# LINEAR AND QUADRATIC INVARIANTS PRESERVING DISCRETIZATION OF EULER EQUATIONS

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Abstract. In the context of the numerical treatment of convective terms in compressible transport equations, general criteria for linear and quadratic invariants preservation, valid on uniform and non-uniform (Cartesian) meshes, have been recently derived by using a matrix-vector approach, for both finite-difference and finite-volume methods ([1, 2]). In this work, which constitutes a follow-up investigation of the analysis presented in [1, 2], this theory is applied to the spatial discretization of convective terms for the system of Euler equations. A classical formulation already presented in the literature is investigated and reformulated within the matrix-vector approach. The relations among the discrete versions of the various terms in the Euler equations are analyzed and the additional degrees of freedom identified by the proposed theory are investigated. Numerical simulations on a classical test case are used to validate the theory and to assess the effectiveness of the various formulations.

# **1** INTRODUCTION

The design of accurate and reliable numerical methods for the numerical simulation of compressible (low-Mach) flows is an important and challenging research topic. An ideal discretization should be locally conservative of linear invariants (a property which is naturally reproduced in finite-volume methods) and globally conservative of quadratic invariants (for which the so-called split forms are typically used in finite-difference methods). Moreover, the correct choice of the setup for the discretization of the (total) energy equation is of paramount importance, as it influences the correct preservation of additional invariants of the Euler equations (e.g. entropy).

Local conservation of primary invariants amounts to the requirement that the discretization of the convective terms, which have a divergence structure, can be cast (in 1D) as the difference of numerical fluxes. This property is mandatory for the convergence of the discretization to the correct weak solution in the case of shocked flows and is satisfied by constructon in finite-volume type formulations, which are focused on the specification of numerical fluxes at cell interfaces. In finite-difference methods the convective terms are approximated by using derivative matrices and the possibility of recasting the discrete operators as a difference of fluxes is not evident in many cases. Previous studies [3, 4] estabilished the possibility of recasting divergence, advective and split forms of the convective derivatives as difference of numerical fluxes for central schemes on uniform meshes and with periodic boundary conditions. Extensions of these initial works have been presented for curvilinear meshes [5] and for the case of non-periodic boundary conditions, within the framework of Summation By Parts (SBP) operators [6]. In all these studies the theory is developed for central schemes, which implies that the derivative operators involved are skew-symmetric (and typically Toeplitz) for internal points.

Conservation of kinetic energy is another important element in the construction of reliable numerical discretizations, for compressible and incompressible flow equations. As regards compressible Euler equations, starting from the pioneering work by Feiereisen et al. [7] many contributions have been presented (cf. [8, 9] and references therein). Recently, a quite complete analysis of the possible kinetic-energy preserving split forms have been presented for finite-difference central schemes on uniform meshes [10]. The theory developed in [10] is based on the SBP property of central schemes in the case of periodic boundary conditions, which is equivalent to the requirement that the derivative matrices are skew symmetric (and typically Toeplitz).

In a recent paper [1] the problem of the discrete local and global preservation of both linear invariants and kinetic energy is studied from an abstract point of view by using a matrix-vector notation. General criteria for local and global conservation of linear invariants and kinetic energy have been obtained for arbitrary derivative matrices (i.e. not necessarily skew symmetric or Toeplitz) and for a wide class of split forms. It is shown that local and global conservation can be assured whithin the usual class of split forms by assuming weakened requirements to the derivative matrices, which typically amount to the vanishing column sums property. An equivalence result is also derived for the concepts of global and local conservation of primary and quadratic (i.e. kinetic energy) invariants. Finally, an intimate relation between globally conservative finite-difference methods and general finite-volume type methods (in which numerical fluxes are specified) is estabilished.

The theory presented in [1] is mainly developed for general transport equations mimicking the fundamental features of compressible flow equations. In this work, a preliminary application is proposed to the two-dimensional system of Euler equation. The theoretical predictions are tested and new formulations exploiting the additional degrees of freedom identified by the theory are investigated.

