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Short Note

Volume consistency in a staggered grid Lagrangian hydrodynamics scheme

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Abstract

Staggered grid Lagrangian schemes for compressible hydrodynamics involve a choice of how internal energy is advanced in time. The options depend on two ways of defining cell volumes: an indirect one, that guarantees total energy conservation, and a direct one that computes the volume from its definition as a function of the cell vertices. It is shown that the motion of the vertices can be defined so that the two volume definitions are identical. A so modified total energy conserving staggered scheme is applied to the Coggeshall adiabatic compression problem, and now also entropy is basically exactly conserved for each Lagrangian cell, and there is increased accuracy for internal energy. The overall improvement as the grid is refined is less than what might be expected.

Keywords: Staggered Lagrangian schemes; Volume consistency; Entropy; Hydrodynamics

1. Introduction

In this note we construct a modification of the classic staggered grid Lagrangian compressible hydrodynamics scheme as described, for example, in [2]. With this modification we remove the ambiguity in the definition of cell volume that results from requiring both total energy conservation and the modeling of the internal energy advance from the differential equation $\frac{de}{dt} + p\frac{d(1/\rho)}{dt} = 0$. This is brought about by appropriately relating the motion of cell vertices to the cell volume change. Our approach is algebraic and simply stated. We then test this modification on the Coggeshall adiabatic compression problem [5]. We observe that now in addition to energy conservation the cell entropies are almost exactly conserved.

In the staggered scheme there are two sets of variables. First, for definiteness specifically in two dimensions, there is a set of indexed nodes or vertices at which the variables are coordinates (x_i, y_i), velocities (u_i, v_i), and nodal masses m^i. Next, there is a set of indexed cells at which the variables are cell volumes V_j, masses m_j, densities ρ_j, specific internal energies e_j, and pressures p_j. The set of cell (resp. node) indexes is $\mathscr{J}$ (resp.

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$\mathscr{I}$). Both sets of data are given at the start of a time step. Nodal and cell masses are Lagrangian, that is, independent of time, and $\rho_j = m_j/V_j$. Pressure is given by an equation of state, $p_j = p(\rho_j, e_j)$. The set of nodes i belonging to the same cell j is $\mathscr{I}_j$. Likewise the set of cells j sharing the same node i is $\mathscr{J}_i$

Two critical but standard assumptions follow, namely:

(i) the volume of any cell is a computable function of the nodal coordinates; typically, the volume of a cell will only depend on those nodes that are the vertices of the cell;
(ii) the velocities are constant during the time step. If those velocities are $(\bar{u}_i, \bar{v}_i)$, we can define the nodal coordinates as functions of time in the interval $(t^n,\ t^{n+1} = t^n + \Delta t)$ for $t \in [t^n, t^{n+1}]$ as

$$x_i(t) = x_i^n + \bar{u}_i(t - t^n), \quad y_i(t) = y_i^n + \bar{v}_i(t - t^n),$$

so that

$$x_i^{n+1} = x_i^n + \bar{u}_i \Delta t, \quad y_i^{n+1} = y_i^n + \bar{v}_i \Delta t.$$

This defines cell volume V_j as a function of time, and we have the identity

$$V_j^{n+1} - V_j^n = \int_{t^n}^{t^{n+1}} \frac{\mathrm{d}V_j}{\mathrm{d}t}\,\mathrm{d}t = \sum_{i\in\mathscr{I}_j} \bar{u}_i \int_{t^n}^{t^{n+1}} \frac{\partial V_j}{\partial x_i}\,\mathrm{d}t + \sum_{i\in\mathscr{I}_j} \bar{v}_i \int_{t^n}^{t^{n+1}} \frac{\partial V_j}{\partial y_i}\,\mathrm{d}t. \tag{1}$$

Noting that $\bar{u}_i = (x_i^{n+1} - x_i^n)/\Delta t, \bar{v}_i = (y_i^{n+1} - y_i^n)/\Delta t$, (1) is just another way of writing the cell volume at time t^{n+1}, V_j^{n+1}, as a function of the coordinates at time t^{n+1}. Specific instances of this are given in Section 2.

