective: Richtmyer-Meshkov instability and towards ALE

The last test case illustrates the necessary balance between numerical stabilization and physically motivated stabilization. We show here, numerical stabilization is needed, but not designed to handle very strong physical shear of the flow appearing at later time of the calculation. Data [3] correspond to a Richtmyer-Meshkov instability [23, 24]. A shock impinges from the right on a sinusoidal interface. It triggers the development of the Richtmyer-Meshkov instability. We display in figure 17 the history of the density map. On the bottom is the Lagrangian calculation without stabilization: it crashes when the mesh tangles due to the appearance of many spurious modes. On the top is a
Figure 13: Numerical solution of the Sedov problem. The parameters are $\mu = 10^{-2}$ on the left and $\mu = 10^{-1}$ on the right. We use decomposition II on the top, and decomposition I on the bottom.

Figure 14: Density plot of the Sedov problem on a Cartesian mesh. The shock is sharp. Some dispersion is visible. The increase of the quality of the mesh insured by the decomposition II seems to be correlated to a better prediction of the peak density: $\rho_{\text{peak}} = 6$ for the exact solution.
Figure 15: The organization of this figure corresponds to the one of figure 13. We plot three curves per figure: one is the total entropy production which is the sum of the Riemann entropy production and of the sub-cell entropy production. An interesting remark about entropy production is the total entropy production is roughly constant, whatever the parameter $\mu$, and the strategy of decomposition of the cell into sub-cells. However, the balance between Riemann entropy and sub-cell entropy is closely related to the stabilization strategy and to the quality of the results. In particular, figure 13 shows the interest of a good calibration of the sub-cell entropy production.

ALE calculation very close to a purely Lagrange+remap calculation: the mesh is of course completely under control. In between is the result of the stabilized Lagrangian calculation: we observe that this calculation is very robust.

At a certain time, it is necessary to continue the calculation with this quite coarse mesh, to adapt the mesh using an ALE procedure. If not, the fundamental robustness of the proposed algorithm necessarily freezes the flow, as displayed in the figure 18. However, consistency properties make us confident in the convergence of the stabilized algorithm, without help of ALE, but at the price of an undesirable increase of the number of degrees of freedom.

9 Conclusion

We have presented a new stabilization approach which is based on subzonal entropy and can be adapted \textit{a priori} to any conservative cell-centered Lagrangian scheme [4, 9, 10, 22]. We have used it to stabilize the cell-centered Lagrangian numerical scheme GLACE [10]. The numerical results in 2D assess the properties of the method: robustness is achieved in all cases. Problems that were before difficult for the low dissipativity GLACE scheme are now easy. The
method allows for an *a posteriori* analysis of the entropy dissipation which is decomposed between a classical Riemann entropy production (for shocks) and the additional sub-cell entropy production (for the correctness of the mesh). The entropy indicators that were used are more or less independent of the mesh size. A prescription that can be drown after numerous test cases is to take the stabilization parameter between $\mu_- = 10^{-3}$ for standard problems and $\mu_+ = 10^{-1}$ for difficult problems like Noh or Sedov problems on Cartesian grids. Intermediate value $\mu = 10^{-2}$ is a good compromise.

By construction the method can be used in any dimension. Further researches will be devoted to the development and optimization of sub-cell decompositions of 3D cells like hexahedrons.

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### A Mimetic analysis

The idea is the following. One has to assume that the fluxes are linear quantities with respect to the space variable. Then one computes the local discrete gradient or the local discrete divergence. If the result is exact, we will say that the scheme is consistent in the mimetic sense. To be more specific we propose to retain the following definition where we focus on the gradient operator.

We assume that $p_{jr}$ is linear with respect to $x_r$, that is $p_{jr} = b + (c, x_r)$. We also assume that all the $q^{i}_{jr}$ are also linear with respect to $x_r$, that is $q^{i}_{jr} =$
\[ b^i_j + (c^i_j, x_r) \]. If
\[
\frac{1}{V_j} \left( \sum_r C_{jr} p_{jr} + \sum_i \sum_r Q_{jr}^i q_{jr}^i \right) = c,
\]
we will say that the gradient operator is consistent in the mimetic sense.

