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AN ASSESSMENT OF VARIOUS DISCRETIZATIONS OF THE ENERGY EQUATION IN COMPRESSIBLE FLOWS

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Abstract. Nonlinear instabilities are one of the major problems in turbulence simulations. One reason behind this problem is the accumulation of aliasing errors produced by the discrete evaluation of the convective term. This can be improved by preserving the quadratic invariants in a discrete sense. However, another source of instabilities is the error due to an incorrect evolution of thermodynamic variables, such as entropy. An appropriate discretization of the energy equation is needed to address this issue. An analysis of the preservation properties of various discretizations of the compressible Euler equations is reported, which includes some of the most common approaches used in the literature, together with some new formulations. Two main factors have been identified and studied: one is the choice of the energy equation to be directly discretized; the other is the particular splitting of the convective terms, chosen among the Kinetic Energy Preserving (KEP) forms. The energy equations analyzed in this paper are total and internal energy, entropy, and speed of sound. All the cases examined are locally conservative and KEP, since this is considered an essential condition for a robust simulation. The differences among the formulations have been theoretically investigated through the study of the discrete evolution equations induced by the chosen energy variable, showing which quantities may be preserved. Both one-dimensional and two-dimensional tests have been performed to assess the advantages and disadvantages of the various options in different cases.

1 INTRODUCTION

The ability to reproduce the symmetries of the compressible Navier-Stokes equations through discretization is the subject of ongoing research [1]. This is due to the fact that respecting this physical realism has been found to mitigate the non-linear instability problem linked to the accumulation of aliasing error. The cause of this error is to be found in the differentiation of the product of two or more variable, and in particular the issue presents itself during the discrete evaluation of the convective terms of the Navier-Stokes equations. In fact, even in the absence of shock waves, straightforward central finite difference approximations of non viscous equations, the Euler equations, present an instability.[2]

A suitable spatial discretization that would preserve the integral value of the kinetic energy was found to be beneficial to the robustness of the simulation for the incompressible case [3, 4,

5, 6, 7] and for the compressible flow [8, 9, 10]. The general criteria, involving the coordinated treatment of the convective terms in the mass and momentum equations, needed to preserve global kinetic energy in compressible flows equations have been recently derived for both finite difference [11] and finite volume [12] methods.

Another sensitive issue is the discretization of the energy equation. The specific equation chosen and the splitting used for its discretization condition the preservation of the integral constrains on thermodynamics quantities of physical importance, such as total energy and entropy. While the direct discretization of the total energy equation is the most common choice [10, 13, 14], it typically fails to globally preserve entropy. Honein and Moin [9] found good numerical stability by directly discretizing the entropy equation; on the other hand, their formulation does not preserve total energy.

The objective of this study is to present an assessment of these and other possible formulations for the discretization of the Euler equations. Particular emphasis will be put on the methods discretizing the internal energy and sound speed equations directly, since these display good robustness and entropy preserving properties, while being able the correctly preserve total energy.

2 EULER EQUATIONS

The compressible Euler equations, together with the equation of state, describe the kinematic and thermodynamic evolution of a fluid in absence of viscosity:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u_\alpha}{\partial x_\alpha} \,, \tag{1}$$

$$\frac{\partial \rho u_\alpha}{\partial t} = -\frac{\partial \rho u_\alpha u_\alpha}{\partial x_\alpha} - \frac{\partial p}{\partial x_\alpha} \,, \tag{2}$$

$$\frac{\partial \rho E}{\partial t} = -\frac{\partial \rho u_\alpha E}{\partial x_\alpha} - \frac{\partial p u_\alpha}{\partial x_\alpha} \,. \tag{3}$$

In these equations ρ is the density, u_α is the Cartesian velocity component, p is the pressure, and E the total energy per unit mass. Equations (1) and (2) express, respectively, the balance of mass and momentum, with the second one being vectorial. From these, using the chain and product rule of differentiation which are valid when smooth flows are considered, it is possible to derive an equation for the evolution of the kinetic energy $k = u_\alpha u_\alpha / 2$:

$$\frac{\partial \rho \kappa}{\partial t} = -\frac{\partial \rho u_\alpha \kappa}{\partial x_\alpha} - u_\alpha \frac{\partial p}{\partial x_\alpha} \,. \tag{4}$$

In principle, this equation is satisfied by the solutions to the system (1)–(3), but this is no longer true when spatially discretized forms are considered. In this case, the rules of calculus that have been used to derive one from the other are no longer valid for spatial derivatives. This means that while the primary variable, the one in the equation that is directly discretized, may be correctly preserved, this is not true for an induced one.

