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Numerical entropy production and error indicator for compressible flows

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Abstract

In the case of multifluid flows, it is classical to refine the mesh in order to improve the precision. As mesh refinement criterion, we propose to use the numerical entropy production. In a refinement procedure by bitree, we check the relevance of this criterion. Our objective is to validate the mesh refinement before integrating it into a three-dimensional parallel code. ***To cite this article: F. Golay, C. R. Mecanique 337 (2009).***

Résumé

Production numérique d'entropie et indicateur d'erreur pour les écoulements compressibles. Dans le cadre des écoulements multifluides, on cherche à raffiner le maillage de manière à optimiser la précision. Comme critère de raffinement, nous proposons d'utiliser la production numérique d'entropie. Dans un prototype de raffinement par *bitree*, on vérifie que ce critère est pertinent. L'objectif est de valider la procédure avant de l'intégrer dans un code tridimensionnel parallèle. ***Pour citer cet article : F. Golay, C. R. Mecanique 337 (2009).***

Keywords: Computational fluid mechanics; Entropy production; Godunov's scheme; Finite volume; Mesh refinement; Error indicator

Mots-clés : Mécanique des fluides numérique ; Production d'entropie ; Schéma de Godunov ; Volumes finis ; Raffinement de maillage ; Indicateur d'erreur

1. Introduction

In finite elements or finite volumes, it is natural to refine or adapt the mesh where "necessary", in order to save computing time while gaining accuracy. For the numerical resolution of hyperbolic conservation laws, it is interesting to use non-conforming meshes because most of industrial cases require complex meshes. In this case, an effective technique is to make a refinement by bitree (1D), quadtree (2D) or octree (3D), as far as the approximation scheme

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manage non-orthogonal meshes [1]. Whereas mesh refinement by quadtree is used in many fields (for example [2]), mesh refinement by octree is more recent, because it is more difficult to built. For instance, we refer to the work of [3,4]. In our work, we are particularly interesting in low Mach number flows to simulate air/water interfaces. We have applied this approach to wave breaking [5]. We have validated a second order, multi domains, three-dimensional Godunov's finite volume scheme with unstructured mesh [6]. In order to compute realistic three-dimensional simulations, we are naturally led to refine the mesh near the air/water interface. To be effective, it is necessary to have an efficient criterion of mesh refinement. Many works concentrate on 'a posteriori error' estimate, which are constructed from mathematical arguments [7]. However, paradoxically, to my knowledge, very few works use a physical criterion as [8]: the entropy production. More recently, Puppo has demonstrated that the numerical entropy production can locate of course the shocks, but also that the local error should be linked to the numerical production of entropy [9,10]. In this Note, we are going to verify that the numerical production of entropy is a relevant criterion for the hyperbolic conservation laws we are studying. Then we will apply this criterion in a prototype (1D) of numerical code, using meshes with macro-cells, which can be refined by bitree.

2. Physical model

In order to simplify the presentation, we consider the one-dimensional compressible Euler model for an ideal gas. The extension to other pressure laws or to the three-dimensional case is not difficult. The conservation laws for the mass and the momentum and the energy without source terms read:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \qquad \frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0, \qquad \frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p)u}{\partial x} = 0 \tag{1}$$

with $p = (\gamma - 1)\rho\varepsilon$ and $E = \varepsilon + u^2/2$.

Here ρ denotes the density, u the velocity, p the pressure, E the total energy, ε the internal specific energy and γ the ratio of the specific heats. Using the conservative variables $w = \langle \rho, \rho u, \rho E \rangle^T$, we classically write (1) as a system of conservation laws:

$$\frac{\partial w(x,t)}{\partial t} + \frac{\partial f(w)}{\partial x} = 0 \tag{2}$$

We associate to w, an entropy $s(w)$ (convex) that must satisfy the Lax entropy inequality:

$$\frac{\partial s(w)}{\partial t} + \frac{\partial \psi(w)}{\partial x} \leqslant 0 \tag{3}$$

where ψ is the entropy flux satisfying the compatibility equation $\nabla_w^T \psi = \nabla_w^T s(w) f'(w)$. In the case where the solution is regular, (3) is an equality, in the case of a shock (3) is a strict inequality. We will use: $s = -\rho \ln(p/\rho^\gamma)$, $\psi = us$.