# 2 TRANSPORT EQUATION AND DISCRETE FORMULATIONS

To briefly recall the results presented in [1, 2], we introduce the system of transport equations for a quantity  $\phi$  which is transported by a flow with mass density  $\rho$  and velocity  $\boldsymbol{u}$  with components  $u_i$ :

$$\frac{\partial \rho}{\partial t} + \mathcal{M} \equiv \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0, \qquad \frac{\partial \rho \phi}{\partial t} + \mathcal{C}\phi \equiv \frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = 0, \qquad (1a,b)$$

where the usual summation convention over repeated indices is assumed. To make the treatment simpler, but without loss of generality, in this and the next section we will work on the 1D version of Eqs. (1a,b), for which  $u_i = u, x_i = x$  and no summation occurs. The extension to multiple dimensions is straightforward and an example is presented in Sec. 4.

A quite general form of a finite-volume or finite-difference (semi)discretization of the system (1) can be expressed by the volume-scaled systems of ordinary differential equations:

$$\mathfrak{H}\frac{\mathrm{d}\rho}{\mathrm{d}t} + \mathfrak{d} = 0; \qquad \mathfrak{H}\frac{\mathrm{d}\mathsf{R}\phi}{\mathrm{d}t} + \mathfrak{C}\phi = 0.$$
 (2a,b)

where  $\mathfrak{H}$  is a diagonal matrix containing the sizes of the control volumes and is chosen such that the sum of the components of the first terms in Eqs. (2a,b) tends to the volume integral of the time derivative when  $|\mathfrak{H}| \to 0$ . In what follows general grid vectors (lower case) and matrices (upper case) are written in a sans-serif font. As an example,  $\mathsf{R} = \operatorname{diag}(\rho)$ is the diagonal matrix gathering the components of the density grid vector  $\rho$  on its main diagonal, in such a way that the product  $\mathsf{R}\varphi$  is the Hadamard (i.e. componentwise) product between  $\rho$  and  $\varphi$ . Quantities with a volume-consistent scaling are written in a  $\mathfrak{Frattur}$  font. With this notation a generic derivative matrix D is related to its scaled version by  $\mathsf{D} = \mathfrak{H}^{-1}\mathfrak{D}$ .

The terms  $\mathfrak{d}$  and  $\mathfrak{C}$  will be assumed to be convex linear combinations of the discrete versions of the following divergence and advective forms (cf. [10]):

$$\mathcal{M}^{D} \equiv \frac{\partial \rho u}{\partial x}, \qquad \mathcal{M}^{A} \equiv u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x}.$$
 (3a,b)

$$\mathcal{C}^{D}\phi \equiv \frac{\partial\rho u\phi}{\partial x}, \quad \mathcal{C}^{\phi}\phi \equiv \phi\frac{\partial\rho u}{\partial x} + \rho u\frac{\partial\phi}{\partial x}, \quad \mathcal{C}^{u}\phi \equiv u\frac{\partial\rho\phi}{\partial x} + \rho\phi\frac{\partial u}{\partial x}, \quad \mathcal{C}^{\rho}\phi \equiv \rho\frac{\partial u\phi}{\partial x} + u\phi\frac{\partial\rho}{\partial x}, \quad (4a-d)$$

in such a way that the most general discretization we will consider is given by

$$\mathfrak{d} = \xi \underbrace{\mathfrak{D}^{\rho u} \mathsf{R} \mathfrak{u}}_{\mathfrak{d}^{D}} + (1 - \xi) \underbrace{(\underbrace{\mathsf{U} \mathfrak{D}^{\rho} \rho + \mathsf{R} \mathfrak{D}^{u} \mathfrak{u}}_{\mathfrak{d}^{A}})}_{\mathfrak{d}^{A}}, \quad (5)$$