A similar consideration could be made about Equation (3), which expresses the balance of total energy. Considering true the ideal gas law $p = \rho R T$ where T is the temperature and R

the gas constant, there are several alternative formulations among which any of the following equations could be used:

$$\frac{\partial \rho e}{\partial t} = -\frac{\partial \rho u_\alpha e}{\partial x_\alpha} - p\frac{\partial u_\alpha}{\partial x_\alpha} \,, \tag{5}$$

$$\frac{\partial \rho c}{\partial t} = -\frac{\partial \rho u_\alpha c}{\partial x_\alpha} - \frac{(\gamma-1)}{2}\rho c\frac{\partial u_\alpha}{\partial x_\alpha} \,, \tag{6}$$

$$\frac{\partial \rho s}{\partial t} = -\frac{\partial \rho u_\alpha s}{\partial x_\alpha} \,. \tag{7}$$

Equation (5) expresses the balance of internal energy $\rho e = \rho E - \rho k = \rho c_v T$, with c_v specific heat at constant volume; Equation (6) is the evolution equation for sound speed $c = \sqrt{\gamma RT} = \sqrt{\gamma(\gamma-1)e}$, in which γ is equal to 1.4 and it is the ratio of c_v and c_p, the specific heat at constant pressure; Equation (7) describes the balance of entropy $s = \rho c_v \log p/\rho^\gamma$. When considering their discretized form, the induced variables may not be preserved.

All the evolution equation can be expressed through a generic formula as the sum of a convective and a pressure term; for a generic variable ϕ this is

$$\frac{\partial \rho\phi}{\partial t} = -\mathcal{C}_{\rho\phi} - \mathcal{P}_{\rho\phi}. \tag{8}$$

To this variable correspond a generalized kinetic energy which evolves following the induced equation

$$\frac{\partial \rho\phi^2/2}{\partial t} = -\left(\phi\mathcal{C}_{\rho\phi} - \frac{\phi^2}{2}\mathcal{M}\right) - \phi\mathcal{P}_{\rho\phi} \tag{9}$$

in which $\mathcal{M} = \mathcal{C}_\rho$.

3 KINETIC ENERGY PRESERVATION

In a paper by Coppola *et al.* [15] it was shown that exists a whole family of splittings of the convective terms capable of preserving kinetic energy. To each value of a parameter ξ corresponds a splitting with such property if the convective terms follow these formulas:

$$\mathcal{M} = \xi\mathcal{M}^D + (1-\xi)\mathcal{M}^A \,, \tag{10}$$

$$\mathcal{C}_{\rho\phi} = \xi\mathcal{C}^F_{\rho\phi} + (1-\xi)\mathcal{C}^C_{\rho\phi} \tag{11}$$

Equation (10) indicates that the convective term of the mass equation $\mathcal{M}$ must be discretized as convex sum of its divergence and its advective forms:

$$\mathcal{M}^D = \frac{\delta \rho u_\alpha}{\delta x_\alpha}, \qquad \mathcal{M}^A = \rho\frac{\delta u_\alpha}{\delta x_\alpha} + u_\alpha\frac{\delta \rho}{\delta x_\alpha} \tag{12}$$

in which the symbol δ stands for the numerical derivative. Similarly, as seen in Equation (11), the convective term for the variable ϕ must be composed by combination of an F and a C form defined as