We define matrices $\mathbf{A}$ and $\mathbf{B}$ by their entries

$$\mathbf{A}_{ji} = \int_{t^n}^{t^{n+1}} \frac{\partial V_j}{\partial x_i}\,\mathrm{d}t, \quad \mathbf{B}_{ji} = \int_{t^n}^{t^{n+1}} \frac{\partial V_j}{\partial y_i}\,\mathrm{d}t, \tag{2}$$

with $j \in \mathscr{J}$ and $i \in \mathscr{I}$, so that $\mathbf{A}$ and $\mathbf{B}$ are rectangular sparse sized $|\mathscr{J}| \times |\mathscr{I}|$ matrices, where $|\mathscr{I}|$ is the size of $\mathscr{I}$. They will play a role in the evolution of the hydrodynamic variables since (1) becomes

$$V_j^{n+1} - V_j^n = \sum_{i\in\mathscr{I}_j} (\mathbf{A}_{ji}\bar{u}_i + \mathbf{B}_{ji}\bar{v}_i). \tag{3}$$

An important point to emphasize here is that $\mathbf{A}$ and $\mathbf{B}$ are not in general simple time averages of the integrands, except in the case of Cartesian coordinates.

2. Momentum, energy, entropy

2.1. Momentum

The differential equations for momentum are

$$\rho \frac{\mathrm{d}u}{\mathrm{d}t} = -(\mathrm{grad}\, p)_x, \quad \rho \frac{\mathrm{d}v}{\mathrm{d}t} = -(\mathrm{grad}\, p)_y.$$

Staggered grid momentum difference equations have the form

$$m^i(u_i^{n+1} - u_i^n) = \sum_{j\in\mathscr{J}_i} p_j \mathbf{a}_{ij}, \quad m^i(v_i^{n+1} - v_i^n) = \sum_{j\in\mathscr{J}_i} p_j \mathbf{b}_{ij}, \tag{4}$$

where the matrix $\mathbf{a}$ involves geometrical grid vectors so that $\sum_{j\in\mathscr{J}_i} p_j \mathbf{a}_{ij}$ is an approximation of the integral of the pressure gradient in x direction over cell indexed j, likewise for $\mathbf{b}$. Matrices $\mathbf{a}$ and $\mathbf{b}$ are rectangular sparse $|\mathscr{I}| \times |\mathscr{J}|$.[1] We now set $\bar{u}_i = \frac{1}{2}(u_i^{n+1} + u_i^n)$, $\bar{v}_i = \frac{1}{2}(v_i^{n+1} + v_i^n)$. To each pressure p_j there will be added an artificial

[1] In [4] the momentum equations corresponding to (4) can be seen on page 575 Eq. (2.1); it involves the "corner force" entity: $f_z^{\vec{p}}$ for a zone/cell z and a point/node p of z. Indeed we urge the reader to consult Section 2 of [4, pp. 575–577] to get a detailed description of the original staggered Lagrangian scheme viewed from a different perspective. The corner force in x direction from this work corresponds in our notation to $\frac{1}{\Delta t} p_j \mathbf{a}_{ij}$.

viscosity q_j to deal with shock waves. However, we take q to be zero in our analysis and in the example presented later.

