Journal of Computational Physics 382 (2019) 86–104

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Numerically stable formulations of convective terms for turbulent compressible flows

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ARTICLE INFO

Article history:
Received 7 May 2018
Received in revised form 12 November 2018
Accepted 10 January 2019
Available online 17 January 2019

Keywords:
Energy conservation
Compressible Navier–Stokes equations
Turbulence simulations

ABSTRACT

A systematic analysis of the discrete conservation properties of non-dissipative, central-difference approximations of the compressible Navier–Stokes equations is reported. A generalized splitting of the nonlinear convective terms is considered, and energy-preserving formulations are fully characterized by deriving a two-parameter family of split forms. Previously developed formulations reported in literature are shown to be particular members of this family; novel splittings are introduced and discussed as well. Furthermore, the conservation properties yielded by different choices for the energy equation (i.e. total and internal energy, entropy) are analyzed thoroughly. It is shown that additional preserved quantities can be obtained through a suitable adaptive selection of the split form within the derived family. Local conservation of primary invariants, which is a fundamental property to build high-fidelity shock-capturing methods, is also discussed in the paper. Numerical tests performed for the Taylor–Green Vortex at zero viscosity fully confirm the theoretical findings, and show that a careful choice of both the splitting and the energy formulation can provide remarkably robust and accurate results.

1. Introduction

It is well known that standard central finite-difference approximations of the equations governing fluid flow are susceptible to numerical nonlinear instability when used at or near zero viscosity, owing to the accumulation of aliasing errors resulting from discrete evaluation of the convective terms [1]. Such shortcoming has also been traced to failure in discretely preserving the secondary quadratic invariants associated with the conservation equations [2,3]. For instance, total kinetic energy is conserved from the Euler equations in the incompressible limit in unbounded or periodic domains, and failure to discretely satisfy this property typically leads to flow divergence, when non-dissipative spatial discretizations are employed. Several attempts have been made over the years to develop numerical methods for the incompressible and the compressible flow equations which replicate quadratic conservation properties in the discrete sense, both in finite-difference and in finite-volume frameworks [4–7]. For incompressible flows, most efforts made so far loosely rely on the idea of expanding the convective derivatives to 'skew-symmetric' split form [8,9], i.e. as the average of divergence ($\nabla \cdot uu$) and advective ($u \cdot \nabla u$) forms, with the objective of either minimizing the aliasing error [10], or to discretely preserve total kinetic energy [8]. In the context of compressible flow equations, where the convective term involves derivatives of triple products, straightforward extensions of 'skew-symmetric' split forms have been proposed, with varying degrees of success [11–13].

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https://doi.org/10.1016/j.jcp.2019.01.007
0021-9991/

Additional numerical robustness in the presence of density variations was gained by Kennedy and Gruber [14] through the use of a 'triple splitting' of the convective terms, i.e. by fully splitting the derivatives of triple products through the product rule. In their paper, the authors analyzed the effects of a full splitting of the cubic nonlinearity on the minimization of both aliasing errors and computational cost, for general multi-component flows.

Although splitting of the convective derivatives may guarantee good numerical stability properties[1] the resulting discrete approximations are not generally expressible in locally conservative form, i.e. a numerical flux cannot always be defined. As a consequence, primary conservation properties may be violated, which is especially concerning if the scheme has to be used as a building block of hybrid shock-capturing algorithms [15]. Pirozzoli [16] showed that locally conservative formulations with arbitrary order of accuracy are possible for some types of splittings, and showed that a particular member of the family of splittings introduced by Kennedy and Gruber [14] yields discrete energy preservation, and it is particularly robust.

Discretization of the energy equation is also known to be a sensitive issue in the numerical solution of the compressible Navier–Stokes equations. Of special importance is the choice of the form of the energy equation among analytically equivalent ones, namely the internal energy, the total energy, the entropy equation and so on. For instance, good numerical stability properties were found by Honein and Moin [17] when using the entropy equation. When the total energy equation is used, several arrangements are possible for the convective and pressure fluxes [12,14,16], which may lead or not to consistency with the internal and the kinetic energy equation, hence leading to different numerical stability properties.

It is the main goal of this paper to present a systematic study of the numerical conservation properties of several central-difference approximations applied to the compressible Navier–Stokes equations. First, in Sections 2 and 3 we focus on the issue of splitting of the convective terms. We show that a more general family of energy-conserving splittings of the mass and momentum equations exists than currently known, some of which also leading to local conservation of the primary invariants. The properties of several members of this wide family are presented and discussed, also in terms of empirically testing their numerical robustness. Second, in Section 4 we focus on the issue of the most appropriate formulation for the energy equation. For that purpose, we consider formulations including the total and internal energy, and the entropy, and bring out discrete conservations properties ensuing from different splittings. We also consider 'dynamic' splittings for the energy equation(s), whereby additional conservation properties are obtained through suitable adaptive selection of a free parameter in the family of available energy-conserving splittings. Numerical experiments are finally presented in Section 5 to support the validity of the theoretical inferences.

2. Problem formulation

The Navier–Stokes equations for a compressible flow can be written as

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u_j}{\partial x_j}\,, \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} = -\frac{\partial \rho u_j u_i}{\partial x_j} - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}\,, \tag{2}$$

$$\frac{\partial \rho E}{\partial t} = -\frac{\partial \rho u_j E}{\partial x_j} - \frac{\partial p u_j}{\partial x_j} + \frac{\partial \tau_{ij} u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)\,, \tag{3}$$

where $E = u_i u_i/2 + c_v T$ is the total energy per unit mass and τ_{ij} is the stress tensor, for which the usual relation is assumed

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k}\delta_{ij}.$$

The standard notation is here adopted whereby ρ is the density, u_i are the Cartesian components of the velocity field, p is the pressure, T is the temperature, κ is the thermal conductivity, c_v the specific heat at constant volume and μ is the molecular viscosity. Closure of the system is achieved by the ideal equation of state $p = \rho R T$, with R the universal gas constant. Equations (1)–(3) represent the viscous balance of mass, momentum and total energy, and fully describe the motion of a compressible viscous fluid, once the equation of state and a suitable dependence of μ with the temperature has been specified.

By introducing the internal energy $e = c_v T$ and the entropy $s = c_v \ln(p/\rho^\gamma)$, with $\gamma = c_p/c_v$ and c_p the specific heat at constant pressure, the following induced balance equations are easily derived

$$\frac{\partial \rho e}{\partial t} = -\frac{\partial \rho u_j e}{\partial x_j} - p\frac{\partial u_j}{\partial x_j} + \tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right), \tag{4}$$

[1] In this work, we will use the term *numerical stability* and its derivatives with exclusive reference to the concept of nonlinear stability introduced by Phillips [1]. In this sense, *stable* formulations are those that enhance the robustness and avoid blow-up of numerical simulations by enforcing secondary conservation properties and/or by alleviating the accumulation of aliasing errors. This work is especially concerned with the former approach.

$$\frac{\partial \rho s}{\partial t} = -\frac{\partial \rho u_j s}{\partial x_j} + \frac{1}{T}\left[\tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial T}{\partial x_j}\right)\right], \tag{5}$$

any of which can be employed in place of the total energy, Eq. (3), to fully describe the motion and the state of the fluid.

The convective terms in Eqs. (1)–(5) have a common structure which can be summarized as

$$\mathcal{C} = \frac{\partial \rho u_j \phi}{\partial x_j}, \tag{6}$$

where ϕ equals unity, u_i, E, e and s for the mass, momentum, total and internal energy and entropy respectively. Integration of the governing equations readily shows that convective terms preserve the total amount of any conserved quantity. The associated invariants are hereafter referred to as linear invariants. By applying the standard product rule, the generic convective term can be written in different analytically equivalent forms. Due to the cubic nonlinearity, there are five basic forms in which it can be expressed

$$\mathcal{C}^D = \frac{\partial \rho u_j \phi}{\partial x_j}, \tag{7}$$

$$\mathcal{C}^\phi = \phi\frac{\partial \rho u_j}{\partial x_j} + \rho u_j \frac{\partial \phi}{\partial x_j}, \tag{8}$$

$$\mathcal{C}^u = u_j\frac{\partial \rho \phi}{\partial x_j} + \rho\phi \frac{\partial u_j}{\partial x_j}, \tag{9}$$

$$\mathcal{C}^\rho = \rho\frac{\partial u_j \phi}{\partial x_j} + \phi u_j \frac{\partial \rho}{\partial x_j}, \tag{10}$$

$$\mathcal{C}^L = \rho\phi\frac{\partial u_j}{\partial x_j} + \rho u_j \frac{\partial \phi}{\partial x_j} + \phi u_j \frac{\partial \rho}{\partial x_j}. \tag{11}$$

Equation (7) is the usual divergence form, whereas Eqs. (8) and (9) were firstly used in conjunction with $\mathcal{C}^D$ by Feiereisen et al. [11] and Blaisdell et al. [12] respectively. These authors applied their splittings for the discretization of both the momentum and continuity equations, and obtained stable simulations. The discretization of Eq. (10) was considered for the first time by Kennedy and Gruber [14], whereas the one in Eq. (11) is named *linear* (L) since only the gradients of linear quantities appear. Note that for the continuity equation, the forms $\mathcal{C}^D$ and $\mathcal{C}^\phi$ reduce to the classical divergence form, whereas $\mathcal{C}^u$, $\mathcal{C}^\rho$ and $\mathcal{C}^L$ are identical and correspond to the usual advective form. Also, only one advective form can be defined for quadratic nonlinearities, whereas four possibilities exist for a cubic product, namely Eqs. (8)–(11).

Any linear convex combination of the above mentioned forms is a consistent expression of the nonlinear convective term. This distinction has little importance in a continuous framework, since all the derived expressions are equivalent once the required analytical manipulations are assumed to be valid. On the other hand, the corresponding discretizations behave differently, mainly because the product rule, which is required to switch from one form to the others, does not hold in general for discrete operators. The differences among the various forms clearly emerge when considering the discrete evolution of induced quantities, such as kinetic energy. As it will be recalled in the next section, a divergence structure for the nonlinear convective term always induces a divergence structure also for the corresponding term in the evolution equation for the generalized energy $\rho\phi^2/2$. This in turn implies that convective terms do not contribute to the evolution of the total amount of generalized energy, a property that is usually lost unless the discretization is properly carried out. Previous experience has shown that retaining this property can yield beneficial effects in terms of numerical stability and physical fidelity of the computations [16,17]. In the next section, we will derive rigorous conditions under which the contribution of convective terms to the evolution of total generalized energy vanishes at the discrete level, when a generic linear combination of the forms (7)–(11) is adopted.