$$\mathcal{C}^F_{\rho\phi} = \frac{\mathcal{C}^D_{\rho\phi} + \mathcal{C}^\phi_{\rho\phi}}{2}, \qquad \mathcal{C}^C_{\rho\phi} = \frac{\mathcal{C}^u_{\rho\phi} + \mathcal{C}^\rho_{\rho\phi}}{2} \,. \tag{13}$$

which are built up from possible ways of discretizing the divergence of the triple product:

$$\begin{aligned} \mathcal{C}^D_{\rho\phi} &= \frac{\delta \rho u_\alpha \phi}{\delta x_\alpha}, \quad \mathcal{C}^\phi_{\rho\phi} = \phi \frac{\delta \rho u_\alpha}{\delta x_\alpha} + \rho u_\alpha \frac{\delta \phi}{\delta x_\alpha}, \\ \mathcal{C}^u_{\rho\phi} &= u_\alpha \frac{\delta \rho \phi}{\delta x_\alpha} + \rho \phi \frac{\delta u_\alpha}{\delta x_\alpha}, \quad \mathcal{C}^\rho_{\rho\phi} = \rho \frac{\delta u_\alpha \phi}{\delta x_\alpha} + \phi u_\alpha \frac{\delta \rho}{\delta x_\alpha}. \end{aligned} \tag{14}$$

Among this family of splitting, there are three notable cases. The C splitting, for which $\xi = 0$, was first considered by Coppola *et al.* [15] ; the KGP splitting, with $\xi = 0.5$, was proposed by Kennedy and Gruber [16] and shown to be energy preserving by Pirozzoli [14]; the F splitting, corresponding to $\xi = 1$, was introduced by Feiereisen [8].

When a Kinetic Energy Preserving (KEP) scheme is chosen for the variable ϕ, the generalized kinetic energy $\phi^2/2$ is preserved and the convective term of its evolution equation, obtained by substituting Equations (10)–(14) into Equation (9), is

$$\mathcal{C}_{\rho\phi^2/2} = \frac{\xi}{2} \left(\phi \frac{\delta \rho \phi u_\alpha}{\delta x_\alpha} + \rho \phi u_\alpha \frac{\delta \phi}{\delta x_\alpha} \right) + \frac{1-\xi}{2} \left(u_\alpha \phi \frac{\delta \rho \phi}{\delta x_\alpha} + \rho \phi \frac{\delta u_\alpha \phi}{\delta x_\alpha} \right). \tag{15}$$

It can be shown that this term can be recast in its flux form [17], meaning that the generalized kinetic energy is locally conserved. In the hypothesis of exact time integration, discretizing according to Equation (15) the generalized kinetic energy would be equivalent to the KEP discretization of the variable ϕ. This means that an alternative interpretation of Equation (15) is that it represent the convective term of a family of splittings that, instead of preserving the kinetic energy of a variable as done by KEP splittings, preserve its square root.

In the case of mass and momentum equation, KEP methods should always be chosen, since preservation of kinetic energy is considered an indispensable characteristic of a robust simulation. On the other hand, this is not necessarily true for the energy equation. In this paper we consider the case of the internal energy: by renouncing to the preservation of ρe^2, it is possible to preserve the more meaningful thermodynamic variable ρc, which is proportional to its square root.

4 ENERGY EQUATION

In this section we briefly present a theoretical analysis of how the choice of primary variable influences the evolution of the other secondary thermodynamic variables. In particular, the choice of internal energy and sound speed has been compared to the more common total energy. A more in depth analysis which includes these and other variables has been presented in a submitted paper [17].