2.2. Energy

Kinetic energy is a nodal quantity for any time t^n, $K_i^n = \frac{1}{2}m^i((u_i^n)^2 + (v_i^n)^2)$, and the total kinetic energy is $K^n = \sum_{i\in\mathscr{I}} K_i^n$. Then since

$$\frac{1}{2}m^i((u_i^{n+1})^2 - (u_i^n)^2) + \frac{1}{2}m^i((v_i^{n+1})^2 - (v_i^n)^2) = \bar{u}_i \sum_{j\in\mathscr{J}_i} p_j \mathbf{a}_{ij} + \bar{v}_i \sum_{j\in\mathscr{J}_i} p_j \mathbf{b}_{ij},$$

that is to say $K_i^{n+1} - K_i^n = \bar{u}_i \sum_{j\in\mathscr{J}_i} p_j \mathbf{a}_{ij} + \bar{v}_i \sum_{j\in\mathscr{J}_i} p_j \mathbf{b}_{ij}$, the change in total kinetic energy is

$$K^{n+1} - K^n = \sum_{i\in\mathscr{I}} \bar{u}_i \sum_{j\in\mathscr{J}_i} p_j \mathbf{a}_{ij} + \sum_{i\in\mathscr{I}} \bar{v}_i \sum_{j\in\mathscr{J}_i} p_j \mathbf{b}_{ij}.$$

The total energy is taken to be the sum of the total nodal kinetic energy and total cell internal energy, that is, $E = \left(\sum_{j\in\mathscr{J}} m_j e_j\right) + K$. Then energy conservation requires that $(E^{n+1} - E^n) = 0$, that is to say $\left(\sum_{j\in\mathscr{J}} m_j(e_j^{n+1} - e_j^n)\right) + (K^{n+1} - K^n) = 0$, or

$$\sum_{j\in\mathscr{J}} \left(m_j(e_j^{n+1} - e_j^n) + p_j \sum_{i\in\mathscr{I}_j} \bar{u}_i \mathbf{a}_{ij} + p_j \sum_{i\in\mathscr{I}_j} \bar{v}_i \mathbf{b}_{ij} \right) = 0.$$

Thus a *sufficient condition* for energy conservation, *no matter how the* **a** *and* **b** *matrices have been defined*, is that for any cell, the internal energy evolution be[2]

$$m_j(e_j^{n+1} - e_j^n) + p_j \sum_{i\in\mathscr{I}_j} (\bar{u}_i \mathbf{a}_{ij} + \bar{v}_i \mathbf{b}_{ij}) = 0. \tag{5}$$

2.3. Entropy

For adiabatic flows the entropy S satisfies $T\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{d}e}{\mathrm{d}t} + p\frac{\mathrm{d}(1/\rho)}{\mathrm{d}t} = 0$. The Lagrangian difference expression of this, according to (3), is

$$m_j(e_j^{n+1} - e_j^n) + p_j(V_j^{n+1} - V_j^n) \equiv m_j(e_j^{n+1} - e_j^n) + p_j \sum_{i\in\mathscr{I}_j} (\bar{u}_i \mathbf{A}_{ji} + \bar{v}_i \mathbf{B}_{ji}) = 0. \tag{6}$$

It can now be seen that there are *two implied volume definitions*,[3] following from (5) and (6). They will be identical if for all $i \in \mathscr{I}$, $j \in \mathscr{J}$

$$\mathbf{a}_{ij} = \mathbf{A}_{ji} \quad \text{and} \quad \mathbf{b}_{ij} = \mathbf{B}_{ji}. \tag{7}$$

and then we will have both total energy conservation and (6).

This is different from the approach in, e.g. [1], where the **a** and **b** matrices are chosen in order to satisfy some symmetry conditions and then the **A** and **B** matrices are defined by (7), in which case (3) cannot be expected to hold. Indeed, the discrepancy between $\sum_{i\in\mathscr{I}_j} (\bar{u}_i \mathbf{a}_{ij} + \bar{v}_i \mathbf{b}_{ij})$ and $(V_j^{n+1} - V_j^n)$ for the area-weighted scheme of [1] and its effect on stability is the subject of [4].

3. Two geometries

For specific examples we need to indicate the relation between nodes and cells and we have to compute the volume change matrices **A** and **B**.

[2] Eq. (5) can be seen in [4, Eq. (2.2), p. 575], or in [2, Eqs. (12) and (13), p. 234–235].