3. Numerical model

We approximate (2) by a finite volume method. The computational domain is split into control volumes C_k of mesh ratio h_k, where $w_k^n \simeq w(x, t_n)$. We use the Godunov scheme, where the numerical flux F at the interface of neighbouring cells is determined from the exact solution of a Riemann problem, and the time step is determined from the CFL's condition. For more details, we can refer to [11] or [12]. If $R(0, w_L, w_R)$ denotes the solution of the Riemann problem between two states, the left one w_L and right one w_R, and if $F_{k+1/2}^n = f(R(0, w_k, w_{k+1}))n_{kk+1}$ denotes the numerical flux between the cell C_k and the neighbouring cell C_{k+1} (edge of normal vector n_{kk+1} taken to 1 in 1D), then (2) becomes:

$$w_k^{n+1} = w_k^n - \frac{\Delta t_n}{h_k}\left(F_{k+1/2}^n - F_{k-1/2}^n\right) \tag{4}$$

Integrating (3) in time and space, with notation $s_k^n = s(w_k^n)$, we define the density of numerical entropy production,

$$S_k^n = \frac{s_k^{n+1} - s_k^n}{\Delta t_n} - \frac{\psi(w_{k+1/2}^n) - \psi(w_{k-1/2}^n)}{h_k} \tag{5}$$

and the total entropy production $S = \sum_k \sum_n S_k^n \Delta t_n h_k$.

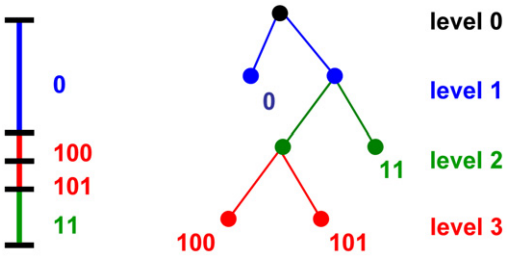

Fig. 1. Mesh refinement example with bi-tree and 4 levels.

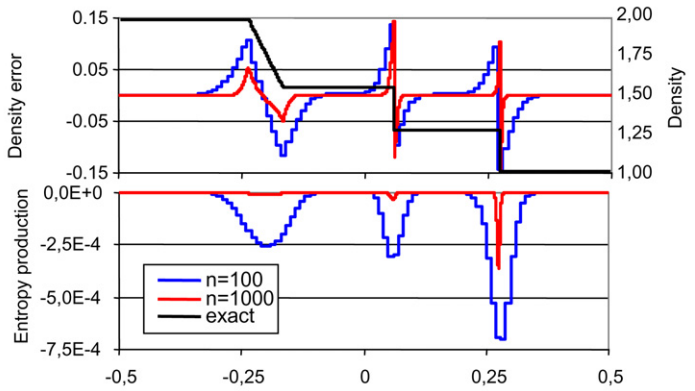

Fig. 2. Density, error of density and entropy production, at $t = 0.2$ s for $n = 100$ and 1000.

4. Mesh refinement by bitree

The aim of this part is to make local mesh refinement on unstructured meshes. In order to reduce the time necessary to manage the refinement, we use "macro-cell" which could be refined by generating hierarchical grids. Each cell can be split in 2, 4 or 8, "daughter" cells, depending on the space dimension (1, 2, or 3). We thus produce a cells graph (bitree, quadtree, octree), whose numbering (in basis 2, 4 or 8) allows a quick computing scan to determine the neighbouring cells. A mesh refinement example is proposed in Fig. 1. The mesh refinement procedure can then simply be expressed. First, the numerical entropy production of each cell is computed. Then the graph is scanned. If $S_k^n > S_{\max}$, the mesh is refined. If $S_k^n < S_{\min}$, as all other "daughter" cells of the same level, the cells are coarsened. Finally, the mesh refinement is adjusted in order to avoid a too great difference of hierarchical level between the cells (generally 2).

5. Results

We present here one example in order to justify the relevance of our criterion. We consider a shock tube, $x \in [-0.5, 0.5]$, with at left side a fluid at rest with $\rho_L = 2$, $u_L = 0$, $p_L = 2$, and at the right side $\rho_R = 1$, $u_R = 0$, $p_R = 1$. The flow is computed until $t = 0.2$ s for some mesh ratio (first order scheme). In Fig. 2, we first verify that the numerical entropy production coincides with the errors on the density (difference between the analytical solution and the density computed numerically). Secondly, we verify that, if the mesh is refined, the numerical entropy production vanishes, except on shock, as predicted by the theory. Then two cases (mr1 and mr2) are computed, beginning with 10 or 50 macro-cells, which could be refined at each time step (hierarchical level $= 4$, $S_{\max} = 75\% \max(S_k^n)$, $S_{\min} = 10\% \max(S_k^n)$). The total number of cells during the computation varies from 10 to 64 for mr1 and from 50 to 104 for mr2 (59 and 89 at the end). In Fig. 3, we verify that the mesh mr2 give better results than the fixed mesh and that the error is more regularly distributed. In Table 1, we notice that, for an equivalent number of cells, the computational error is clearly lower with adapted mesh. In Fig. 4, we verify that the mesh refinement procedure follows well the evolution of physical singularities. Moreover, if we take classically the gradient of the density as a mesh refinement

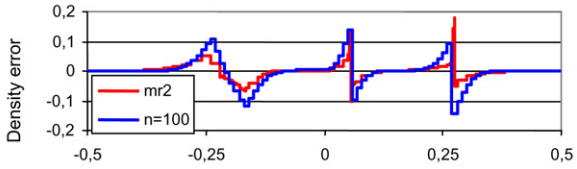

Fig. 3. Error of density at $t = 0.2$ s for $n = 100$ and the mesh refinement mr2.