In what follows we will assume that the governing equations are numerically treated by adopting a semidiscretization procedure, in which the equations are firstly discretized in space, and then integrated in time. Hence, we assume that all the manipulations involving time derivatives can be carried out at the continuous level. The effects of discrete time integration will not be discussed in detail in this paper. It is worth mentioning that temporal errors are typically of dissipative character (especially when using Runge–Kutta schemes) and can be controlled by using sufficiently small time steps [18]. Although the ensuing discussion will focus on the case of spatially periodic computational domains, the analysis herein carried out only assumes that the space discretization operators satisfy the summation-by-parts (SPB) property, namely the discrete counterpart of integration by parts. Given two scalar grid functions u, v, and D a finite difference approximation of the first derivative operator, the SBP property can be expressed as $\langle u, Dv\rangle = -\langle Du, v\rangle + \text{b.t.}$, where $\langle\cdot,\cdot\rangle$ is a suitable discrete scalar product and b.t. are boundary terms. This property is satisfied in the periodic case (in which the boundary terms vanish) by central difference operators of any order [19], but SBP operators can also be derived for non-periodic domains [20]. In that general case, physical boundary conditions can be effectively handled through the simultaneous-approximation-terms (SAT) approach [21]. Hence, for the sake of simplicity but with no loss of generality, we will assume that space derivatives are approximated with central formulas, both explicit or compact, on a collocated mesh layout, which allows to infer the

effect on the evolution of induced quantities through analytical manipulations of the time derivatives, upon use of the SBP property.

3. Energy-preserving formulations

3.1. Derivation of the new forms

For a generic scalar variable ϕ, one can easily obtain the simple relation

$$\frac{\partial \rho\phi^2/2}{\partial t} = \phi \frac{\partial \rho\phi}{\partial t} - \frac{\phi^2}{2}\frac{\partial \rho}{\partial t}, \tag{12}$$

whose derivation only employs manipulation of temporal derivatives. If ϕ satisfies an equation of the type $\partial\rho\phi/\partial t = -\mathcal{C}$, the evolution equation for the generalized energy $\rho\phi^2/2$ is given by

$$\frac{\partial \rho\phi^2/2}{\partial t} = -\left(\phi\mathcal{C} - \frac{\phi^2}{2}\mathcal{M}\right), \tag{13}$$

where $-\mathcal{M}$ is the right-hand-side of Eq. (1). Assuming that $\mathcal{C}$ has the divergence structure of Eq. (6), simple analytical manipulation of the spatial derivatives can be applied to Eq. (13) to yield

$$\frac{\partial \rho\phi^2/2}{\partial t} = -\frac{\partial \rho u_i \phi^2/2}{\partial x_i} \tag{14}$$

which shows that a divergence structure for $\mathcal{C}$ and $\mathcal{M}$ induces a divergence structure for the right-hand-side of the evolution equation for the generalized energy $\rho\phi^2/2$. This in turn implies that the *global* energy (i.e. the energy integrated over the entire domain) is always conserved when periodic or homogeneous boundary conditions are applied. The associated invariants are hereafter referred to as quadratic invariants.

When the evolution equation has a more complex form, as in the cases of Eqs. (2)–(5), the considerations made above apply only to the convective terms, which always have a structure of the type (6), whereas global energy conservation is spoiled by viscous and pressure forces. This property holds in the continuous case for all the balanced quantities reported in Eqs. (1)–(5), and its reproduction at the discrete level is usually considered to be an important target for the choice of the spatial discretization. More specifically, when ϕ equals u_i (i.e. for the momentum equation) the generalized energy is exactly the kinetic energy of the fluid. In the case of incompressible flows, for which kinetic energy is globally conserved in the inviscid limit, energy-preserving numerical methods are highly desirable because of their inherent nonlinear stability [10,9,22]. When ϕ equals E, e or s, the corresponding generalized energies read ρE^2, ρe^2 and ρs^2 respectively. While these quantities have no direct physical meaning, numerical discretizations capable of ensuring that the convective terms do not contribute to the rate of variation of their volume integrals are likewise appealing. Indeed, experience shows that enforcement of these additional requirements typically yields enhanced numerical robustness [17].

The derivation of Eq. (14) from Eq. (13) employs the classical product rule for spatial derivatives, which is generally violated by discrete operators. As a consequence, the divergence structure of the convective term in Eq. (14) is in general not reproduced at a discrete level, and the analytically equivalent forms, Eqs. (7)–(11), behave differently when discretized. In what follows, when a discretization reproduces the physical property that nonlinear terms do not contribute to the generalized global energy balance, we will term it a *globally energy-preserving* discretization. This concept is usually not related to the classical conservative approximation property, which consists in the discrete preservation of the linear invariants. Following the standard usage, we will term *globally conservative* discretizations those for which the volume integral of the discretized convective term is zero. On the other hand, local conservation is achieved when the discretization of the convective term can be cast as difference of fluxes at adjacent nodes, this in turn implying global conservation through the telescoping property [16].

The condition that has to be satisfied so that the discretized nonlinear terms do not spuriously contribute to the global energy balance is easily derived by integrating Eq. (13) over the entire domain, and by equating it to zero

$$\int_\Omega \left(\phi\mathcal{C} - \frac{\phi^2}{2}\mathcal{M}\right) \mathrm{d}\Omega = 0. \tag{15}$$

The fulfilment of Eq. (15) by a central-difference discretization requires that a suitable form for $\mathcal{C}$ and $\mathcal{M}$ has to be chosen among Eqs. (7)–(11) (or among any linear combination of them), such that the integral at the l.h.s. can be shown to vanish by virtue of the integration by parts rule only, assuming that boundary terms are zero because of periodic or homogeneous boundary conditions.

Following the steps of Kennedy and Gruber [14], we express the convective terms for mass and for the generic variable ϕ as a linear combination of different, analytically equivalent, forms (7)–(11):

$$\mathcal{M} = \xi\,\mathcal{M}^D + (1-\xi)\,\mathcal{M}^A, \tag{16}$$

$$\mathcal{C} = \alpha\,\mathcal{C}^D + \beta\,\mathcal{C}^\phi + \gamma\,\mathcal{C}^u + \delta\,\mathcal{C}^\rho + \varepsilon\,\mathcal{C}^L, \tag{17}$$

where ξ is an arbitrary coefficient and $\alpha+\beta+\gamma+\delta+\varepsilon=1$. In Eq. (16) $\mathcal{M}^D = \partial\rho u_j/\partial x_j$ and $\mathcal{M}^A = \rho\partial u_j/\partial x_j + u_j\partial\rho/\partial x_j$ are the divergence and advective forms of the nonlinear term in the continuity equation. Upon substitution of Eqs. (16)–(17) in Eq. (15), and by transforming the resulting terms by making use only of the integration by parts rule, one can easily derive that satisfying the condition of Eq. (15) leads to the following constraints on the coefficients

$$\begin{cases} \alpha &= 1/2 - \delta \\ \beta &= \xi/2 \\ \gamma &= \delta \\ \varepsilon &= \dfrac{1-\xi}{2} - \delta. \end{cases} \tag{18}$$

The system (18) defines a two-parameter family of discretizations having the property that nonlinear convective terms do not contribute to the global energy balance, as it happens for the continuous equations. Note that by assuming that the coefficient ξ is independent of the coefficients appearing in Eq. (17), we are somehow deviating from the usual assumption that the same splitting is applied to the continuity and to the other balance equations. Removing this assumption greatly enlarges the range of possible energy-preserving formulations, although it affects global conservation of the linear invariants, as discussed later on.

Split forms which are found in the literature, and for which energy preservation has been already shown, are but two. The first is the Feiereisen (F) form, which is obtained by setting the free parameters $\xi=1$, $\delta=0$, resulting in the divergence form for the continuity equation and in the employment of the forms $\mathcal{C}^D$ and $\mathcal{C}^\phi$, both weighted with $1/2$, in the balance equation for ϕ. The second is the splitting obtained by uniformly weighting the forms $\mathcal{C}^D$, $\mathcal{C}^\phi$, $\mathcal{C}^u$ and $\mathcal{C}^\rho$ with weight $1/4$. This last splitting, which was firstly considered by Kennedy and Gruber [14] and later shown to be energy preserving by Pirozzoli [16], is obtained by choosing the free parameters $\xi=1/2$, $\delta=1/4$ and will be denoted as KGP (Kennedy–Gruber–Pirozzoli) hereinafter. The Blaisdell form, which has been used in the past as an extension of the so-called 'skew symmetric' form in the incompressible case, cannot be obtained by choosing specific values of δ and ξ, and is, in fact, not energy preserving.

The present analysis shows that the two mentioned examples are particular cases of a two-parameter family of energy-preserving forms that can be obtained by weighting the five forms of Eqs. (7)–(11). In the next section an analysis of this family is proposed, and new particular energy-preserving split formulations are introduced.

3.2. Analysis of the new forms

Starting from the general expression given in Eq. (18), two special one-parameter families of energy-preserving discretizations can be deduced. The first one is obtained by setting $\varepsilon=0$ in Eq. (17). Indeed, by performing an analysis similar to that employed for the case of the energy preservation, it can be easily shown that this condition is related to the possibility of attaining a formulation which discretely preserves linear invariants. In fact, the presence of the form $\mathcal{C}^L$ in Eq. (17) prevents the possibility of nullifying the integral of the convective term over the entire domain by just applying the integration by parts rule. In Appendix A it is shown that the requirement $\varepsilon=0$ is also a sufficient condition for writing the discretization in *locally* conservative form for central, explicit schemes.

When $\varepsilon=0$, the following one-parameter family of energy-preserving, globally conservative forms is thus obtained

$$\begin{cases} \xi = 1-2\delta \\ \alpha = \beta = 1/2 - \delta \\ \gamma = \delta \\ \varepsilon = 0. \end{cases} \tag{19}$$

The F and KGP forms are members of this family corresponding to $\delta=0$ and $\delta=1/4$. Note that this family satisfies $\xi=\alpha+\beta$, which implies that both the ϕ-equation and the continuity are discretized by employing the same split form. Hence, a necessary condition for a split form to be energy preserving and globally conservative of linear invariants is that the same form is employed for continuity and ϕ-equation, which in turn is equivalent to require that $\varepsilon=0$.