[3] See the discussion in [2, Section 2.3, pp. 244–245], where this volume inconsistency is referred as to an entropy error.

3.1. 1D spherical coordinates

Each cell at half-index $i+\frac{1}{2}$ has vertices r_i and r_{i+1}. The volume of the cell is $V_{i+\frac{1}{2}} = \frac{1}{3}(r_{i+1}^3 - r_i^3)$, so

$$V_{i+\frac{1}{2}}^{n+1} - V_{i+\frac{1}{2}}^{n} = \left(\bar{u}_{i+1} \int_{t^n}^{t^{n+1}} (r_{i+1}^n + \bar{u}_{i+1}(t-t^n))^2 \,\mathrm{d}t - \bar{u}_i \int_{t^n}^{t^{n+1}} (r_i^n + \bar{u}_i(t-t^n))^2 \,\mathrm{d}t \right)$$
$$= \left(\mathbf{A}_{i+\frac{1}{2},i+1} \bar{u}_{i+1} + \mathbf{A}_{i+\frac{1}{2},i} \bar{u}_i \right), \tag{8}$$

where

$$\mathbf{A}_{i+\frac{1}{2},k} = \begin{cases} -\frac{\Delta t}{3}((r_i^n)^2 + (r_i^{n+1})^2 + r_i^n r_i^{n+1}) & \text{if } k = i \\ \frac{\Delta t}{3}((r_{i+1}^n)^2 + (r_{i+1}^{n+1})^2 + r_{i+1}^n r_{i+1}^{n+1}) & \text{if } k = i+1 \\ 0 & \text{if } k \neq i,\ k \neq i+1 \end{cases}$$

By (7) the momentum equation must therefore be given by

$$m^i(u_i^{n+1} - u_i^n) = \mathbf{a}_{i,i+\frac{1}{2}} p_{i+\frac{1}{2}} + \mathbf{a}_{i,i-\frac{1}{2}} p_{i-\frac{1}{2}} \equiv \mathbf{A}_{i+\frac{1}{2},i} p_{i+\frac{1}{2}} + \mathbf{A}_{i-\frac{1}{2},i} p_{i-\frac{1}{2}},$$

or,

$$m^i(u_i^{n+1} - u_i^n) = -\Delta t \frac{1}{3}((r_i^n)^2 + (r_i^{n+1})^2 + r_i^n r_i^{n+1}) \left(p_{i+\frac{1}{2}} - p_{i-\frac{1}{2}} \right). \tag{9}$$

Then, in order to get the volume consistency in 1D spherical symmetry the approximate pressure gradient must be given by the right hand side of (9). As seen in Section 1 it uniquely implies the discretization of the energy equation (5) to get total energy conservation.

3.2. 2D cylindrical coordinates

In cylindrical r–z coordinates, for a generic quadrilateral cell V_j with counter-clockwise ordered vertices $(1,2,3,4)$ with coordinates (r_i, z_i) (functions of t),[4] the cell volume is (with indices defined by periodicity)

$$V_j = \frac{1}{6} \sum_{i=1}^{4} (r_i^2 + r_{i+1}^2 + r_i r_{i+1})(z_{i+1} - z_i). \tag{10}$$

Looking at vertex i, $\frac{\partial V_j}{\partial r_i} = \frac{1}{6}((2r_i + r_{i+1})(z_{i+1} - z_i) + (2r_i + r_{i-1})(z_i - z_{i-1}))$. However, the volume also is

$$V_j = \frac{1}{6} \sum_{i=1}^{4} (r_i z_{i+1} + r_{i+1} z_i + 2(r_i z_i + r_{i+1} z_{i+1}))(r_{i+1} - r_i), \tag{11}$$

so $\frac{\partial V_j}{\partial z_i} = \frac{1}{6}((2r_i + r_{i+1})(r_{i+1} - r_i) + (2r_i + r_{i-1})(r_i - r_{i-1}))$. Now we just need to use the fact that for two functions $\alpha(s)$ and $\beta(s)$ linear in $[0,1]$

$$\int_0^1 \alpha(s)\beta(s)\,\mathrm{d}s = \frac{1}{6}[\alpha(0)\beta(1) + \alpha(1)\beta(0) + 2\{\alpha(0)\beta(0) + \alpha(1)\beta(1)\}].$$