4.1 Internal energy

When total energy is chosen as primary variable and Equation (3) discretized directly, the internal energy evolves with an induced equation which has convective and pressure terms given by

$$\mathcal{C}_{\rho e} = \mathcal{C}_{\rho E} - \underbrace{\left(u_\alpha \mathcal{C}_{\rho u_\alpha} - \frac{u_\alpha u_\alpha}{2} \mathcal{M} \right)}_{\mathcal{C}_{\rho\kappa}}; \qquad \mathcal{P}_{\rho e} = \mathcal{P}_{\rho E} - \underbrace{u_\alpha \mathcal{P}_{\rho u_\alpha}}_{\mathcal{P}_{\rho\kappa}} \tag{16}$$

The total energy convective term is in conservative form and this is the case for the one of the kinetic energy, if a KEP splitting is used for mass and momentum equations [11]. This means that internal energy is locally conserved as well. A similar reasoning could be applied when internal energy is chosen as the primary variable [18, 19, 20]. The induced evolution of the total energy can be derived by inverting Equation (16). It can be shown that, by discretizing the internal energy equation, total energy is preserved, provided that kinetic energy is preserved and that the pressure term is properly discretized [17, 21].

4.2 Sound Speed

The direct discretization of the internal energy equation induces an evolution of sound speed with convective and pressure terms that, in the case of a perfect gas, are

$$\mathcal{C}_{\rho c} = \frac{\gamma(\gamma-1)}{2c}\boldsymbol{\mathcal{C}}_{\rho e} + \frac{c}{2}\boldsymbol{\mathcal{M}}, \tag{17}$$

$$\mathcal{P}_{\rho c} = \frac{\gamma(\gamma-1)}{2c}\boldsymbol{\mathcal{P}}_{\rho e}. \tag{18}$$

This terms are generally not in conservative form, and spurious production from the convective term can effect the discrete evolution of ρc.

However, sound speed can be chosen as the primary variable, as done by Kok [22]. The induced convective and pressure terms for the internal energy can be obtained by inverting Equations (17) and (18):

$$\mathcal{C}_{\rho e} = \frac{2}{\gamma(\gamma-1)}\left(c\boldsymbol{\mathcal{C}}_{\rho c} - \frac{c^2}{2}\boldsymbol{\mathcal{M}}\right), \tag{19}$$

$$\mathcal{P}_{\rho e} = \frac{2c}{\gamma(\gamma-1)}\boldsymbol{\mathcal{P}}_{\rho c}. \tag{20}$$

By comparing these terms with those in Equation (9), it can be observed that the induced evolution of internal energy corresponds to that of a generalized kinetic energy. From this we can derive that a direct KEP discretization of the sound speed equation locally conserves internal energy. This also implies the local preservation of total energy, when kinetic energy is preserved.

An alternative interpretation of this formulation is to consider it equivalent to a direct discretization of the internal energy in which the convective term is discretized as in Equation (15). In this case the preservation of ρe^2 is lost in favour of $\rho\sqrt{e}$, proportional to sound speed.

In this paper, the formulations employing C form and KGP form splittings on the convective term of the sound speed equations are tested, in addition to the previously studied F form [22].

5 NUMERICAL RESULTS

Numerical tests have been performed to study a selection of the possible discrete formulations of the Euler equations among those using a KEP splitting for the mass and momentum equation.

Starting with the discretization of the internal energy equation, (ρe) is the KEP scheme using the KGP splitting for the convective term, which in the hypothesis of exact time integration is equivalent to the KEEP schemes proposed by Kuya *et al.* [23]. In addition, splittings with Pressure Equilibrium Preservation (PEP) property have also been studied. These are able to

preserve the equilibrium of velocity and pressure when they are constant at the initial time [24, 17]. The formulation $(\rho e)_{\mathrm{PEP}}$, is the PEP formulation presented by Shima *et al.* [24], in which the the $\partial up/\partial x$ term is discretized as an average of its advective and divergence form. The formulation $(\rho e)_{\mathrm{div}}$ is the analogous PEP scheme in which only the divergence form of the term is used. The choice of the speed of sound as primary variable has been tested with the KEP forms F, C and KGP and they are indicated as $(\rho c)_{\mathrm{F}}$, $(\rho c)_{\mathrm{C}}$ and $(\rho c)_{\mathrm{KGP}}$, respectively. The formulation employing the F form, $(\rho c)_{\mathrm{F}}$, was initially used by Kok [22].