Another interesting one-parameter family can be obtained by requiring that Eq. (17) has the symmetric structure given by $\beta=\gamma=\delta$, as done by Kennedy and Gruber [14], yielding the following one-parameter family

$$\begin{cases} \xi = 2\delta \\ \alpha = 1/2 - \delta \\ \beta = \gamma = \delta \\ \varepsilon = 1/2 - 2\delta. \end{cases} \tag{20}$$

Actually, the symmetry assumption is not strictly needed, since the special role played by the continuity equation breaks the symmetry among the 'quadratic' forms $\mathcal{C}^\phi$, $\mathcal{C}^u$ and $\mathcal{C}^\rho$ of the convective term. In this respect, the family of energy-preserving split forms identified by Kennedy and Gruber [14] does not have any special significance, but it is here highlighted to allow

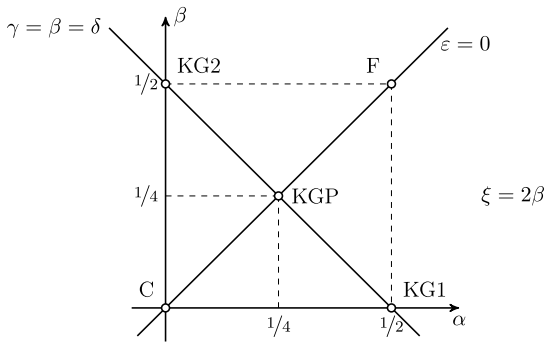

Fig. 1. Chart showing two families of energy-conserving schemes.

Table 1
Coefficients of classical and new energy-preserving split forms analyzed in Sec. 3.2.

	ξ	α	β	γ	δ	ε
F	1	1/2	1/2	0	0	0
C	0	0	0	1/2	1/2	0
KGP	1/2	1/4	1/4	1/4	1/4	0
KG1	0	1/2	0	0	0	1/2
KG2	1	0	1/2	1/2	1/2	−1/2

for a comparison with the work of these authors. In this respect, we note that in Fig. 7 of [14], a chart was reported showing the output in terms of blown-up or completed simulations for compressible isotropic turbulence tests. Several splittings of the momentum and energy equations in the $\alpha - \beta$ plane (same convention for the coefficients of Eq. (17) is used here) were employed. The authors' comment on that test campaign was that *a diagonal band of α–β pairs result in the DNS code not crashing*. That 'diagonal band' in fact coincides with the energy-preserving family of forms identified by Eq. (20), which is a first indirect confirmation of the validity of the present analysis.

The only form belonging to both classes is the one obtained by substituting $\delta = 1/4$ in (20) or (19), i.e. the KGP form, which turns out to be the only globally conservative and energy-preserving form among the ones analyzed by Kennedy and Gruber. A chart showing the two one-parameter families on a $\alpha - \beta$ plane is given in Fig. 1. In this graph, both the F and KGP forms are highlighted, together with three new forms with a particularly simple structure, which are briefly outlined below. A summary of the coefficients of these energy-preserving forms is also given in Table 1.

1. The form denoted as KG1 has parameters $\alpha = \varepsilon = 1/2$ and $\xi = \beta = \gamma = \delta = 0$. It is energy preserving, but is not globally conservative of linear invariants. The continuity equation is discretized with the advective form and the $\mathcal{C}^D$ and $\mathcal{C}^L$ forms are used with weight 1/2,
$$\frac{\partial \rho}{\partial t} = \rho \frac{\partial u_j}{\partial x_j} + u_j \frac{\partial \rho}{\partial x_j} \tag{21}$$
$$\frac{\partial \rho\phi}{\partial t} = \frac{1}{2}\left(\frac{\partial \rho u_j \phi}{\partial x_j} + \rho\phi \frac{\partial u_j}{\partial x_j} + \rho u_j \frac{\partial \phi}{\partial x_j} + \phi u_j \frac{\partial \rho}{\partial x_j} \right). \tag{22}$$
Equation (22) was used by Kennedy and Gruber in their direct numerical simulations of decaying compressible isotropic turbulence. However, in their implementation the form corresponding to the case $\xi = 1/2$ was adopted for continuity equation, hence the global scheme used in their paper is not strictly energy preserving.
2. The form denoted with KG2 has parameters $\xi = 1, \alpha = 0, \beta = \gamma = \delta = 1/2$ and $\varepsilon = -1/2$. As for the KG1 form, this form is energy preserving, but it does not globally preserve linear invariants. The continuity equation is discretized with the divergence form, whereas in the ϕ-equation the forms $\mathcal{C}^\phi$, $\mathcal{C}^u$ and $\mathcal{C}^\rho$ are used with equal weights 1/2, while $\mathcal{C}^L$ is weighted with $-1/2$. The ϕ-equation has only "quadratic" terms, i.e. terms of the type $f\nabla(gh)$
$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho u_j}{\partial x_j} \tag{23}$$
$$\frac{\partial \rho\phi}{\partial t} = \frac{1}{2}\left(\phi \frac{\partial \rho u_j}{\partial x_j} + u_j \frac{\partial \rho\phi}{\partial x_j} + \rho \frac{\partial u_j \phi}{\partial x_j} \right). \tag{24}$$
3. The form denoted as C has parameters $\xi = \alpha = \beta = \varepsilon = 0$ and $\gamma = \delta = 1/2$. This is an energy-preserving form which also globally preserves linear invariants. The continuity equation is discretized with the advective form and in the momentum equation $\mathcal{C}^u$ and $\mathcal{C}^\rho$ forms are both weighted with 1/2

$$\frac{\partial \rho}{\partial t} = \rho \frac{\partial u_j}{\partial x_j} + u_j \frac{\partial \rho}{\partial x_j} \tag{25}$$

$$\frac{\partial \rho\phi}{\partial t} = \frac{1}{2}\left(u_j \frac{\partial \rho\phi}{\partial x_j} + \rho\phi \frac{\partial u_j}{\partial x_j} + \rho \frac{\partial u_j \phi}{\partial x_j} + \phi u_j \frac{\partial \rho}{\partial x_j} \right). \tag{26}$$

This new form is in some sense symmetric to the classical F form and seems to have never been considered in the literature. Note that the one-parameter family of forms (19) can be equivalently expressed as a linear combination of the F and C forms with weight ξ and $1-\xi$ respectively, the KGP form corresponding to the case $\xi = 1/2$.

An important issue related to energy-preserving and globally conservative discretizations is local conservation of linear invariants. As shown by Pirozzoli [16], when central explicit finite-difference formulas of arbitrary order are used to discretize the derivatives, both the F and the KGP forms can be recast in a locally conservative form, i.e. as the difference of numerical fluxes at successive intermediate nodes. Besides the important implications on the convergence to weak solutions and the improvement in computational efficiency, this result implies that discrete local and global conservation of the linear invariants is guaranteed when the F or KGP forms are employed. This result directly extends to the family of forms defined by Eq. (19), which may cast as a convex linear combination of F and KGP forms. For the F and KGP forms, particularly simple and cost-effective flux functions have been show to exist. In Appendix A we show that similar simple flux function can also be derived for the C form, thus establishing a complete analogy with the F form.

4. Splitting of the energy equation

Regardless of the splitting selected for the convective terms in the continuity and momentum equations, the issue remains of which additional equation for energy is most suitable among the equivalent formulations (3)–(5), and which type of splitting to apply to it. A variety of splittings of the energy equation have been considered in the previous literature. Blaisdell et al. [12] applied their splitting to the internal energy equation, whereas Feiereisen et al. [11] used the evolution equation for pressure. Kennedy and Gruber [14] and Pirozzoli [16] used total energy, although the approach adopted by Kennedy and Gruber separately splits the convective term for ρE and the pressure term, whereas Pirozzoli applied the splitting directly to the total enthalpy $E + p/\rho$. Honein and Moin [17] applied the Feiereisen splitting to continuity, momentum and entropy equations, and reported great advantages in terms of robustness of the simulations. In this section, a systematic overview of the possible approaches is presented.

In the case of vanishing viscosity, the system of Eqs. (1)–(5) can be symbolically written as

$$\frac{\partial \rho}{\partial t} = -\mathcal{M}\,, \tag{27}$$

$$\frac{\partial \rho u_i}{\partial t} = -\mathcal{Q}_i - \mathcal{G}_i, \tag{28}$$

$$\frac{\partial \rho E}{\partial t} = -\mathbb{E} - \mathcal{D}, \tag{29}$$

$$\frac{\partial \rho e}{\partial t} = -\mathcal{E} - \mathcal{P}, \tag{30}$$

$$\frac{\partial \rho s}{\partial t} = -\mathcal{S}, \tag{31}$$

where $\mathcal{M}, \mathcal{Q}_i, \mathbb{E}, \mathcal{E}$ and $\mathcal{S}$ are the nonlinear convective terms for ρ, u_i, E, e and s respectively, and $\mathcal{G}_i = \partial p/\partial x_i$, $\mathcal{D} = \partial p u_j/\partial x_j$, $\mathcal{P} = p\partial u_j/\partial x_j$.

From the definitions of E, e and s the following general relations are easily derived by manipulating only temporal derivatives,

$$\frac{\partial \rho E}{\partial t} = \frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i^2/2}{\partial t}, \tag{32}$$

$$\frac{\partial \rho s}{\partial t} = \frac{c_v}{e}\frac{\partial \rho e}{\partial t} + (s - \gamma c_v)\frac{\partial \rho}{\partial t}. \tag{33}$$

From these relations, it is easy to obtain the effects of the spatial discretization of any quantity among E, e, s on the balance of the other ones. In the following sections we will separately explore the possible alternatives.

4.1. Discretization of the total energy equation

Discretization of the continuity and momentum equations according to Eqs. (27)–(28) induces a discrete evolution equation for $\rho u_i^2/2$ of the form

$$\frac{\partial \rho u_i^2/2}{\partial t} = -\left(u_i \mathcal{Q}_i - \frac{u_i^2}{2}\mathcal{M}\right) - u_i \mathcal{G}_i, \tag{34}$$

which is analogous to Eq. (13) in the case $\phi = u_i$. By construction, in the absence of pressure gradients (from now on this assumption will be tacitly made when referring to local and global conservation properties) kinetic energy is globally conserved, since energy-preserving splittings are used for $\mathcal{Q}_i$ and $\mathcal{M}$. Local conservation is however not guaranteed in general, even when locally conservative discretizations are used for $\mathcal{Q}_i$ and $\mathcal{M}$. The additional discretization of the total energy equation, Eq. (29), through a locally conservative and globally energy-preserving form, ensures that ρE is conserved locally and ρE^2 is conserved globally. By virtue of Eq. (32), this in turn ensures that ρe is conserved globally, and it evolves through an equation of the form (30), where $\mathcal{E}$ and $\mathcal{P}$ are expressed as

$$\mathcal{E} = \mathbb{E} - u_i \mathcal{Q}_i + \frac{u_i^2}{2}\mathcal{M}, \tag{35}$$

$$\mathcal{P} = \mathcal{D} - u_i \mathcal{G}_i. \tag{36}$$

This implies that, according to Eqs. (13) and (32), the discrete evolution equation for $\rho e^2/2$ is

$$\frac{\partial \rho e^2/2}{\partial t} = -e\left(\mathbb{E} - u_i \mathcal{Q}_i + \frac{u_i^2}{2}\mathcal{M}\right) + \frac{e^2}{2}\mathcal{M} - e\left(\mathcal{D} - u_i \mathcal{G}_i\right), \tag{37}$$

which readily shows that ρe^2 is not conserved globally in general, i.e. a locally conservative, energy-preserving discretization of $\rho, \rho u_i$ and ρE is globally conservative but not energy preserving for ρe.