Thus, if we define

$$R_{i\to j} = (2r_i^n + r_j^n)(z_j^{n+1} - z_i^{n+1}) + (2r_i^{n+1} + r_j^{n+1})(z_j^n - z_i^n) + 2\{(2r_i^n + r_j^n)(z_j^n - z_i^n) + (2r_i^{n+1} + r_j^{n+1})(z_j^{n+1} - z_i^{n+1})\},$$

$$Z_{i\to j} = (2r_i^n + r_j^n)(r_j^{n+1} - r_i^{n+1}) + (2r_i^{n+1} + r_j^{n+1})(r_j^n - r_i^n) + 2\{(2r_i^n + r_j^n)(r_j^n - r_i^n) + (2r_i^{n+1} + r_j^{n+1})(r_j^{n+1} - r_i^{n+1})\},$$

it is seen that

$$V_j^{n+1} - V_j^n = \frac{\Delta t}{36}\{(\bar{u}_1[R_{1\to2} - R_{1\to4}] + \bar{u}_2[R_{2\to3} - R_{2\to1}] + \bar{u}_3[R_{3\to4} - R_{3\to2}] + \bar{u}_4[R_{4\to1} - R_{4\to3}])$$
$$+ (\bar{v}_1[Z_{1\to2} - Z_{1\to4}] + \bar{v}_2[Z_{2\to3} - Z_{2\to1}] + \bar{v}_3[Z_{3\to4} - Z_{3\to2}] + \bar{v}_4[Z_{4\to1} - Z_{4\to3}])\},$$

[4] For example see Fig. 1 in [4, p. 575].

and this defines the matrix elements of (3). **A** and **B** being defined, it uniquely implies the discretizations of (4) and (5) in order to get volume consistency and total energy conservation.

The above expressions were easily incorporated into the ALE-INCUBATOR [3] code in order to obtain the computations in Section 4.

4. The full predictor corrector scheme and the Coggeshall cylindrical adiabatic compression problem

This is a modification of the predictor corrector scheme of [2]. The scheme solves the implicit system

$$m^i(u_i^{n+1}-u_i^n)=\sum_{j\in\mathscr{I}_i}p_j\mathbf{a}_{ij},\quad m^i(v_i^{n+1}-v_i^n)=\sum_{j\in\mathscr{I}_i}p_j\mathbf{b}_{ij}, \tag{12}$$

$$x_i^{n+1}=x_i^n+\bar{u}_i\Delta t,\quad y_i^{n+1}=y_i^n+\bar{v}_i\Delta t. \tag{13}$$

This is solved by simple substitution, keeping the pressures fixed. That is, predict the nodal coordinates in the right sides of (12) to get predicted $\bar{u}$ and $\bar{v}$, and then use (13) to obtain corrected coordinates. Let us call this the *inner consistency iteration*. This produces the new cell volumes V_j^{n+1} which can then be entered in the internal energy Eq. (6) to get a new internal energy and then a new pressure. But then we can iterate on the pressure (*outer iteration*), putting $p_j=\frac{1}{2}(p_j^{n+1}+p_j^n)$. The currently used method does the consistency iteration to convergence,[5] and then just one outer corrector iteration.[6]

4.1. The Coggeshall problem

The ALE-INCUBATOR [3] code is used to obtain the following numerical tests. The code is run without artificial viscosity and without anti-hourglass forces (see [3] and the references therein), so that only pressure forces enter the calculation as described in this note.

