Kinetic energy control in the MAC discretization of compressible Navier-Stokes equations

Raphaele Herbin, Jean-Claude Latché

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A KINETIC ENERGY PRESERVING CONVECTION OPERATOR FOR THE MAC DISCRETIZATION OF COMPRESSIBLE NAVIER-STOKES EQUATIONS

R. Herbin[1] and J.-C. Latché[2]

Abstract. We present in this short note a simple construction of the convection operator in variable density Navier-Stokes equations (*i.e.* the discrete analogue of $\partial_t(\rho \boldsymbol{u}) + \mathrm{div}(\rho \boldsymbol{u} \times \boldsymbol{u})$, where ρ stands for the density and $\boldsymbol{u}$ for the velocity) for MAC discretizations which ensures the control of the kinetic energy. We thereby adapt a similar construction performed in previous works for staggered finite element non-conforming discretizations, and so we extend the stability results which were obtained for implicit or pressure correction schemes for compressible barotropic flows.

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1. Introduction

Let Ω be a domain of $\mathbb{R}^d$, $d = 2$ or $d = 3$, suitable for a discretization with the MAC scheme (*i.e.* with boundaries parallel to the hyperplanes spanned by $d-1$ vectors of the canonical basis of $\mathbb{R}^d$), and let ρ and $\boldsymbol{u}$ be regular density and velocity fields defined on Ω and satisfying the mass balance:

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0. \tag{1}$$

Let z be a regular scalar function defined over Ω. Supposing for short that the velocity $\boldsymbol{u}$ vanishes at the boundary of Ω, the following identity holds:

$$\int_\Omega \big[\partial_t(\rho z) + \mathrm{div}(\rho z \boldsymbol{u})\big]\, z \,\mathrm{d}\boldsymbol{x} = \frac{1}{2}\,\frac{d}{dt}\int_\Omega \rho z^2 \,\mathrm{d}\boldsymbol{x}. \tag{2}$$

If z is the i^{th} component of $\boldsymbol{u}$, $\partial_t(\rho z) + \mathrm{div}(\rho z \boldsymbol{u})$ is the convection part of the momentum balance equation projected along the i^{th} vector of the canonical basis of $\mathbb{R}^d$; applying identity (2) to each component of $\boldsymbol{u}$ thus yields the central argument of the proof of the kinetic energy theorem.

The aim of this short note is to propose a discrete convection operator for the MAC scheme (see [8] for the seminal paper, [6, 7] for the first implementations for compressible flows and [9] for a review) which satisfies a discrete counterpart of (2). The result given here is the only ingredient necessary to extend to the MAC

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[1] Université de Provence, France (herbin@cmi.univ-mrs.fr)

[2] Institut de Radioprotection et de Sûreté Nucléaire (IRSN) (jean-claude.latche@irsn.fr)

discretization the stability studies already performed for staggered discretizations based on low-order nonconforming finite elements (namely the Couzeix-Raviart or Rannacher-Turek elements) for incompressible [2] or barotropic compressible [4, 5] flows.

This note is organized as follows: we first give an abstract discrete analogue to Identity (2), which holds for general meshes and was proved in [4]. We then show how to apply it to a MAC discretization.

2. An abstract discrete stability result

In this section, we consider a general mesh of Ω and state a stability result which was proved in [4]. Let Ω be split into control volumes $\bar\Omega = \cup_{K\in\mathcal{M}} \bar K$. The internal faces of the mesh are denoted by $\sigma = K|L$ and we suppose given two families of positive real numbers $(\rho^*_K)_{K\in\mathcal{M}}$ and $(\rho_K)_{K\in\mathcal{M}}$ satisfying the following set of equations:

$$\forall K \in \mathcal{M}, \qquad \frac{|K|}{\delta t}\,(\rho_K - \rho^*_K) + \sum_{\sigma=K|L} F_{\sigma,K} = 0, \tag{3}$$