For the discretization of the total energy, three classical formulations have been selected: the stardard (ρE) discretizes the total energy equation directly discretized with a a divergence form for the pressure term; $(\rho E)_{\mathrm{JP}}$ is the Jameson-Pirozzoli variant [13, 14] with the total enthalpy appearing in the convective term through the inclusion of the scaled pressure term; finally a PEP scheme, $(\rho E)_{\mathrm{PEP}}$, proposed by Singh and Chandrashekar [25]. The KGP splitting is used for the discretization of the convective fluxes in all the three cases.

The entropy equation has been discretized using the C, F and KGP forms: $(\rho s)_{\mathrm{C}}$, $(\rho s)_{\mathrm{F}}$ and $(\rho s)_{\mathrm{KGP}}$.

To display the results of the tests, the $\sim$ sign over a generic variable f will be used to denote integration over the spatial domain; the brackets will indicate normalization with respect to its initial value $\widetilde{f}_0$: $\langle\widetilde{f}\rangle = (\,\widetilde{f} - \widetilde{f}_0\,)/\widetilde{f}_0$.

5.1 Isentropic vortex

In this two-dimensional test, a vortex is convected without entropy production in a square domain of unitary side with periodic boundary conditions. The vortex, with core radius $r_v = 1/15$ and center initially located in $(x_0, y_0) = (0.5, 0.5)$, has initial conditions

$$\frac{u(x,y)}{u_\infty} = 1 - \frac{M_v}{M_\infty}\frac{y-y_0}{r_v}e^{(1-\hat{r}^2)/2}\,; \qquad \frac{v(x,y)}{u_\infty} = \frac{M_v}{M_\infty}\frac{x-x_0}{r_v}e^{(1-\hat{r}^2)/2} \tag{21}$$

$$\frac{T(x,y)}{T_\infty} = \left(\frac{p(x,y)}{p_\infty}\right)^{(\gamma-1)/\gamma} = \left(\frac{\rho(x,y)}{\rho_\infty}\right)^{\gamma-1} = 1 - \frac{\gamma-1}{2}M_v^2 e^{1-\hat{r}^2} \tag{22}$$

in which $u_\infty = \rho_\infty = 1$, $M_v = M_\infty = 0.5$, and $T_\infty = 720 M_v r_v$ and $\hat{r} = r/r_v$. The pressure is normalized with $p_\infty = \rho_\infty^\gamma/(\gamma M_\infty^2)$. A uniform Cartesian grid with 40^2 nodes is used to discretize the domain. For the spatial derivatives fourth-order accurate central schemes are employed; the classical fourth-order Runge-Kutta (RK4) is used for time integration. The Courant number of the simulations is CFL = 0.01.

Due to the periodic conditions and the non viscosity of the flow, the integral value of density, momentum and total energy are supposed to stay constant throughout the simulation. This was true up to machine precision for all methods but the ones using entropy as the primary variable, for which an error is committed on the total energy. This is because the induced evolution equation is not conservative [15, 17]. It is however evident from Figure 1(i) that the the choice of the KGP splitting for the convective term greatly reduces the error committed.

For all the other formulations, more interesting observations can be made about the evolution of the integral value of entropy, initially equal to zero. When the entropy equation is directly discretized, $\widetilde{\rho s}$ stays exactly equal to zero; all the other methods cause an error, but its magnitude varies greatly depending on the discretization (Figure 2). The methods that provide the best