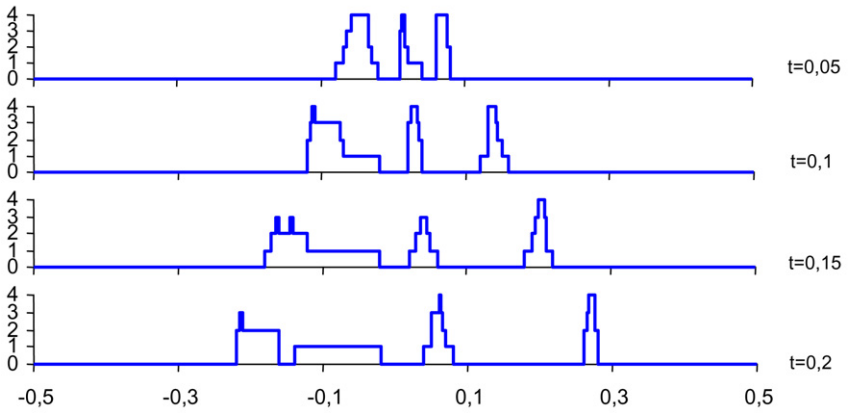

Fig. 4. Hierarchical levels from mr2's mesh at $t = 0.05, 0.10, 0.15, 0.20$.

Table 1
Error of density and total entropy at $t = 0.2$ s for some meshes.

Maillage	$n = 10$	$n = 50$	$n = 100$	$n = 500$	$n = 1000$	mr1	mr2	mr2bis
$\|\Delta\rho\|_2$	1.0×10^{-1}	5.2×10^{-2}	4.0×10^{-2}	2.2×10^{-2}	1.1×10^{-2}	4.1×10^{-2}	2.3×10^{-2}	5.0×10^{-2}
$-S$	1.2×10^{-3}	9.2×10^{-5}	3.1×10^{-5}	2.7×10^{-6}	9.9×10^{-7}	4.1×10^{-4}	2.1×10^{-5}	–

criterion, then, with an initial mesh of 50 'macro-cells' (case mr2bis), we verify that the entropy criterion is more relevant (see Table 1).

6. Conclusion

We have verified the relevance of the numerical entropy production as a mesh refinement criterion for a gas compressible flow. This work can be extended to any hyperbolic systems of conservation laws. We have, for instance, verified it in the context of multiphase flows. We have validated the use of 'macro-cell' on unstructured mesh refined by bitree. We are then going to develop the three-dimensional extension with octree.

References

[1] F. Boyer, F. Hubert, Finite volume method for 2D linear and nonlinear elliptic problems with discontinuities, SIAM J. Numer. Anal. 46 (6) (2008) 3032–3070.
[2] J.S. Bai, P. Li, L.Y. Zou, T. Wang, A quadtree adaptive level set method for capturing interfacial instability on Cartesian grid, Eng. App. Comp. Fluid Mech. 1–4 (2007) 263–372.
[3] F. Losasso, R. Fedkiw, S. Osher, Spatially adaptive techniques for level set methods and incompressible flow, Comput. Fluids 35 (2006) 995–1010.
[4] S. Popinet, Gerris: a tree-based adaptive solver for the incompressible Euler equations in complex geometries, J. Comp. Phys. 190 (2003) 572–600.
[5] P. Helluy, F. Golay, J.P. Caltagirone, P. Lubin, S. Vincent, D. Drevard, R. Marcer, P. Fraunie, N. Seguin, S. Grilli, A.N. Lesage, A. Dervieux, O. Allain, Numerical simulation of wave breaking, M2AN 39 (3) (2005) 591–607.
[6] P. Helluy, F. Golay, Numerical schemes for low Mach wave breaking, Int. J. Comput. Fluid Dyn. 21 (2) (2007) 69–86.

[7] X.D. Zhang, J.Y. Trépanier, R. Camarero, A posteriori error estimation for finite-volume solutions of hyperbolic conservation laws, Comp. Meth. App. Eng. 185 (2000) 1–19.
[8] J.P. Croisille, Contribution à l'étude théorique et à l'approximation par elements finis du système hyperbolique de la dynamique des gaz multidimensionnelle et multi-espèce, Thèse de l'université Paris VI, 1990.
[9] G. Puppo, Numerical entropy production on shocks and smooth transitions, SIAM J. Sci. Comput. 17 (1–4) (2002) 263–271.
[10] G. Puppo, Numerical entropy production for central schemes, SIAM J. Sci. Comput. 25 (4) (2003) 1382–1415.
[11] T. Barberon, P. Helluy, S. Rouy, Practical computation of axisymmetrical multifluid flows, Int. J. Finite 1 (2003) 1–34.
[12] E.F. Toro, Riemann Solvers and Numerical Methods for Fluid Dynamics, 2nd ed., Springer, New York, 1999.