where $F_{\sigma,K}$ is a quantity associated to the edge σ and to the control volume K; we suppose that the property of local conservativity (or conservativity of the numerical fluxes) is satisfied, *i.e.*, for any internal edge $\sigma = K|L$, $F_{\sigma,K} = -F_{\sigma,L}$. The relation (3) may be seen as a discrete mass balance, namely the finite volume discretization of (1); in this case, ρ^*_K and ρ_K stand for the approximation of the density ρ over K respectively at the beginning and at the end of the time step δt, $|K|$ is the measure of K and $F_{\sigma,K}$ is the mass flux coming out of K through σ, *i.e.* an approximation of the integral over σ of the quantity $\rho\boldsymbol{u}\cdot\boldsymbol{n}_{K,\sigma}$ where $\boldsymbol{n}_{K,\sigma}$ stands for the normal vector to σ outward K. Note that the sum of the fluxes is retricted to the internal edges of the mesh, which implicitly reflects the fact that the normal velocity is supposed to be zero at the boundary.

Let $(z^*_K)_{K\in\mathcal{M}}$ and $(z_K)_{K\in\mathcal{M}}$ be two families of real numbers. For any internal edge $\sigma = K|L$, we define z_σ by $z_\sigma = (z_K + z_L)/2$, and the convection operator $C_\mathcal{M}$ by:

$$\forall K \in \mathcal{M}, \quad (C_\mathcal{M} z)_K = \frac{1}{\delta t}\,(\rho_K\, z_K - \rho^*_K\, z^*_K) + \frac{1}{|K|}\sum_{\sigma=K|L} F_{\sigma,K}\, z_\sigma \tag{4}$$

The quantity $(C_\mathcal{M}\, z)_K$ may be seen as a finite volume approximation over K of $\partial_t(\rho z) + \mathrm{div}(\rho\boldsymbol{u} z)$, where z is a generic scalar function. Then the following stability property holds:

$$\sum_{K\in\mathcal{M}} |K|\; z_K\; (C_\mathcal{M}\, z)_K \geq \frac{1}{2}\sum_{K\in\mathcal{M}} \frac{|K|}{\delta t}\;\Big[\rho_K\, z_K^2 - \rho^*_K\, {z^*_K}^2\Big] \tag{5}$$

This relation is a discrete analogue of (2), which is thus satisfied provided that the convection operator $C_\mathcal{M}$ satisfies a consistency property with the discrete mass balance, namely (3), which can be reformulated by saying that $(C_\mathcal{M}\, z)_K = 0$, $\forall K \in \mathcal{M}$ for any constant discrete function z (*i.e.*, without loss of generality, if $z_K = 1$, $\forall K \in \mathcal{M}$).

3. A kinetic energy preserving operator for the MAC scheme

We now need to specialize the presentation to the MAC discretization. We suppose that $d = 2$ for the sake of simplicity and use the notations given on Figure 1.

On the cell $K_{i,j} = (x_{i-\frac12}, x_{i+\frac12}) \times (y_{j-\frac12}, y_{j+\frac12})$, the discretization of the mass balance (1) obtained by a backward Euler discretization reads:

$$\frac{|K_{i,j}|}{\delta t}\,(\rho_{i,j} - \rho^*_{i,j}) + F^x_{i+\frac12,j} + F^y_{i,j+\frac12} - F^x_{i-\frac12,j} - F^y_{i,j-\frac12} = 0 \tag{6}$$

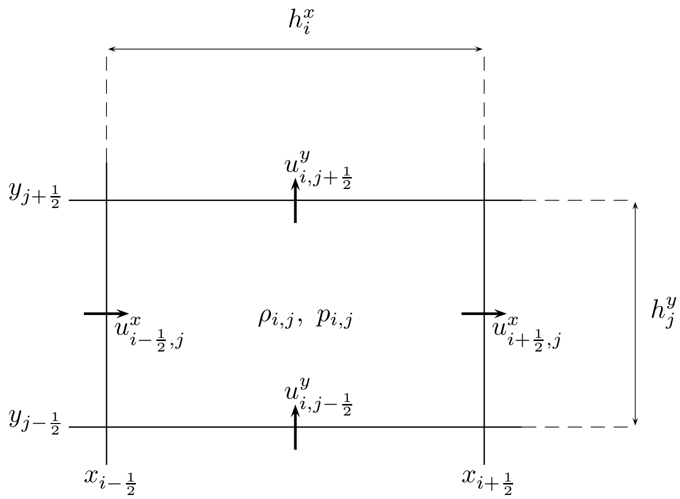

FIGURE 1. Mesh and unknowns.

with, for instance, $F^x_{i+\frac{1}{2},j} = h^y_j\ u^x_{i+\frac{1}{2},j}\ \tilde\rho_{i+\frac{1}{2},j}$, where $\tilde\rho_{i+\frac{1}{2},j}$ stands for an approximation of the density at the face, which, for the aim pursued here, may be obtained by any reasonable interpolation formula.