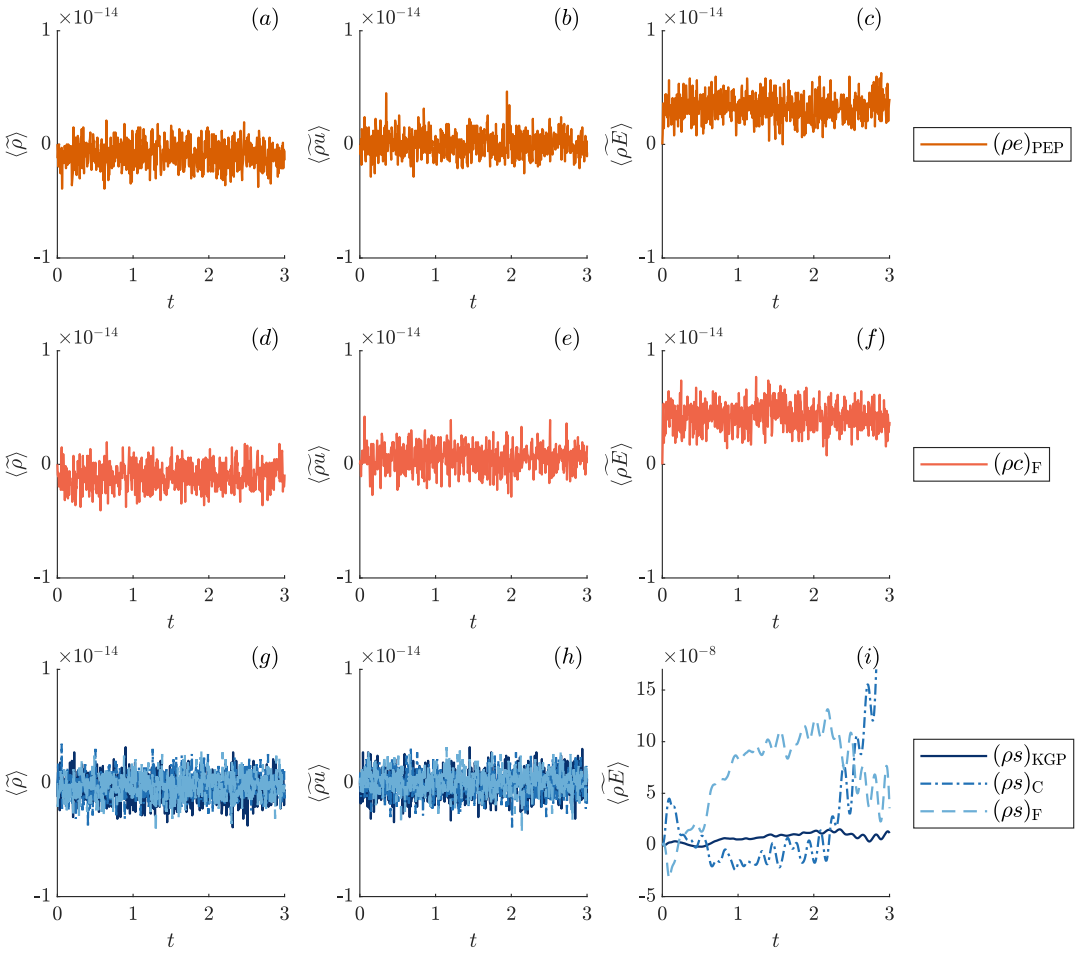

Figure 1: Evolution of linear invariants for the isentropic vortex flow simulated on a 40^2 uniform Cartesian mesh using different primary energy variables: internal energy, sound speed, and entropy. Spatial derivatives are discretized with fourth-order central schemes.