Concerning the divergence operator a similar property can be checked as a consequence of the fact that the divergence of a vector field is equal to the trace of its gradient. So the consistency in the mimetic sense of the gradient implies the consistency in the mimetic sense of the divergence.

**Proposition 17.** The gradient operator is consistent in the mimetic sense.

One has
\[
\sum_r C_{jr} p_{jr} = \sum_r C_{jr} b + \sum_r C_{jr} (c, x_r) = \left( \sum_r C_{jr} \right) b + \left( \sum_r C_{jr} \otimes x_r \right) c.
\]

Using (7-8) one obtains
\[
\frac{1}{V_j} \sum_r C_{jr} p_{jr} = 0 + \frac{1}{V_j} V_j c = c.
\]

On the other hand for all \( i \)
\[
\sum_r Q_{jr}^i q_{jr}^i = \sum_r Q_{jr}^i b^i_j + \sum_r Q_{jr}^i (c^i_j, x_r) = \left( \sum_r Q_{jr}^i \right) b^i_j + \left( \sum_r Q_{jr}^i \otimes x_r \right) c^i_j.
\]

Using (14-16) one obtains directly \( \sum_r Q_{jr}^i q_{jr}^i = 0 \). Therefore the gradient operator is consistent in the mimetic sense.

## B Other subzonal decompositions

The subzonal entropy proposed in section 2 is based on the choice of a convenient concave function on the one hand, and is applied to a particular decomposition of the cell on the other hand. In what follows we discuss two other natural decompositions of a quadrangle.

### B.1 Decomposition in sub-quadrangles

It corresponds to the figure 19. A useful choice is to take \( L = \frac{1}{2} (A + B) \) and so on for all edges. The center is
\[
O = \frac{1}{4} (A + B + C + D) = \frac{1}{4} (K + L + M + N).
\]

This decomposition is common to many authors. In our context we do not see any advantage of using this decomposition instead of the one depicted in figure 1. Indeed the \( A \rightarrow D \) limit of such a quad, figure 20, is more difficult to analyze. The volume fraction of the sub-quad \( ALOK \) doe not tend to zero. So a subzonal entropy cannot prevent tangling in this situation.
B.2 Decomposition in two sub-triangles

The last configuration that we consider is more appealing. Let us consider the figure 21. If one uses a subzonal entropy in this case, the four different volume fractions remain positive. Tangling will be controlled as in the situation analyzed in section 2. By construction the quad will also remain convex: for example the node $A$ cannot cross the line $BD$ because it would force the volume fraction of the sub-triangle $ABD$ to go to zero, and this is forbidden by the subzonal entropy. It is worthwhile to notice that such a decomposition is purely a numerical one and has absolutely nothing physical.

References


Figure 17: A shock comes from the right on a sinusoidal interface and triggers a Richtmyer-Meshkov instability. The ALE calculation is on top, the Lagrangian calculation without stabilization on bottom and the Lagrangian calculation with stabilization in between. All these results have been computed with $\mu = 10^{-3}$. 

$t = 0$

$t = 0.025 \text{ s}$

$t = 0.027 \text{ s}$

$t = 0.031 \text{ s}$

$t = 0.0315 \text{ s}$

$t = 0.031 \text{ s}$
Figure 18: Time $t = 0.005$ s. The purely Lagrangian stabilized calculation on the bottom inhibits the development of the Richtmyer-Meshkov instability at latest times. An ALE procedure is mandatory to continue the calculation with reasonable accuracy.

Figure 19: Sub-cell decomposition of a quad into four quads.

Figure 20: Pathological evolution of the quad.
Figure 21: Decomposition of a quad in two different sets of triangles.