Let us now turn to the discretization of the momentum balance equation, which reads:

$$\partial_t(\rho \boldsymbol{u}) + \nabla\cdot(\rho\boldsymbol{u}\otimes\boldsymbol{u}) + D(u) - \nabla p = 0, \tag{7}$$

where $D(u)$ stands for a diffusion term which does not need to be detailed here. The discrete equations are obtained by writing a balance equation corresponding to (7) on staggered cells, which are of the form $K^x_{i-\frac{1}{2},j} = (x_{i-1}, x_i)\times(y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}})$ for the x component and $K^y_{i,j-\frac{1}{2}} = (x_{i-\frac{1}{2}}, x_{j+\frac{1}{2}})\times(x_{j-1}, x_j)$ for the y component. Our aim is to produce a discrete set of equations such that the kinetic energy is preserved: hence, we wish the theory of Section 2 to apply (and so, in particular, the resulting convection operator to be such that it vanishes for any constant velocity field); the convection term $\partial_t(\rho\boldsymbol{u}) + \nabla\cdot(\rho\boldsymbol{u}\otimes\boldsymbol{u})$ should therefore be discretized under the form (4) where z represents each of the velocity component, and with fluxes $F_{K,\sigma}$ constructed in such a way that the discrete equations (3) are also satisfied on the cells $K^x_{i-\frac{1}{2},j}$.

Using the notations given on Figure 2, the discrete equation for the x-component of $\boldsymbol{u}$ posed over the control volume $K^x_{i-\frac{1}{2},j}$ reads, with a backward Euler discretization:

$$\begin{aligned}\frac{|K^x_{i-\frac{1}{2},j}|}{\delta t}\ \Big[\rho_{i-\frac{1}{2},j}\, u^x_{i-\frac{1}{2},j} - \rho^*_{i-\frac{1}{2},j}\,(u^x_{i-\frac{1}{2},j})^*\Big]& \\ +F^x_{i,j}\ u^x_{i,j} + F^y_{i-\frac{1}{2},j+\frac{1}{2}}\ u^x_{i-\frac{1}{2},j+\frac{1}{2}} - F^x_{i-1,j}\ u^x_{i-1,j} - F^y_{i-\frac{1}{2},j-\frac{1}{2}}\ u^x_{i-\frac{1}{2},j-\frac{1}{2}}& \\ +(T_d)_{i-\frac{1}{2},j} + (\boldsymbol{\nabla} p)_{i-\frac{1}{2},j} = 0,&\end{aligned}$$

where $(T_d)_{i-\frac{1}{2},j}$ and $(\boldsymbol{\nabla} p)_{i-\frac{1}{2},j}$ stand for the approximation of the diffusion term $D(u)$ and pressure gradient term ∇p respectively, and denoting by $(u^x_{i-\frac{1}{2},j})^*$ the beginning-of-step x-component of the velocity on $K^x_{i-\frac{1}{2},j}$. Our task is now to define the approximation of the densities $\rho_{i-\frac{1}{2},j}$ and $\rho^*_{i-\frac{1}{2},j}$, the mass fluxes $F^x_{i,j}$, $F^y_{i-\frac{1}{2},j+\frac{1}{2}}$, $F^x_{i-1,j}$ and $F^y_{i-\frac{1}{2},j-\frac{1}{2}}$ and the velocities $u^x_{i,j}$, $u^x_{i-\frac{1}{2},j+\frac{1}{2}}$, $u^x_{i-1,j}$ and $u^x_{i-\frac{1}{2},j-\frac{1}{2}}$ so as to meet the requirements of