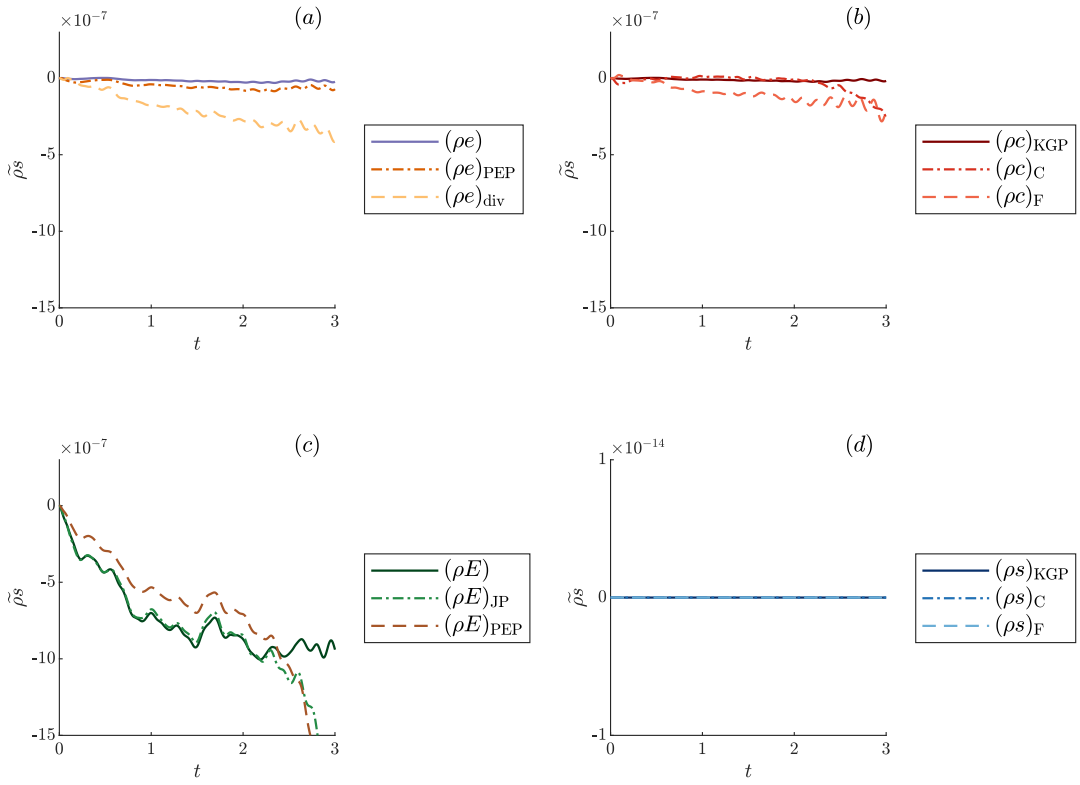

Figure 2: Evolution of the entropy integral for the isentropic vortex flow simulated on a 40^2 uniform Cartesian mesh using different primary energy variables: internal energy, sound speed, total energy, and entropy. Spatial derivatives are discretized with fourth-order central schemes.

performance in this respect are those that have as primary variables internal energy and sound speed. They are directly compared in Figure 3 and the error is lowest when KGP splitting is used for the convective terms. The integral values of kinetic energy and internal energy are also shown in Figure 3 and are supposed to stay constant throughout the simulation, since the motion is a pure translation of the vortex. The displayed error is due to the mesh discretization and present in all simulations regardless of the conservation properties of the formulation employed.

5.2 Robustness test

In order to better evaluate the stability of the different formulations, the isentropic vortex test was run again with a longer end time, $T_{\mathrm{fin}} = 50$, on a coarser 30^2 mesh and with CFL $= 0.1$. Table 1 reports the values of blow-up times for all the different cases. All the methods employing total energy as primary variables diverged, with the use of the Jameson-Pirozzoli approach and

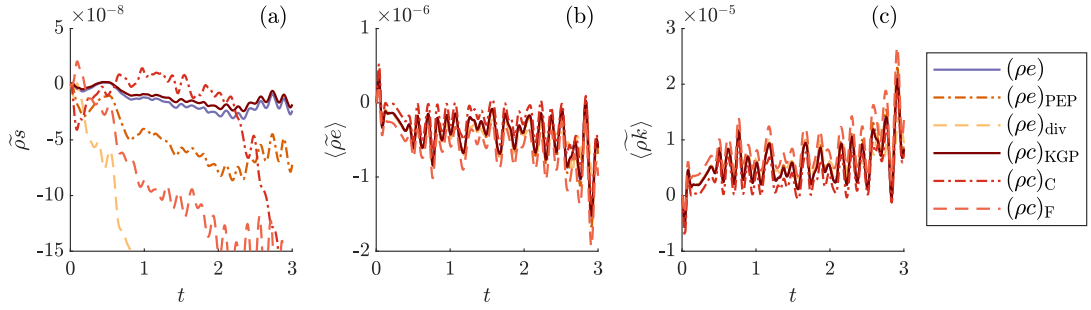

Figure 3: Evolution of conserved integral quantities for the isentropic vortex flow simulated on a 40^2 uniform Cartesian mesh using internal energy and sound speed equations. Spatial derivatives are discretized with fourth-order central schemes.

of the PEP scheme seemingly improving robustness.