The choice of numerical tests is limited to tests free of shock waves and hourglass spurious modes; the Coggeshall adiabatic compression is described in [6].

The geometry is 2D r–z cylindrical. A sphere of initial radius $R=1.0$ is filled with a perfect gas ($\gamma=5/3$) in motion leading to the following exact solution $u^{\mathrm{ex}}(t)=-\frac{r(t)}{1-t}$, $v^{\mathrm{ex}}(t)=-\frac{z(t)}{4(1-t)}$, $\rho^{\mathrm{ex}}(t)=(1-t)^{-9/4}$, $e^{\mathrm{ex}}(t)=\left(\frac{3z(t)}{8(1-t)}\right)^2$. At each boundary, the exact velocity is imposed up to the final time $t^n=0.7$. Initial and final meshes can be seen [6].[7] We then look at various errors, comparing Consistent control Volume (CV) method, as described in this note, to the original discrete compatible formulation of Lagrangian hydrodynamics scheme, referred as in Consistent control Volume method and labeled (iCV) see [1,2]. The grid is rectangular polar made of $n_r\times n_z$ nodes, and refined several times in r and z directions by a factor 2.

4.2. Entropy, density and specific internal energy errors

For any mesh we compute the error in density ρ, entropy S and energy e, (the number of cells being n_c, $\mathbf{x}_j=(r_j,z_j)^t$ and Q stands for ρ, S, or e) as

$$\varepsilon_Q^n=\frac{1}{n_c}\sum_{j\in\mathscr{J}}|Q^{\mathrm{ex}}(\mathbf{x}_j,t^n)-Q_j^n|/\max_{j\in\mathscr{J}}|Q^{\mathrm{ex}}(\mathbf{x}_j,t^n)|.$$

Fig. 1 compares the errors ε_Q^n as functions of time ($t_n\leqslant 0.7$) for different mesh sizes. This figure shows that: (i) errors decrease as the mesh is refined for iCV and CV, (ii) asymptotically, a ratio 2 (first order convergence) is

[5] That is to say if ν is the iteration indices and $\mathbf{x}_i=(x_i,y_i)$, convergence of the inner consistency iteration is attained if $\epsilon=\frac{\sum_{i\in\mathscr{I}}\|\mathbf{x}_i^{\nu+1}-\mathbf{x}_i^{\nu}\|^2}{\sum_{i\in\mathscr{I}}\|\mathbf{x}_i^{\nu+1}\|^2}\leqslant 10^{-10}$.

[6] The predictor corrector scheme from [2] simply does one inner iteration and one outer iteration. In the case of cylindrical geometry, in [2] the Cartesian geometrical vector $\vec{a}_1$ (see Fig. 4, p. 249) is modified into $\vec{a}_1(3r_1+r_2)/4$ on p. 261: This can not fulfill consistency of volumes and total energy conservation. In this new method $\vec{a}_1$ is replaced by $\frac{1}{6}\left(\left(\frac{2}{3}r_1^*+\frac{1}{3}r_2^*\right)(2\vec{a}_1^*+\vec{a}_1^n)+\left(\frac{2}{3}r_1^n+\frac{1}{3}r_2^n\right)(\vec{a}_1^*+2\vec{a}_1^n)\right)$ with * referring to the most updated value from the inner consistency iteration.

[7] See Fig. 2, p. 5 for a 20×20 mesh of [6].