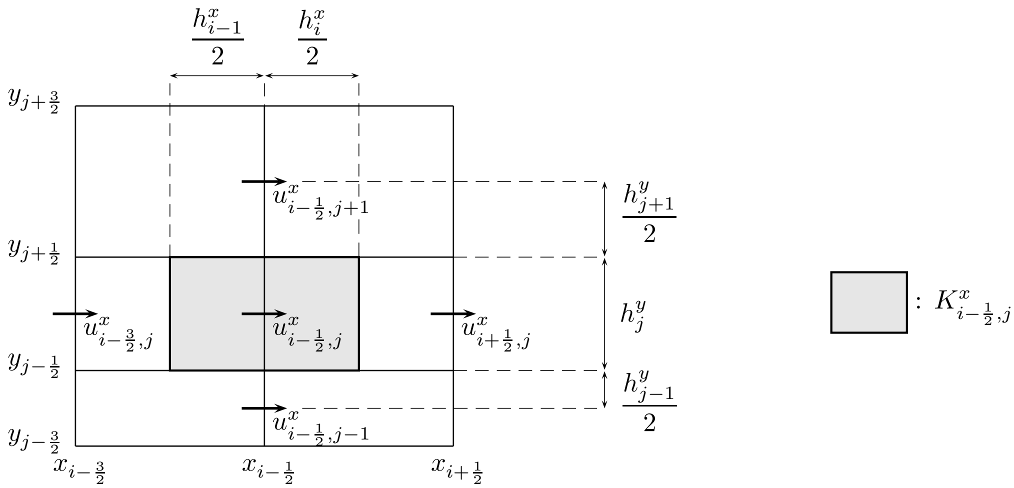

FIGURE 2. Notations for the control volume $K^x_{i-\frac{1}{2},j}$.

Section 2. Hence, we first discretize the face velocities by a centered approximation:

$$u^x_{i,j} = \frac{1}{2}\ (u^x_{i-\frac{1}{2},j} + u^x_{i+\frac{1}{2},j}), \qquad u^x_{i-\frac{1}{2},j+\frac{1}{2}} = \frac{1}{2}\ (u^x_{i-\frac{1}{2},j} + u^x_{i-\frac{1}{2},j+1}),$$
$$u^x_{i-1,j} = \frac{1}{2}\ (u^x_{i-\frac{3}{2},j} + u^x_{i-\frac{1}{2},j}), \qquad u^x_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{1}{2}\ (u^x_{i-\frac{1}{2},j} + u^x_{i-\frac{1}{2},j-1}).$$

Next, we wish the following discrete mass balance on cell $K^x_{i-\frac{1}{2},j}$ to hold:

$$\frac{|K^x_{i-\frac{1}{2},j}|}{\delta t}\ \Big[\rho_{i-\frac{1}{2},j} - \rho^*_{i-\frac{1}{2},j}\Big] + F^x_{i,j} + F^y_{i-\frac{1}{2},j+\frac{1}{2}} - F^x_{i-1,j} - F^y_{i-\frac{1}{2},j-\frac{1}{2}} = 0. \tag{8}$$

Let us then write the discrete mass balance (6) for the mesh $K_{i-1,j}$, and sum with (6). We get:

$$\begin{aligned} &\frac{1}{\delta t}\ \Big[(|K_{i-1,j}|\ \rho_{i-1,j} + |K_{i,j}|\ \rho_{i,j}) - (|K_{i-1,j}|\ \rho^*_{i-1,j} + |K_{i,j}|\ \rho^*_{i,j})\Big] \\ &\quad + \Big[F^x_{i-\frac{1}{2},j} + F^x_{i+\frac{1}{2},j}\Big] + \Big[F^y_{i-1,j+\frac{1}{2}} + F^y_{i,j+\frac{1}{2}}\Big] - \Big[F^x_{i-\frac{3}{2},j} + F^x_{i-\frac{1}{2},j}\Big] - \Big[F^y_{i-1,j-\frac{1}{2}} + F^y_{i,j-\frac{1}{2}}\Big] = 0. \end{aligned} \tag{9}$$