The induced equation for entropy is of the type (31), where by virtue of Eq. (33), $\mathcal{S}$ reads

$$\mathcal{S} = \frac{c_v}{e}\left(\mathbb{E} - u_i \mathcal{Q}_i + \frac{u_i^2}{2}\mathcal{M}\right) + \left(s - \gamma c_v\right)\mathcal{M} + \frac{c_v}{e}\left(\mathcal{D} - u_i \mathcal{G}_i\right), \tag{38}$$

from which it can be readily seen that ρs is in general not conserved globally.

Note that, due to the divergence structure of the pressure term in the total energy equation, Eq. (29) can be equivalently expressed as

$$\frac{\partial \rho E}{\partial t} = -\mathbb{E} - \mathcal{D} = -\mathcal{H} \tag{39}$$

where $\mathcal{H}$ has the classical structure of Eq. (6) with $\phi = E + p/\rho$. We will hereafter refer to 'total energy splitting' as the classical splitting of $\mathbb{E}$ with accompanying discretization of $\mathcal{D}$ in divergence form, and to 'total enthalpy splitting' as the splitting directly applied to $\mathcal{H}$.

4.2. Discretization of the internal energy equation

Discretization of the internal energy equation, Eq. (30), in addition to continuity and momentum equations, through a globally (and locally) conservative and a globally energy-preserving discretization, of course guarantees that ρe is conserved locally, and ρe^2 is conserved globally. As for the previous case, by virtue of Eq. (32) this guarantees that ρE is conserved globally and it evolves through an equation of the form (29) where $\mathbb{E}$ and $\mathcal{D}$ read

$$\mathbb{E} = \mathcal{E} + u_i \mathcal{Q}_i - \frac{u_i^2}{2}\mathcal{M}, \tag{40}$$

$$\mathcal{D} = \mathcal{P} + u_i \mathcal{G}_i. \tag{41}$$

According to Eqs. (13) and (32), the discrete evolution equation for $\rho E^2/2$ is

$$\frac{\partial \rho E^2/2}{\partial t} = -E\left(\mathcal{E} + u_i \mathcal{Q}_i - \frac{u_i^2}{2}\mathcal{M}\right) + \frac{E^2}{2}\mathcal{M} - E\left(\mathcal{P} + u_i \mathcal{G}_i\right), \tag{42}$$

from which it is again easily seen that ρE^2 is not conserved globally in general, i.e. a locally conservative, energy-preserving discretization of $\rho, \rho u_i$ and ρe is globally conservative but not energy preserving for ρE.

The induced equation for entropy is of the type (31), where by virtue of Eq. (33) $\mathcal{S}$ has the form

$$\mathcal{S} = \frac{c_v}{e}\mathcal{E} + \left(s - \gamma c_v\right)\mathcal{M} + \frac{c_v}{e}\mathcal{P}, \tag{43}$$

from which it can be readily seen that ρs is in general not conserved globally.

Table 2
Conservation properties induced by different energy balance equations discretized in split form. ⊙: variable conserved locally and globally, ◯: variable conserved globally but not locally, ×: variable not conserved.

		Conserved variable								
		ρ	ρu_i	ρE	ρe	ρs	ρu_i^2	ρE^2	ρe^2	ρs^2
Discretized energy equation	ρE	⊙	⊙	⊙	◯	×	◯	◯	×	×
	ρe	⊙	⊙	◯	⊙	×	◯	×	◯	×
	ρs	⊙	⊙	×	×	⊙	◯	×	×	◯
	ρe (dyn)	⊙	⊙	◯	⊙	◯	◯	×	◯	×
	ρs (dyn)	⊙	⊙	◯	◯	⊙	◯	×	×	◯

4.3. Discretization of the entropy equation

A discussion on the equations induced by a direct discretization of the entropy equation can be conducted similarly to the previous two cases. A discretization of Eq. (31), in addition to continuity and momentum equations, through a globally (and locally) conservative and a globally energy-preserving discretization, guarantees that $\rho, \rho u_i$ and ρs are conserved locally, and ρu_i^2 and ρs^2 are conserved globally. By virtue of Eq. (33) and of Eqs. (40) and (41), this implies that ρe and ρE evolve through equations of the form (30) and (29) respectively, where $\mathcal{E}+\mathcal{P}$ and $\mathbb{E}+\mathcal{D}$ are expressed in the form

$$\mathcal{E}+\mathcal{P} = \frac{e}{c_v}\mathcal{S} - \frac{e}{c_v}\left(s-\gamma c_v\right)\mathcal{M}, \tag{44}$$

$$\mathbb{E}+\mathcal{D} = \frac{e}{c_v}\mathcal{S} - \frac{e}{c_v}\left(s-\gamma c_v\right)\mathcal{M} + u_i\mathcal{Q}_i - \frac{u_i^2}{2}\mathcal{M} + u_i\mathcal{G}_i, \tag{45}$$

from which it is seen that in general, neither ρe nor ρE are globally conserved. Note that the application of Feiereisen splitting to Eqs. (44) and (45) yields exactly the non-viscous versions of Eqs. (18) and (19) of Honein and Moin [17].

4.4. Adaptive selection of the split form

The results of the above made considerations are summarized in Table 2, showing that by discretizing directly the internal or the total energy equation, global conservation of entropy is not guaranteed. On the other hand, discretizing the entropy equation ensures that ρs is conserved locally and ρs^2 globally, but conservation of the total and internal energy is lost, even in a global sense.

Since the possible split forms which are energy preserving and globally (and locally) conservative of linear invariants constitute a one-parameter family, it is tempting to exploit the degree of freedom given by the free parameter in order to satisfy additional conservation properties. As shown below, this can be achieved under certain conditions, through an adaptive procedure that selects the splitting within the family in a dynamic way, by enforcing an additional global conservation constraint. This procedure can in fact be designed in different ways. Here we provide some possibilities to illustrate the general idea.

Let us consider the case in which the continuity and momentum equations are discretized together with the internal energy equation with a globally (and locally) conservative discretization and with an energy-preserving split form. According to Eq. (43), the condition for global conservation of entropy is given by

$$\int_\Omega \left(\frac{c_v}{e}\mathcal{E} + \left(s-\gamma c_v\right)\mathcal{M} + \frac{c_v}{e}\mathcal{P}\right)\mathrm{d}\Omega = 0. \tag{46}$$

Since ρ is globally conserved, the space integral of $\mathcal{M}$ is zero, and Eq. (46) reduces to

$$\int_\Omega \left(\frac{c_v}{e}\mathcal{E} + s\mathcal{M} + \frac{c_v}{e}\mathcal{P}\right)\mathrm{d}\Omega = 0. \tag{47}$$

Note that, if $\mathcal{M}$ and $\mathcal{E}$ are discretized through a split form of the family (19), they may be expressed as

$$\mathcal{M} = \xi\mathcal{M}^D + (1-\xi)\mathcal{M}^A, \tag{48}$$

$$\mathcal{E} = \xi\mathcal{E}^F + (1-\xi)\mathcal{E}^C, \tag{49}$$

where $\mathcal{E}^F$ and $\mathcal{E}^C$ are the convective terms of the internal energy equation discretized in the F and in the C form, respectively. By substituting Eqs. (48) and (49) into Eq. (47) one is left with

$$\int_\Omega \xi\left[\frac{c_v}{e}\left(\mathcal{E}^F-\mathcal{E}^C\right) + s\left(\mathcal{M}^D-\mathcal{M}^A\right)\right] + \left(\frac{c_v}{e}\mathcal{E}^C + s\mathcal{M}^A + \frac{c_v}{e}\mathcal{P}\right)\mathrm{d}\Omega = 0. \tag{50}$$

In Eq. (50), the free parameter ξ can be selected in order to satisfy Eq. (47). In fact, dynamically adjusting ξ in time according to

$$\xi_e = -\frac{\int_\Omega \left(\frac{c_v}{e}\mathcal{E}^C + s\mathcal{M}^A + \frac{c_v}{e}\mathcal{P}\right) \mathrm{d}\Omega}{\int_\Omega \frac{c_v}{e}\left(\mathcal{E}^F - \mathcal{E}^C\right) + s\left(\mathcal{M}^D - \mathcal{M}^A\right) \mathrm{d}\Omega} \tag{51}$$

guarantees that Eq. (47) is satisfied at each time instant, and the procedure will conserve locally ρ, ρu_i and ρe and globally ρu_i^2, ρE, ρe^2 and ρs.

Similarly, if one considers the case in which the entropy equation is discretized together with the continuity and the momentum equations, according to Eq. (44), the condition for global conservation of internal energy is given by

$$\int_\Omega \left(\frac{e}{c_v}\mathcal{S} - \frac{e}{c_v}\left(s - \gamma c_v\right)\mathcal{M} - \mathcal{P}\right) \mathrm{d}\Omega = 0. \tag{52}$$

By expressing $\mathcal{M}$ through Eq. (48) and $\mathcal{S}$ as $\mathcal{S} = \xi\mathcal{S}^F + (1-\xi)\mathcal{S}^C$, Eq. (52) reduces to

$$\int_\Omega \xi\frac{e}{c_v}\left[\left(\mathcal{S}^F - \mathcal{S}^C\right) - \left(s - \gamma c_v\right)\left(\mathcal{M}^D - \mathcal{M}^A\right)\right] + \frac{e}{c_v}\left(\mathcal{S}^C - \left(s - \gamma c_v\right)\mathcal{M}^A\right) - \mathcal{P}\,\mathrm{d}\Omega = 0, \tag{53}$$

from which one may infer that dynamically adjusting ξ in time according to

$$\xi_s = -\frac{\int_\Omega \left(\frac{e}{c_v}\left(\mathcal{S}^C - \left(s - \gamma c_v\right)\mathcal{M}^A\right) - \mathcal{P}\right) \mathrm{d}\Omega}{\int_\Omega \frac{e}{c_v}\left[\left(\mathcal{S}^F - \mathcal{S}^C\right) - \left(s - \gamma c_v\right)\left(\mathcal{M}^D - \mathcal{M}^A\right)\right] \mathrm{d}\Omega} \tag{54}$$

guarantees that Eq. (52) is satisfied at each time instant, and the procedure will conserve locally ρ, ρu_i and ρs and globally ρu_i^2, ρs^2, ρe and ρE.