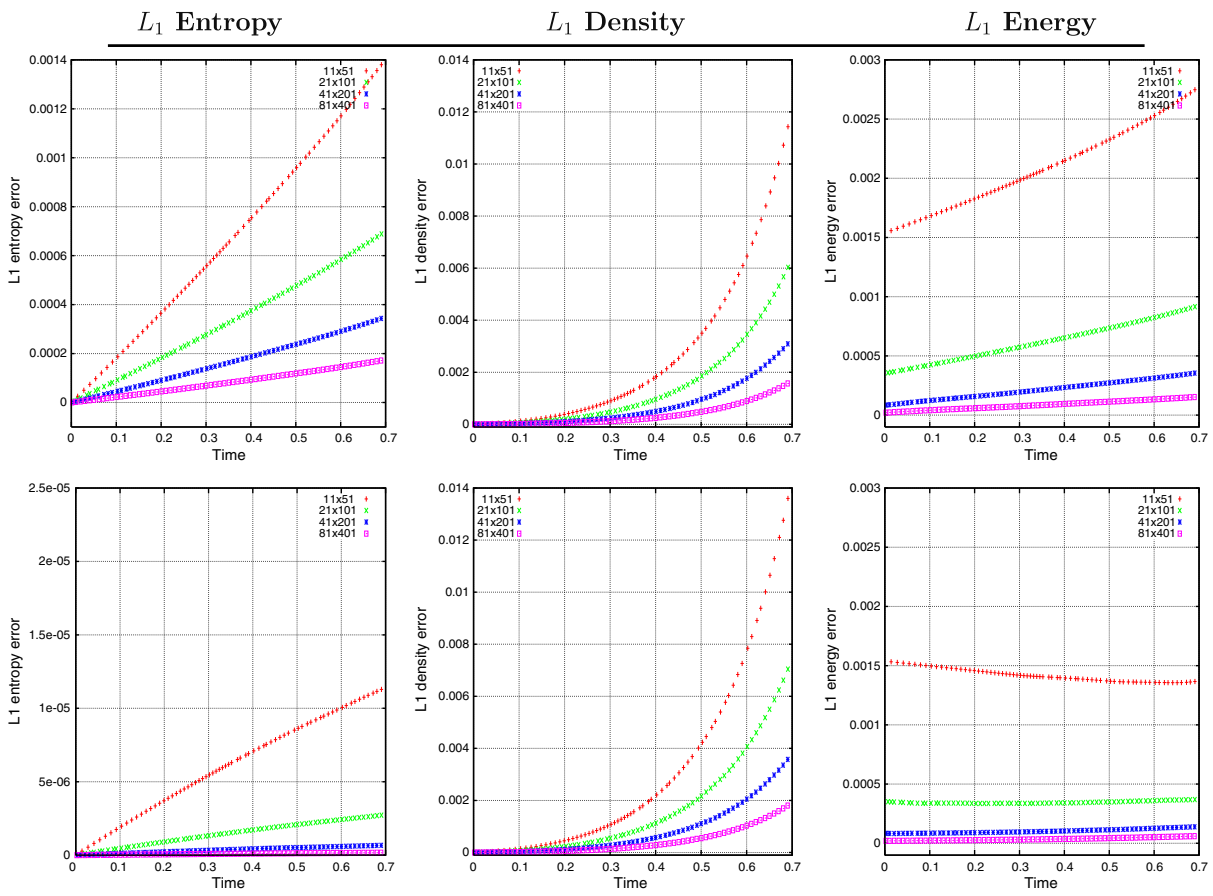

Fig. 1. Coggeshall problem on a quarter of a disk in r–z geometry – Entropy (left panels), density (middle panels), energy (right panels) – L_1 errors as functions of time for successively refined meshes 11×51 up to 81×401 for a CFL condition 1/4. *Top*: Inconsistent control Volume (iCV) scheme. *Bottom*: Consistent control Volume (CV) scheme. The scales for the entropy error plots are different as the consistent control Volume scheme exhibits a quasi-exact entropy conservation.

obtained for any variable, (iii) CV is nearly exact for entropy and more accurate for internal energy, but density accuracy is not increased.

Finally then, we have proposed a staggered Lagrangian numerical scheme with the following properties:

- It is volume consistent: there is no ambiguity in the cell volume definition.
- Total energy is conserved.
- For the adiabatic compression Coggeshall problem, with the artificial viscosity set to zero, cell entropies are almost exactly conserved.

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