An easy identification of the terms in (8) and (9) shows that we will obtain the desired stability property taking for the densities:

$$|K^x_{i-\frac{1}{2},j}|\ \rho_{i-\frac{1}{2},j} = \frac{1}{2}\ \Big[|K_{i-1,j}|\ \rho_{i-1,j} + |K_{i,j}|\ \rho_{i,j}\Big], \qquad |K^x_{i-\frac{1}{2},j}|\ \rho^*_{i-\frac{1}{2},j} = \frac{1}{2}\ \Big[|K_{i-1,j}|\ \rho^*_{i-1,j} + |K_{i,j}|\ \rho^*_{i,j}\Big],$$

and for the mass fluxes:

$$F^x_{i,j} = \frac{1}{2}\ \Big[F^x_{i-\frac{1}{2},j} + F^x_{i+\frac{1}{2},j}\Big] \qquad F^y_{i-\frac{1}{2},j+\frac{1}{2}} = \frac{1}{2}\ \Big[F^y_{i-1,j+\frac{1}{2}} + F^y_{i,j+\frac{1}{2}}\Big]$$
$$F^x_{i-1,j} = \frac{1}{2}\ \Big[F^x_{i-\frac{3}{2},j} + F^x_{i-\frac{1}{2},j}\Big] \qquad F^y_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{1}{2}\ \Big[F^y_{i-1,j-\frac{1}{2}} + F^y_{i,j-\frac{1}{2}}\Big]$$

This construction may be easily transposed to the y-component of the velocity, and, more generally, to the three-dimensional case.

Remark 3.1. Note that, for instance, depending on the discretization of the mass fluxes in the mass balance equation, the density in the cells $K_{i-1,j}$ or $K_{i+1,j}$ may appear in the expression of the $F^x_{i,j}$, even if this flux is associated to a face included in $K_{i,j}$.

Remark 3.2 (Boundary conditions)**.** Usually, when using a MAC discretization, the Dirichlet boundary conditions for the velocity are directly prescribed to the boundary velocity degrees of freedom. In this case, the theory of Section 2 needs to be slightly adapted, because no balance equation is satisfied on the (half-) dual cells associated to these degrees of freedom. The proof that the stability inequality (5) still holds is given in [2, proof of Theorem 3.1]. Note however that, because of this particular feature of staggered discretizations, if the velocity is not prescribed to zero (but, let us say, to $\boldsymbol{u}_D$) at the boundary, the kinetic energy flux entering the domain is consistent with what may be anticipated from the boundary condition (*i.e.* $\frac{1}{2}\ \rho_D\ |\boldsymbol{u}_D|^2\ \boldsymbol{u}_D \cdot \boldsymbol{n}$, with ρ_D the density at the boundary and $\boldsymbol{n}$ the outward normal vector), but cannot be expressed as a function of the boundary data only [2, Remark 3].
When the velocity is not prescribed, an explicit expression of the kinetic energy flux across the boundary of the domain can be established, and this result may be used to derive a discrete artificial boundary condition able to cope with inward flows, purposely built to yield an energy estimate (see [3] for a work following similar ideas in the incompressible case). This artificial condition has been succesfully tested to compute natural convection external flows [1].

Remark 3.3 (Upwinding of the velocity)**.** If an upwind approximation is used for the velocity in the momentum flux through the faces of the dual cells, Inequality (5) is still satisfied, and an additional dissipation (non-negative) term appears at the right hand side [2, Remark 2].

Remark 3.4 (Using this construction in a pressure correction algorithm)**.** The implementation of the proposed construction of the convection operator is not straightforward in a pressure correction algorithm, since, usually, the mass balance equation is solved after the momentum balance equation. The choice which has been made in [2,4,5] is to start from the mass balance (*i.e.* to use for Equation (6)) at the previous time step. Denoting by the superscript n the time level, in the time semi-discrete setting and with a linearly-implicit time discretization, this yields to a space discretization of the convection term under the form $(\rho^n\, \boldsymbol{u}^{n+1} - \rho^{n-1}\, \boldsymbol{u}^n)/\delta t + \mathrm{div}(\rho^n \boldsymbol{u}^{n+1} \times \boldsymbol{u}^n)$.

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