5. Numerical tests: the inviscid Taylor–Green flow

In this section, the inviscid compressible Taylor–Green flow is used as a test case for comparing the performance of the various split forms analyzed in Sec. 3.2. Different splittings of the energy equation are also considered as explained in Sec. 4, resulting in a test matrix of 20 different formulations. We should point out that for convenience of computational implementation, and as suggested by Honein and Moin [17] the total energy equation is solved in all cases, however with the right-hand side rearranged either according to Eqs. (40), (41) to emulate the splitting of the internal energy equation, or to Eq. (45), to emulate the splitting of the entropy equation. Spatial discretization is performed in all cases by standard explicit central schemes of order 2, 4 and 6, and time integration is carried out by means of the third-order TVD Runge–Kutta scheme of Shu and Osher [23] and by the standard fourth-order Runge–Kutta scheme (RK4). The flow is integrated in a triply periodic cube of size 2π with zero viscosity, with the following initial conditions [15]

$$\begin{aligned}
\rho &= 1,\\
u &= \sin(x)\cos(y)\cos(z),\\
v &= -\cos(x)\sin(y)\cos(z),\\
w &= 0,\\
p &= 100 + \frac{(\cos(2x) + \cos(2y))\,(\cos(2z) + 2) - 2}{16},
\end{aligned}$$

where pressure is taken to be sufficiently high to provide a flow which is effectively incompressible. The ratio of specific heats γ is set to 1.4. It is well known that, after an initial transient, the initially smooth flow experiences distortion and stretching, and quickly undergoes instabilities characterized by the formation of smaller and smaller scales. For any given grid, after a sufficiently long time interval the flow develops unresolved scales, entering a thermalized random regime. This behaviour makes this flow a convenient testbed to check the stability of numerical methods in strongly under-resolved situations, and the absence of viscosity allows rigorous verification of the conservation of the invariants of motion.

Table 3
Test matrix for inviscid Taylor–Green flow numerical simulations. ✓numerically stable; × numerically unstable. Refer to Table 1 for the definition of the various split forms.

		Order	Forms for convective terms				
			KGP	F	C	KG1	KG2
Formulation of energy equation	Internal energy	2	✓	×	×	×	×
		4	✓	×	×	×	×
		6	✓	×	×	×	×
	Total energy with total energy splitting	2	✓	×	×	×	×
		4	✓	×	×	×	×
		6	✓	×	×	×	×
	Total energy with total enthalpy splitting	2	✓	✓	✓	×	×
		4	✓	✓	✓	×	×
		6	✓	✓	✓	×	×
	Entropy	2	✓	✓	✓	×	×
		4	✓	✓	✓	×	×
		6	✓	✓	✓	×	×

5.1. Robustness assessment

A numerical simulation campaign was first carried out to verify the computational robustness of the various formulations. The Euler equations are discretized on a 32^3 uniform grid and integrated in time with the third-order TVD Runge–Kutta scheme up to the final time $t = 256$ with CFL $= 1$.

The results of the tests are summarized in Table 3, in terms of numerical stability or instability, at least within the time integration interval. The data have been checked to be sufficiently general by performing additional spot calculations at different CFL numbers and changing the time integration scheme to RK4. The table shows that among the various split forms, the KGP form is most robust, allowing to achieve stable computations when applied in conjunction with any of the formulations for the energy equation. Furthermore, use of the total energy equation with total enthalpy splitting or of the entropy equation is found to be the most robust choice for the energy equation, yielding numerical stability also for the F and C split forms. In all other cases the simulations diverged within the time integration interval. The order of accuracy of the spatial discretization seems to have no influence on stability, although it is clearly expected to play a role on the accuracy of the solution.

In order to verify the predictions developed in the previous sections, selected calculations have been carried out with the more accurate RK4 scheme and with CFL $= 0.1$, in order to reduce temporal errors as much as possible. The results are shown in Figs. 2, 3 in terms of the time evolution of linear and quadratic invariants. In these plots, the overbar denotes spatial integration over the entire domain, whereas the brackets indicate the normalization

$$\langle \overline{f} \rangle = \frac{\overline{f} - \overline{f_0}}{\left| \overline{f_0} \right|},$$

where the absolute value at the denominator is taken to correctly represent time variations in the case that the initial value is negative.

The data reported in Fig. 2 were obtained by integrating the equations of mass, momentum and total energy with total enthalpy splitting, and by testing all the energy-preserving split forms discussed in Sec. 3. Central second-order approximations were used for all the space derivatives. It is found that the formulations employing the KG1 and KG2 forms diverge before $t = 10$, and the corresponding curves are seen as vertical lines (not labelled). On the other hand, the energy-preserving and locally-conservative forms KGP, F and C are found to be stable over the entire integration interval. As seen in panels (a)–(c), global values of mass, momentum and total energy are accurately conserved in time, up to machine precision (all calculations have been carried out using double-precision arithmetics). Although globally preserved by convection, ρe and ρu_i^2 are not conserved in time as their evolution is also affected by exchange of energy through the exchange terms $\mathcal{P}$, $u_i \mathcal{G}_i$ (see Eqs. (30), (34), respectively). Similarly, the quantity $\overline{\rho E^2}$, although preserved by convective terms, is affected by the pressure-type term $E\,(\mathcal{P} + u_i \mathcal{G}_i)$, which causes slight increase in time. On the other hand, $\overline{\rho s}$ and $\overline{\rho s^2}$, should stay constant in the inviscid case, hence their variations are entirely attributable to the lack of global discrete conservation.

The data reported in Fig. 3 support this analysis. In this case, splitting is applied to the mass, momentum and entropy equations, again with all the energy-preserving forms discussed in Sec. 3. The plots clearly show that mass, momentum and entropy are exactly globally conserved in time, together with $\overline{\rho s^2}$. The total energy displays slight deviations from constancy, because the entropy formulation does not guarantee global preservation of total and internal energy. Note that for this formulation of the energy equation the C split form performs worse than the KGP and the F forms, as larger deviations from the expected behaviour are observed starting at $t \simeq 50$; however, no blow-up is observed. At $t = 100$, $\langle \overline{\rho u^2} \rangle$, $\langle \overline{\rho E} \rangle$ and $\langle \overline{\rho s} \rangle$ reach values of 0.22, 3.8×10^{-4} and 4.1×10^{-10}, respectively. Note also that, in contrast to what observed in Fig. 2,

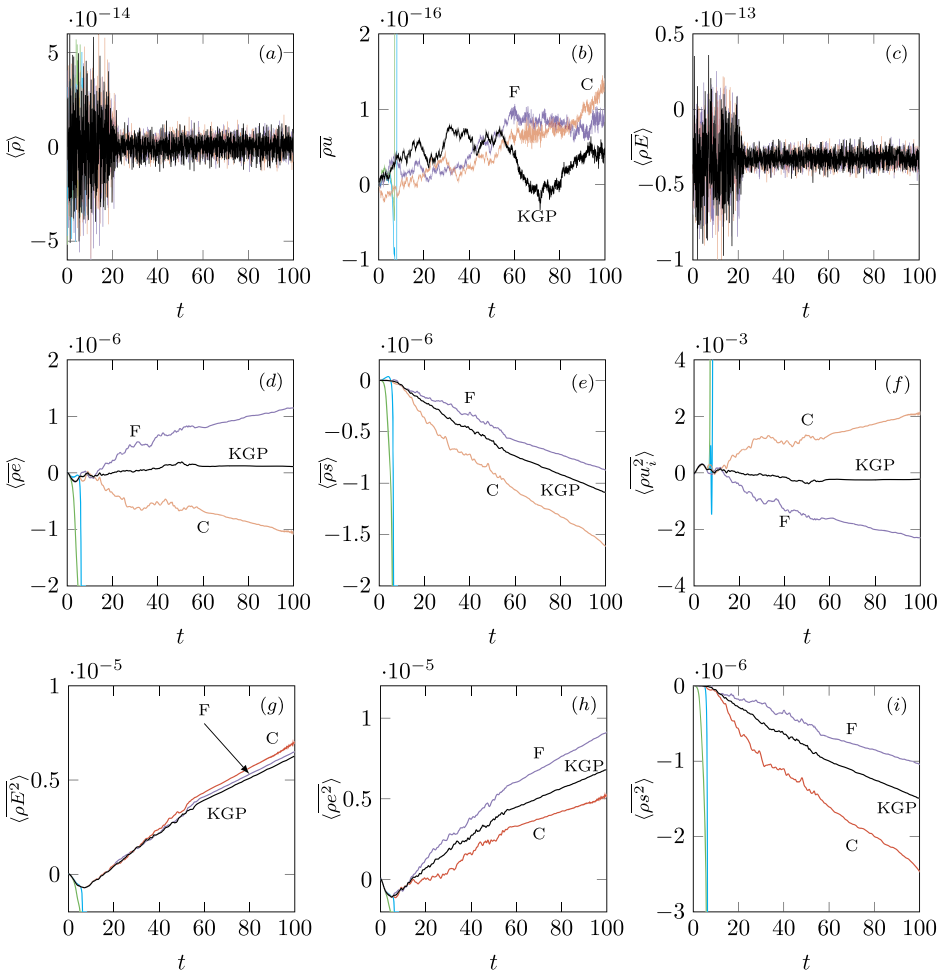

Fig. 2. Time evolution of linear and quadratic invariants for inviscid Taylor–Green flow using different splittings of the convective terms, with second-order central discretization of the space derivatives. Black lines refer to KGP form, blue lines to F form, red lines to C form and green and cyan lines refer to KG1 and KG2 forms, respectively. The total energy equation is used with total enthalpy splitting. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

the deterioration of the performances of the C form also affects the quantities $\overline{\rho s}$ and $\overline{\rho s^2}$, which should be conserved by construction (see the C curves in panels (e) and (i)). This behaviour may be traced to the previously noted use of a surrogate total energy equation in the place of the entropy equation. In this formulation, the entropy is strictly a derived variable (it is evaluated from ρE through $\rho s = \rho c_v \ln\left((\gamma-1)\left(\rho E - \rho u_i^2/2\right)/\rho^{\gamma-1}\right)$, and therefore, accumulation of numerical errors may also spoil variables which should be globally conserved by construction. The deterioration of the accuracy of the C form, on the other side, does not affect the global conservation of mass and momentum, whose equations are directly solved for (see panels (a) and (b)).

A further observation on Fig. 3 relates to the total energy evolution obtained from the KGP split form applied to the entropy formulation. The curve labelled as KGP in Fig. 3(c) actually shows that, in contrast to the C and F curves, in the entropy formulation the total energy is globally conserved with good accuracy during the whole integration interval (its maximum absolute value is about 2×10^{-10}). This additional conservation property of the KGP split form in the context of the discretization of the entropy equation is further investigated in the forthcoming section.