On the other hand, when using the KGP splitting on the convective term, the methods using internal energy, sound speed and entropy all managed to produce a full simulation until the end time. The PEP scheme based on the internal energy also showed a good stability, but only when the splitting taking the average was employed, the one simply using the divergence blew up.

Recent studies [24, 25, 26] tried to assess the ability of different discretizations of the compressible Euler equations to withstand instabilities due to pressure oscillations. A test that highlights this kind of instability is that of a one dimensional density wave with periodic boundary conditions. The initial conditions are of velocity u and pressure p unitary in the whole domain, defined as $x \in [0, 1]$, while the density has a distribution given by

$$\rho(x) = 2 + \sin(2\pi x) \tag{23}$$

The domain is uniformly discretized with 41 nodes; second-order accurate central schemes are used for spatial derivatives; the time integrator is the RK4 with CFL = 0.1.

All the formulation with PEP prevented the simulation from becoming unstable, included those that failed the previous test. On the other hand, among the others only the methods using entropy as a primary variable managed to avoid blow-up. It can be noted, however, that the methods using sound speed also showed an advantage with an increased blow-up time.

6 CONCLUSIONS

In this work, numerical test have been performed to verify theoretical predictions about various formulation of the energy equation in non viscous compressible flows and to compare their robustness and ability to preserve invariants of the system of equations.

By simulating the isentropic vortex, it was shown that, as expected, the schemes preserved total energy up to machine precision with the only exception being the schemes discretizing entropy as a primary variable. These, on the other hand, were the only ones capable of correctly conserving the entropy integral.

Among the other formulations, the smallest error on entropy was produced when internal energy and sound speed where discretized with a KGP splitting. An interesting note is that

	Blow-up times	
	Isentropic Vortex	Density Wave
(ρE)	28	13
$(\rho E)_{\mathrm{JP}}$	34	11
$\rho E)_{\mathrm{PEP}}$	44	–
(ρe)	–	13
$(\rho e)_{\mathrm{PEP}}$	–	–
$(\rho e)_{\mathrm{div}}$	26	–
$(\rho c)_{\mathrm{F}}$	29	22
$(\rho c)_{\mathrm{C}}$	19	24
$(\rho c)_{\mathrm{KGP}}$	–	29
$(\rho s)_{\mathrm{F}}$	44	–
$(\rho s)_{\mathrm{C}}$	34	–
$(\rho s)_{\mathrm{KGP}}$	–	–

Table 1: Blow-up times using different discretizations of the energy equation. Fourth-order accurate central schemes are employed for spatial derivatives in the isentropic vortex case, they are second-order accurate for the density wave; Courant number is CFL = 0.1; the meshes are of 30^2 for the isentropic vortex and of 41 nodes for the density wave. The symbol '–' indicates no divergence until the end of the simulation, which is $T_{\mathrm{fin}} = 50$ for the isentropic vortex and $T_{\mathrm{fin}} = 200$ for the density wave.

actually the choice of sound speed as a primary variable could also be seen as discretizing the internal energy in such a way that it is not its kinetic energy to be preserved, but the variable based on its square root $\rho\sqrt{e}$.

These schemes also showed good robustness on a longer simulation of the isentropic vortex, when compared to formulations based on total energy. For the monodimensional density wave test case, due to the spurious pressure oscillation, most schemes diverged, while the schemes provided with the PEP property showed no instability until the end of the simulation. However, the use of the sound speed had a longer blow-up time when compared to other non PEP methods. An exception to that were the schemes discretizing the entropy equation, which did not diverge despite the lack of the PEP property.

The results presented suggest that the use of a KEP splitting for the energy equation may not always be the best approach, when the preservation of other quantities such as the square root could provide similar robustness and the reproduction of physical properties in the discrete setting.

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