$$\mathfrak{C} = \alpha \underbrace{\mathfrak{D}^{\rho u} \mathsf{R} \mathfrak{U}}_{\mathfrak{C}^{D}} + \beta \underbrace{[\mathsf{R} \mathfrak{U} \mathfrak{D}^{0} + \operatorname{diag} (\mathfrak{D}^{\rho u} \mathsf{R} \mathfrak{u})]}_{\mathfrak{C}^{\phi}} + \gamma \underbrace{[\underbrace{\mathsf{U} \mathfrak{D}^{\rho} \mathsf{R} + \operatorname{diag} (\mathsf{R} \mathfrak{D}^{u} \mathfrak{u})]}_{\mathfrak{C}^{u}} + \delta \underbrace{[\mathsf{R} \mathfrak{D}^{u} \mathsf{U} + \operatorname{diag} (\mathsf{U} \mathfrak{D}^{\rho} \rho)]}_{\mathfrak{d}^{\rho}}, \quad (6)$$

with  $\alpha + \beta + \gamma + \delta = 1$ . Note that to have a more general formulation, in Eqs. (5) and (6) we allowed the use of different derivative matrices acting on the various terms. The matrices  $\mathfrak{D}^{\rho u}, \mathfrak{D}^{\rho}, \mathfrak{D}^{u}$  and  $\mathfrak{D}^{0}$  are at the moment arbitrary scaled first-order derivative matrices, typically having vanishing row sums. The condition of global and local conservation of linear and quadratic invariants for the discretization defined in Eqs. (5) and (6) will put additional constraints on the derivative matrices and their relations and on the coefficients  $\xi, \alpha, \beta, \gamma$  and  $\delta$ .

# 3 GENERAL RESULTS ON LINEAR AND QUADRATIC INVARIANTS PRESERVATION

The theory developed in [1] estabilishes the following general results:

The split family of methods (5) and (6) globally and locally conserve:

1) mass, if and only if  $\mathfrak{D}^{\mathsf{pu}}$  has vanishing column sums and the duality condition

$$\mathfrak{D}^{\rho} = -\mathfrak{D}^{\mathsf{u}\mathrm{T}} \tag{7}$$

is satisfied.

2) momentum, if and only if the extended duality conditions

$$\mathfrak{D}^{0} = -\mathfrak{D}^{\rho \mathbf{u} \mathbf{T}} \quad and \quad \mathfrak{D}^{\rho} = -\mathfrak{D}^{\mathbf{u} \mathbf{T}} \tag{8}$$

are satisfied. When  $\alpha = 1$  only the vanishing column sums of  $\mathfrak{D}^{\mathsf{pu}}$  is required.

3) kinetic energy, if and only if next to the duality conditions (8) also Coppola's conditions [10]:

$$\alpha = \beta = \frac{1}{2}\xi \quad and \quad \gamma = \delta = \frac{1}{2}(1 - \xi) \tag{9a,b}$$

are satisfied.

These results allows one to conclude that, given the duality relations (8), the most general formulation preserving mass, momentum and kinetic-energy (within the class of split forms here considered) is given by

$$\mathfrak{d} = \xi \,\mathfrak{d}^D + (1-\xi) \,\mathfrak{d}^A; \qquad \mathfrak{C} = \frac{1}{2} \xi \big( \mathfrak{C}^D + \mathfrak{C}^\phi \big) + \frac{1}{2} (1-\xi) \big( \mathfrak{C}^u + \mathfrak{C}^\rho \big), \tag{10}$$

where  $\mathfrak{d}^{(\cdot)}$  and  $\mathfrak{C}^{(\cdot)}$  are defined in Eqs. (5) and (6).

In all existing studies of the conservation properties for the split convective formulations a central discretization is assumed for derivatives. This implies that all the derivative matrices are skew symmetric. Moreover, since typically the same numerical scheme is adopted at each computational node, the matrices are also Toeplitz (or circulant, for periodic boundary conditions). The analysis developed in [1] shows that a much wider class of derivative matrices are allowed for global and local conservation of primary invariants and kinetic energy. As examples, directionally-biased discretizations are allowed, provided they satisfy the duality relations (8). Moreover, pointwise dependent schemes (giving rise to non-Toeplitz derivative matrices) are permitted. In Sec. 4 some examples of these more general discretizations will be shown. Note also that when the derivative matrices are the same, the duality conditions (8) reduce to the classical skew-symmetry condition.