5.2. Test of adaptive splitting procedures

With the aim of further analyzing the properties of the various split forms in connection to the enforcement of additional balance equations, the adaptive procedures proposed in Sec. 4.4 have been tested. The test case and the space and time discretization setup are the same as in Sec. 5.1, but the split form is now dynamically adjusted within the family of Eq. (19), by adapting the value of ξ according to either Eq. (51) or Eq. (54).

In Fig. 4(a) the value of the coefficient ξ_s obtained from Eq. (54) is shown as a function of time. In this simulation, the mass, momentum and entropy equations are solved in split form, and the free coefficient is dynamically adjusted to

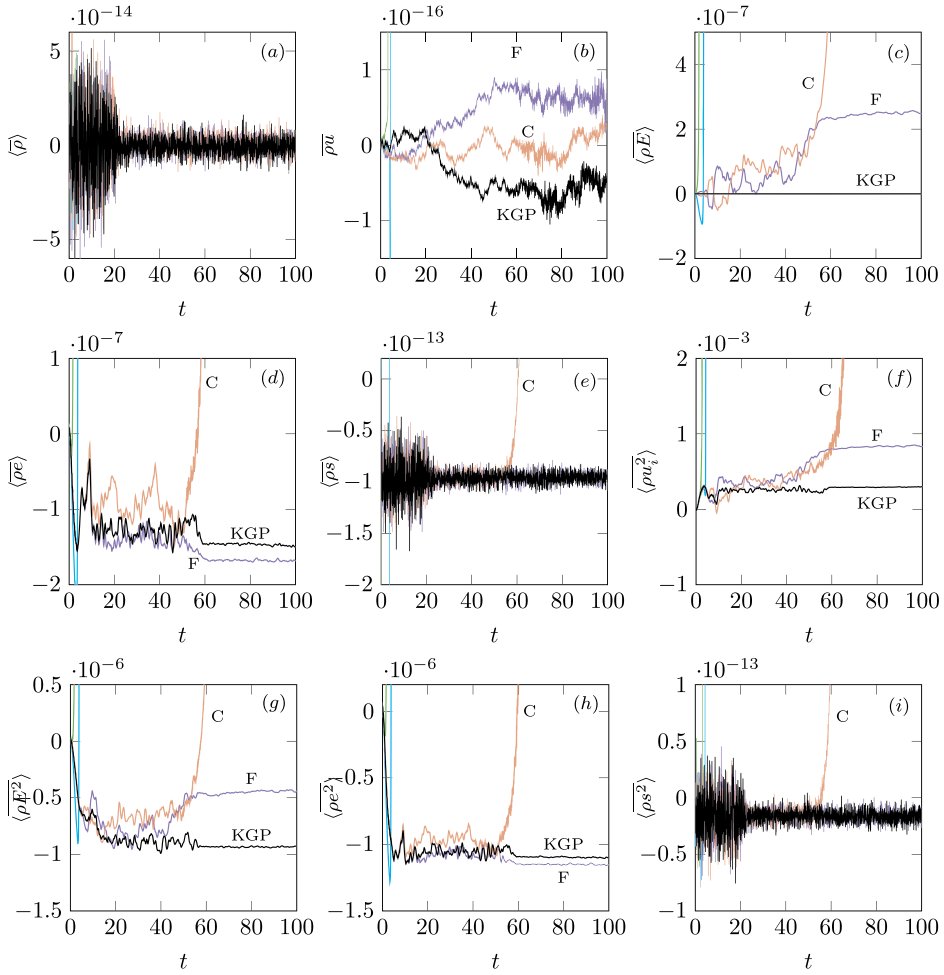

Fig. 3. Time evolution of linear and quadratic invariants for inviscid Taylor–Green flow using different splittings of the convective terms, with second-order central discretization of the space derivatives. Black lines refer to KGP form, blue lines to F form, red lines to C form and green and cyan lines refer to KG1 and KG2 forms, respectively. The entropy energy equation is used.

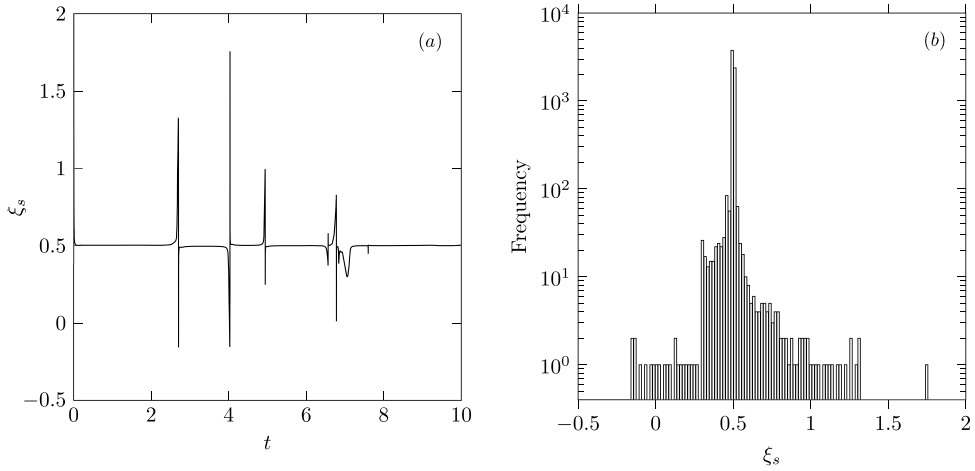

Fig. 4. Time evolution (a) and frequency distribution histogram (b) of the ξ_s coefficient for the adaptive procedure of Eq. (54).

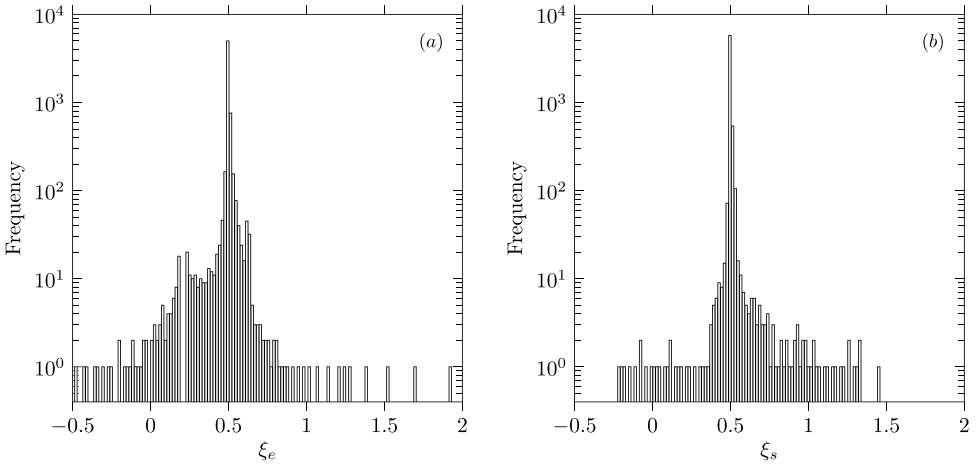

Fig. 5. Frequency distribution histograms of the ξ_e coefficient for the adaptive procedure of Eq. (51) for inviscid Taylor–Green flow (a) and of ξ_s for the adaptive procedure of Eq. (54) for viscous Taylor–Green flow at $\mathrm{Re} = 1600$ (b).

guarantee the additional global preservation of ρe. From this plot it can be seen that, with the exception of isolated spikes due to the possibly singular character of Eq. (54), the value of ξ_s obtained from the dynamic procedure settles around 0.5. In practice, this stands to indicate that the KGP form applied to the entropy equation also guarantees global conservation of the internal energy, and as a consequence global conservation of ρE. This finding is in perfect agreement with the results obtained in the previous section with the KGP form applied to the entropy equation (recalling Fig. 3(c)), which was shown to yield negligible variation of global total energy. The frequency distribution of ξ_s is shown in Fig. 4(b), where bars outside the interval $[-0.5, 2]$ are not displayed. From these data it may be estimated that ξ_s falls in the interval 0.5 ± 0.01 in the 90% of the cases, and in the interval 0.5 ± 0.05 in more than 95% of the cases (note that semi-logarithmic representation is used).

A similar situation also occurs for the dynamical procedure applied to the internal energy equation. In this case the mass, momentum and internal energy equations are integrated in time, whereas the split form is dynamically selected by the value of ξ_e given by Eq. (51), which guarantees additional global preservation of ρs. Fig. 5(a) shows the frequency distribution histogram of ξ_e. The convergence to the 0.5 value corresponding to the KGP form is confirmed also for this procedure, and cases in which ξ_e falls in the interval 0.5 ± 0.05 are estimated to be around 92% of the total.

As far as additional global conservation properties are concerned, both simulations show that the KGP form is almost optimal over the entire time integration interval. This includes smooth states in the initial transient, as well as fully thermalized states in later stages. The robustness of this finding has been further investigated by applying the dynamic procedure to a viscous calculation. The same initial condition and the same domain size are employed for numerical integration of the viscous Taylor–Green flow on a 32^3 grid at Reynolds number of 1600. The mass, momentum and entropy equations are solved, and the split form is adaptively determined through application of Eq. (54). In Fig. 5(b) the frequency distribution histogram of the dynamically calculated coefficient ξ_s is reported. The histogram again shows a strong tendency of the dynamical procedure to select values of ξ_s around 0.5. In this case the number of occurrences of ξ_s in the interval 0.5 ± 0.05 is around 97% of the total.

5.3. Effect of formulations of the energy equation

The effect of the formulation used for the energy equation on the reliability of numerical simulations remains to be explored. Indeed, we find the KGP split form to be equally robust, regardless of the energy formulation employed (among those introduced in Sec. 4), whereas the F and C forms proved to be stable only when either the total energy equation (with total enthalpy splitting) or the entropy equation are used. In this section we attempt to give additional insights regarding the accuracy of the various (stable) formulations, with the aim of establishing the most reliable one.

As a measure for reliability, we monitor the evolution of thermodynamic fluctuations in time, and in particular we consider density and temperature fluctuations. It is expected that after an initial transient, these quantities should level off to a constant value, similarly to what reported for inviscid isotropic homogeneous turbulence [17,16]. In Fig. 6, the r.m.s. density and temperature fluctuations obtained with selected numerical simulations are shown. The parameters of the simulations are the same as in Figs. 2 and 3, except for the spatial discretization, which was carried out through fourth-order central explicit formulas. All formulations for the energy equation are considered along with the KGP splitting (the corresponding cases are denoted as KPG(X)), whereas the total energy equation with total enthalpy splitting is used with the C splitting (the corresponding case is denoted as C(ρH)), and the entropy equation is used with the F splitting (the corresponding case is denoted as F(ρs)). Note that the two formulations KGP(ρH) and F(ρs) match those considered by Pirozzoli [16] and by Honein & Moin [17] respectively, although in the latter case compact differencing was used in space.