As a final remark, it is worth noting that since derivative matrices must have vanishing row sums, the duality conditions (8) imply that they have vanishing column and row sums. As shown in [1], this property allows one to explicitly decompose them as 'difference of fluxes' operators. This means that in all the cases in which global conservation is guaranteed (for both primary invariants and kinetic energy) also local conservation follows and explicit formulas for the numerical fluxes are available.

### 4 TWO-DIMENSIONAL EULER EQUATIONS

## 4.1 Discrete formulation

In this section we apply the recalled theory to the full system of compressible Euler equations. There exist several ways to formulate the thermodynamic terms (cf. for example [11, 12]); we choose the formulation used by Pirozzoli [4]:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u}); \quad \frac{\partial \rho \boldsymbol{u}}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u} \boldsymbol{u}) - \nabla p; \quad \frac{\partial \rho e_{\text{tot}}}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u} h). \tag{11}$$

Here  $e_{\text{tot}}$  is the total energy, sum of the kinetic and internal energies  $e_{\text{tot}} = \frac{1}{2} \boldsymbol{u} \cdot \boldsymbol{u} + e$ , p is the pressure, obtained from the equation of state  $p = (\gamma - 1)\rho e$  and h is the specific enthalpy  $h = e_{\text{tot}} + p/\rho$ .

Upon semi-discretization, the 2D version of the system (11) can be written as

$$\mathfrak{H}\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\mathfrak{d}; \quad \mathfrak{H}\frac{\mathrm{d}\mathsf{R}\mathsf{u}}{\mathrm{d}t} = -\mathfrak{C}\mathsf{u} - \mathfrak{D}_x^p\mathsf{p}; \quad \mathfrak{H}\frac{\mathrm{d}\mathsf{R}\mathsf{v}}{\mathrm{d}t} = -\mathfrak{C}\mathsf{v} - \mathfrak{D}_y^p\mathsf{p}; \quad \mathfrak{H}\frac{\mathrm{d}\mathsf{R}\mathsf{e}_{\mathrm{tot}}}{\mathrm{d}t} = -\mathfrak{C}\mathsf{h}, \quad (12)$$

with the usual meaning of the symbols.

The convective terms are treated by assuming a finite-difference energy-preserving discretization as in Eq. (10) where the two-dimensional extension of Eqs. (5)-(6) reads

$$\begin{split} \mathfrak{d}^{D} &= \mathfrak{D}_{x}^{\rho \mathsf{u}}\mathsf{R}\mathsf{u} + \mathfrak{D}_{y}^{\rho \mathsf{u}}\mathsf{R}\mathsf{v}, \\ \mathfrak{d}^{A} &= \mathsf{U}\mathfrak{D}_{x}^{\rho}\rho + \mathsf{R}\mathfrak{D}_{x}^{\mathsf{u}}\mathsf{u} + \mathsf{V}\mathfrak{D}_{y}^{\rho}\rho + \mathsf{R}\mathfrak{D}_{y}^{\mathsf{u}}\mathsf{v}, \\ \mathfrak{C}^{D} &= \mathfrak{D}_{x}^{\rho \mathsf{u}}\mathsf{R}\mathsf{U} + \mathfrak{D}_{y}^{\rho \mathsf{u}}\mathsf{R}\mathsf{V}, \\ \mathfrak{C}^{\phi} &= \mathsf{R}\mathsf{U}\mathfrak{D}_{x}^{0} + \mathsf{R}\mathsf{V}\mathfrak{D}_{y}^{0} + \operatorname{diag}\left(\mathfrak{D}_{x}^{\rho \mathsf{u}}\mathsf{R}\mathsf{u} + \mathfrak{D}_{y}^{\rho \mathsf{u}}\mathsf{R}\mathsf{v}\right), \\ \mathfrak{C}^{u} &= \mathsf{R}\mathfrak{D}_{x}^{\mathsf{u}}\mathsf{U} + \mathsf{R}\mathfrak{D}_{y}^{\mathsf{u}}\mathsf{V} + \operatorname{diag}\left(\mathsf{R}\mathfrak{D}_{x}^{\mathsf{u}}\mathsf{u} + \mathsf{R}\mathfrak{D}_{y}^{\mathsf{u}}\mathsf{v}\right), \\ \mathfrak{C}^{\rho} &= \mathsf{U}\mathfrak{D}_{x}^{\rho}\mathsf{R} + \mathsf{V}\mathfrak{D}_{y}^{\rho}\mathsf{R} + \operatorname{diag}\left(\mathsf{U}\mathfrak{D}_{x}^{\rho}\rho + \mathsf{V}\mathfrak{D}_{y}^{\rho}\rho\right). \end{split}$$