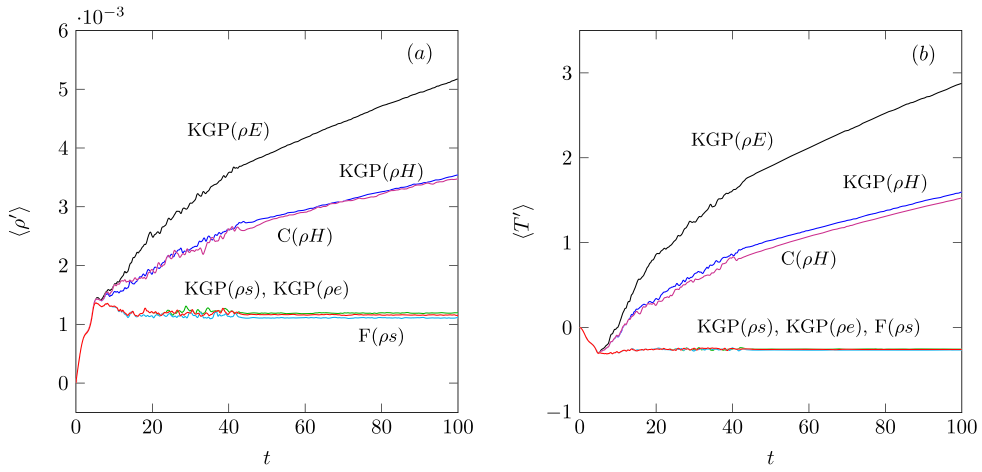

Fig. 6. Density (a) and temperature (b) fluctuations for inviscid Taylor–Green flow using different formulations of the energy equation coupled with different splittings. Black lines refer to the KGP(ρE) formulation, blue lines to KGP(ρH), magenta lines to C(ρH), red, green and cyan lines refer to KGP(ρs), KGP(ρe) and F(ρs) formulations, respectively.

The data in Fig. 6 show that not all the stable formulations yield asymptotic stabilization. Numerical simulations with the KGP form using the total energy equation (irrespective of the use of total energy or total enthalpy splitting) exhibit a non-negligible increase of density and temperature fluctuations, which, however, does not lead to numerical divergence. Similar results are obtained with the F and C split forms in conjunction with the total energy equation, although only the C(ρH) formulation is displayed. This behaviour was previously highlighted by Pirozzoli [16]. On the other hand, application of the KGP or F split forms together with the entropy equation provides much better results, both formulations yielding an asymptotically constant level of the fluctuations. Use of the internal energy yields contrasting results, as the F and C splittings yield numerical divergence, whereas the KPG splitting is effective in maintaining thermodynamic fluctuations to a constant asymptotic value similar to that given by entropy-based formulations. This is the likely consequence of the previously noted empirical evidence that the KPG(ρe) formulation is capable of nearly conserving the total entropy, although we cannot offer a rigorous proof at this stage.

As a further check of the predicted conservation properties, as listed in Table 2, we have carried out additional numerical simulations of nonlinear steepening of a one-dimensional acoustic wave. For that purpose a $[0, \pi]$ periodic interval was considered, with the following initial conditions

$$\rho(x,0) = \rho_0(1 + 0.2\sin x), \quad u(x,0) = 0.2c_0 \sin x, \quad p = p_0 + 0.2\rho_0 c_0^2 \sin x. \tag{55}$$

Nonlinear breakdown of the wave occurs at $t \approx 3$, at which a shock wave forms, and as a consequence entropy and internal energy are no longer conserved. Our purpose here is to verify that the mathematical conservation properties imparted to the numerical algorithm still apply. As a reference for the physically 'correct' results, a numerical solution has been computed with a fifth-order weighted essentially-non-oscillatory (WENO) scheme on a fine mesh to converge to the entropy solution with minimal amount of numerical dissipation. The computed density distributions using the KGP splitting with different formulations of the energy equations are shown in Fig. 7, where 32 cells are used. All the schemes yield visually indistinguishable results up to $t = 2$, at which the solution is still smooth. Some wiggles are observed at $t = 3$, after which large Gibbs oscillations arise, which are not found in the reference solution. Nevertheless, all formulations yield visually similar results. The global flow parameters are monitored in time in Fig. 8. The entropy solution yields dissipation of kinetic energy into heat starting at $t \approx 3$, and accordingly entropy starts to increase in time. As expected, this feature is not found in any of our conservative formulations. In particular, consistent with the results previously presented, we find that the entropy formulation fails to conserve the total energy, and vice-versa. We are also able to confirm that the formulation based on the internal energy, besides conserving internal and total energy, also yields near conservation of the total entropy.

6. Conclusions

A general framework for the derivation of energy-preserving split forms for convective terms in the compressible Navier–Stokes equations has been presented. In contrast to the incompressible case, for which the skew-symmetry of the discretized convective operator was shown to be the essential ingredient for global preservation of kinetic energy, energy-preserving formulations in the compressible case were not completely characterized. The theory herein developed fills this gap and provides a wide generalization of existing split forms for the compressible Navier–Stokes equations. Although illustrative examples are only provided for the case of spatially periodic computational domains, the analysis merely relies on use of the SBP property, hence it equally applies to the case of non-periodic domains, when supplemented with suitable SAT numerical boundary conditions. The classical Feiereisen et al. [11] splitting, and the more recent form introduced by Kennedy

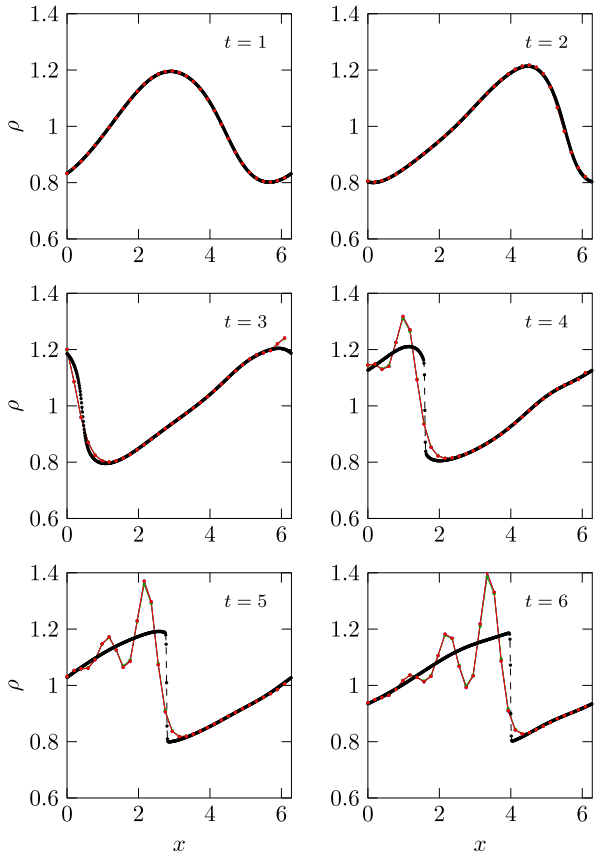

Fig. 7. Time evolution of density distribution for the one-dimensional acoustic wave test case. Black dashed lines refer to fifth order WENO scheme on a 512-cells mesh, used as reference solution. The solid lines refer to simulations obtained by using the KGP splitting of the convective terms on a 32-cells mesh, and by discretizing different energy balance equations. Blue lines refer to the KGP(ρH) formulation, green lines to KGP(ρe) and red lines to KGP(ρs). These last three formulations produce very similar results and the curves are hardly distinguishable in the scale of the plot.

and Gruber [14] and employed by Pirozzoli [16] (here referred to as KGP form), have been shown to be just two particular cases of a two-parameter family of energy-preserving forms. The analysis of the new forms has been conducted by considering also the topic of global conservation of primary quantities. It has been shown that even in the case in which the preservation of both linear and quadratic invariants is required, the set of admissible split forms constitutes a one-parameter family. Locally conservative formulations, on the other hand, have shown to be possible for this restricted class (for central explicit schemes of arbitrary order) by extending the approach used by Pirozzoli [16], and particularly simple and economic flux functions have been derived also for the new splitting forms.

In compressible flows the choice of a suitable energy-preserving split form for the discretization of convective terms does not strictly guarantee nonlinear stability. Another important and influential topic is the choice of which energy equation is most suitable among the various equivalent possibilities. A systematic analysis of the induced conservation properties of each formulation has been presented, and the employment of the free parameters stemming from the proposed theory on the split forms has led to the idea of 'dynamic' procedures which are able to provide additional discrete conservation properties by adaptively selecting the split form within a one-parameter family.

Numerical tests on the inviscid compressible Taylor–Green flow confirmed the theoretical predictions and provided new insights toward the selection of an optimal formulation in terms of stability and reliability. The numerical experiments showed that global conservation of linear invariants is a important issue, since energy-preserving formulations which are not globally conservative of primary variables are typically unstable in the inviscid case. This result is somehow in contrast to what happens in incompressible flows, for which kinetic energy conservation alone is typically sufficient to prevent instabilities arising from the accumulation of aliasing errors. Among the various split forms, the newly derived C form has robustness properties analogous to the classical F form, while the KGP form has proved to be the most robust, in conjunction with all the energy equation formulations. This behaviour has been confirmed by the application of adaptive procedures, which revealed that the KGP form is the optimal choice also with respect to additional induced conservation requirements. Finally, an analysis conducted on thermodynamic fluctuations has confirmed that the conservation of global entropy is an important ingredient. This is true not only for robustness, but also with respect to the reliability of numerical simulations, since the unphysical increase in amplitude of the fluctuations, arising in some stable formulations, is not present

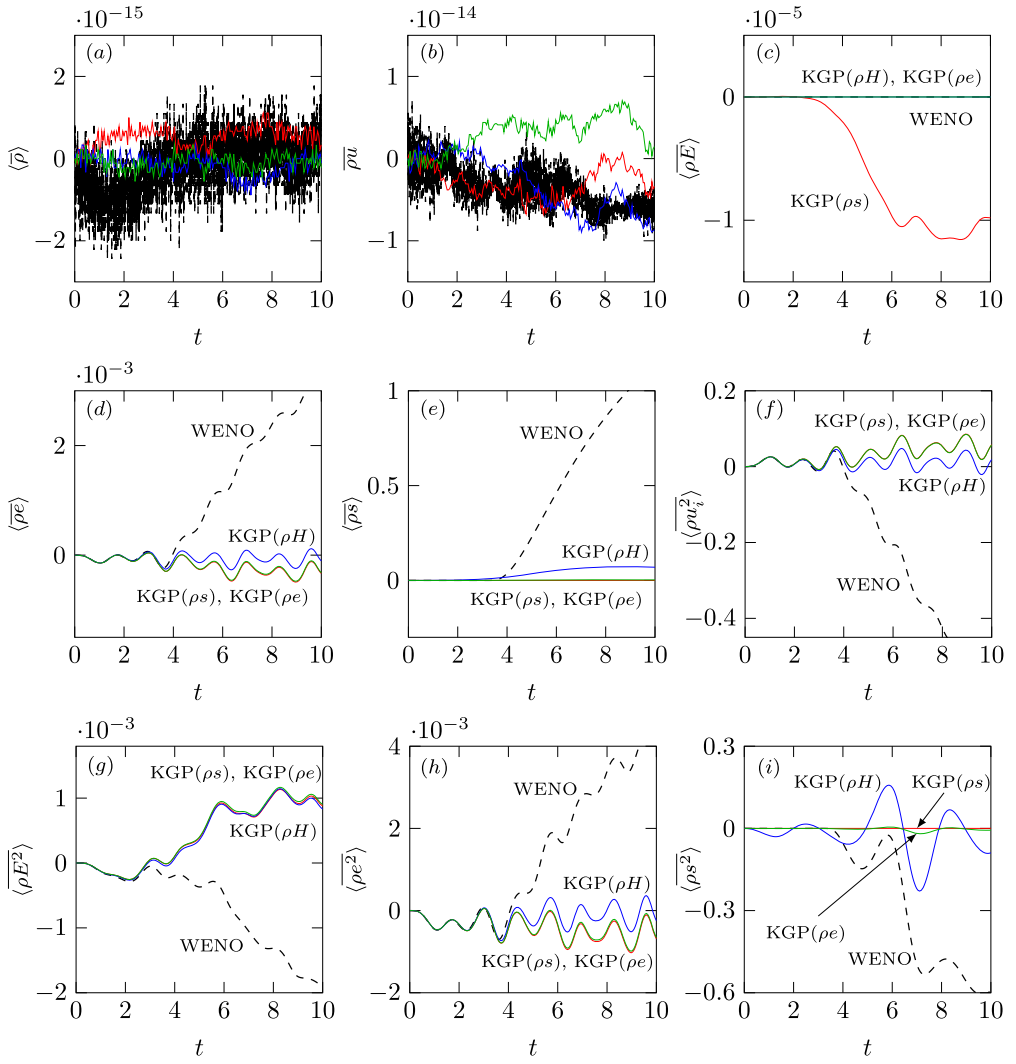

Fig. 8. Time evolution of linear and quadratic invariants for the one-dimensional acoustic wave test case. Black dashed lines refer to fifth order WENO scheme on a 512-cells mesh, used as reference solution. The solid lines refer to simulations obtained by using the KGP splitting of the convective terms on a 32-cells mesh, and by discretizing different energy balance equations. Blue lines refer to the KGP(ρH) formulation, green lines to KGP(ρe) and red lines to KGP(ρs).

when global entropy is preserved, both as a primary effect of the direct discretization of the entropy equation or as a hidden advantage of the adopted splitting. Additional numerical simulations for a one-dimensional sinusoidal acoustic wave developing into a shock confirm the predicted conservation properties discussed in the paper, and provide further support to the theoretical inferences.

Appendix A. Locally conservative formulations

By assuming a central finite difference explicit differentiation formula of the form

$$\widehat{\left.\frac{\partial \phi}{\partial x}\right|}_i = \sum_{k=1}^{L} a_k \delta_k \phi_i,$$

where $\delta_k \phi_i = (\phi_{i+k} - \phi_{i-k})/(2kh)$, the derivative of a product of two functions f and g can be expressed in locally conservative form, namely as the difference of numerical flux functions $(\hat{F}_{i+1/2} - \hat{F}_{i-1/2})/h$ where $\hat{F}_{i+1/2}$ has the form:

$$\hat{F}_{i+1/2} = 2 \sum_{k=1}^{L} a_k \sum_{m=0}^{k-1} \mathcal{I}(f, g)_{i-m,k}\,. \tag{A.1}$$

In Eq. (A.1), $\mathcal{I}(f,g)_{i,k}$ is a suitable two-function two-point interpolation operator. The *divergence* and *advective* forms of the product fg have the associated interpolation operators,

$$\begin{aligned}\widehat{\frac{\partial fg}{\partial x}} &\longrightarrow \mathcal{I}(f,g)_{i,k} = (\overline{f,g})_{i,k} \equiv \frac{f_{i+k}g_{i+k} + f_i g_i}{2},\\ \left(f\widehat{\frac{\partial g}{\partial x}} + g\frac{\partial f}{\partial x}\right) &\longrightarrow \mathcal{I}(f,g)_{i,k} = (\overline{\overline{f,g}})_{i,k} \equiv \frac{f_{i+k}g_i + f_i g_{i+k}}{2}.\end{aligned} \tag{A.2}$$

Any linear combinations of these two forms has a flux function given by the same linear combination of the corresponding fluxes. The associated interpolations follow the same rule,

$$\alpha\widehat{\frac{\partial fg}{\partial x}} + \beta\left(f\widehat{\frac{\partial g}{\partial x}} + g\frac{\partial f}{\partial x}\right) \longrightarrow \mathcal{I}(f,g)_{i,k} = \alpha(\overline{f,g})_{i,k} + \beta(\overline{\overline{f,g}})_{i,k}. \tag{A.3}$$

A particularly simple structure is obtained for the case of $\alpha = \beta = 1/2$, for which the interpolation operator assumes the form

$$\frac{1}{2}\left[\widehat{\frac{\partial fg}{\partial x}} + \left(f\widehat{\frac{\partial g}{\partial x}} + g\frac{\partial f}{\partial x}\right)\right] \longrightarrow \mathcal{I}(f,g)_{i,k} = (\widetilde{f,g})_{i,k} = \frac{1}{4}\left(f_i + f_{i+k}\right)\left(g_i + g_{i+k}\right). \tag{A.4}$$

In the case of three functions ρ, u and ϕ there are five basic ways of expressing the derivative of the triple product, analogous to the five forms (7–11). Four of them can be expressed in locally conservative form with the associated numerical flux

$$\hat{F}_{i+1/2} = 2\sum_{k=1}^{L} a_k \sum_{m=0}^{k-1} \mathcal{I}(\rho,u,\phi)_{i-m,k}, \tag{A.5}$$

where $\mathcal{I}(\rho,u,\phi)_{i,k}$ is a suitable three-function two-point interpolation operator. The list of forms and associated interpolation operators is

$$\frac{\partial \rho u\phi}{\partial x} \longrightarrow \mathcal{I}(\rho,u,\phi)_{i,k} = (\overline{\rho,u,\phi})_{i,k} = \frac{(\rho u\phi)_{i+k} + (\rho u\phi)_i}{2}, \tag{A.6}$$

$$\phi\frac{\partial \rho u}{\partial x} + \rho u\frac{\partial \phi}{\partial x} \longrightarrow \mathcal{I}(\rho,u,\phi)_{i,k} = (\overline{\overline{\rho u,\phi}})_{i,k} = \frac{(\rho u)_{i+k}\phi_i + \phi_{i+k}(\rho u)_i}{2}, \tag{A.7}$$

$$u\frac{\partial \rho\phi}{\partial x} + \rho\phi\frac{\partial u}{\partial x} \longrightarrow \mathcal{I}(\rho,u,\phi)_{i,k} = (\overline{\overline{\rho\phi,u}})_{i,k} = \frac{(\rho\phi)_{i+k}u_i + u_{i+k}(\rho\phi)_i}{2}, \tag{A.8}$$

$$\rho\frac{\partial u\phi}{\partial x} + \phi u\frac{\partial \rho}{\partial x} \longrightarrow \mathcal{I}(\rho,u,\phi)_{i,k} = (\overline{\overline{\phi u,\rho}})_{i,k} = \frac{(\phi u)_{i+k}\rho_i + \rho_{i+k}(\phi u)_i}{2}. \tag{A.9}$$

Any linear combination of these forms has a flux function whose associated interpolation operator $\mathcal{I}$ is a linear combination of the corresponding basic interpolation operators. Particularly simple structures are obtained in the following cases:

1. the F form, whose interpolation operator is

$$\mathcal{I}(\rho,u,\phi)_{i,k} = \frac{1}{2}\left((\overline{\rho,u,\phi})_{i,k} + (\overline{\overline{\rho u,\phi}})_{i,k}\right) = (\widetilde{\rho u,\phi})_{i,k}; \tag{A.10}$$

2. the KGP form, whose interpolation operator is

$$\mathcal{I}(\rho,u,\phi)_{i,k} = \frac{1}{4}\left((\overline{\rho,u,\phi})_{i,k} + (\overline{\overline{\rho u,\phi}})_{i,k} + (\overline{\overline{\rho\phi,u}})_{i,k} + (\overline{\overline{\phi u,\rho}})_{i,k}\right) = (\widetilde{\rho,u,\phi})_{i,k}, \tag{A.11}$$

   where

$$(\widetilde{\rho,u,\phi})_{i,k} = \frac{1}{8}\left(\rho_i + \rho_{i+k}\right)\left(u_i + u_{i+k}\right)\left(\phi_i + \phi_{i+k}\right);$$

3. the C form, whose interpolation operator is

$$\mathcal{I}(\rho,u,\phi)_{i,k} = \frac{1}{2}\left((\overline{\overline{\rho\phi,u}})_{i,k} + (\overline{\overline{\phi u,\rho}})_{i,k}\right) = (\overline{\overline{\phi|\rho,u}})_{i,k}, \tag{A.12}$$

   where

$$(\overline{\overline{\phi|\rho,u}})_{i,k} = \frac{1}{2}\left(\phi_i + \phi_{i+k}\right)(\overline{\overline{\rho,u}})_{i,k}.$$

A comparison of the computational effort required for the calculation of the fluxes for each form can be made by considering the cost required for the evaluation of the relevant interpolation operators, since the additional cost of assembling the flux through Eq. (A.5) is the same for all the locally conservative forms. The F form interpolation operator given by Eq. (A.10) requires $2L$ sums and L multiplications per node (cfr. Eq. (A.4)), in addition to a single multiplication per node in order to calculate the products of variables appearing in Eq. (A.10). The KGP form interpolation operator requires an effort of $3L$ sums and $2L$ multiplications, with no additional cost for the pre-storage of product of variables, whereas the C form requires $3L$ multiplications and $2L$ sums, with again no additional pre-storage cost. In summary, the F form interpolation requires $N(1+3L)$ floating point operations, while the C and KGP form interpolations require $5NL$ operations.

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