To complete the method, the pressure terms have to be discretized. In the limit of incompressible flow, the discrete gradient operator acting on p should be equal to minus the transposed divergence in the continuity equation [13, Req. 3.2]. This gives for the *x*-direction:

$$\mathfrak{D}_x^{\mathsf{p}} = -\left[\xi\mathfrak{D}_x^{\mathsf{pu}} + (1-\xi)\mathfrak{D}_x^{\mathsf{u}}\right]^{\mathrm{T}} = \xi\mathfrak{D}_x^0 + (1-\xi)\mathfrak{D}_x^{\mathsf{p}},$$

and similar for the y-direction. As  $\nabla p$  does not depend on  $\rho$ , we can use it also for compressible flow. This reasoning also defines the discretization of the dilatation term in an eventual equation for internal energy. Note that for this two-dimensional case the matrices  $\mathfrak{D}_x^{(\cdot)}$  and  $\mathfrak{D}_y^{(\cdot)}$  are operators acting on the whole set of variables on the twodimensional domain, i.e. they have dimensions of the order  $N_x N_y$ , where  $N_x$  and  $N_y$  are the number of points along each direction.

In the tests shown below we use the following discretizations: (i) central discretizations (2nd- and 4th-order) on uniform and non-uniform meshes with different choices for the control volumes, (ii) derivatives based on Lagrangian (i.e. maximum order) interpolations (2nd- and 4th-order) on non-uniform meshes, and (iii) a dual-sided, 2nd-order discretization described below.

### 4.2 Numerical test case

The numerical tests have been performed by discretizing the convection of a circular isentropic vortex in a uniform flow [5, 14], whose initial velocity, density and pressure are:

$$\begin{aligned} \frac{u(x,y)}{U_{\infty}} &= 1 - \frac{M_v}{M_{\infty}} \frac{y - y_0}{r_v} e^{(1 - \bar{r}^2)/2}; & \frac{v(x,y)}{U_{\infty}} &= \frac{M_v}{M_{\infty}} \frac{x - x_0}{r_v} e^{(1 - \bar{r}^2)/2}; \\ \frac{\rho(x,y)}{\rho_{\infty}} &= \left(1 - \frac{\gamma - 1}{2} M_v^2 e^{(1 - \bar{r}^2)}\right)^{\frac{1}{\gamma - 1}}; & \frac{p(x,y)}{p_{\infty}} &= \left(\frac{\rho}{\rho_{\infty}}\right)^{\gamma}, \end{aligned}$$

where  $M_v$  is the vortex Mach number,  $M_\infty$  is the free-stream Mach number,  $r_v$  is the radius of the vortex core,  $(x_0, y_0)$  are the initial coordinates of the vortex core and  $\bar{r} = r/r_v$ . In all the calculations shown below the equations are integrated on a domain with extension  $L_x = L_y = 1$  and periodic boundary conditions. The vortex is initially located at  $(x_0, y_0) = (L_x/3, L_y/2)$  with radius  $r_v = L_x/15$  and strength given by  $M_v = M_\infty = 0.5$ . Time integration is performed through a classical RK4 scheme with Courant number C = 0.1 (based on the maximum velocity component of the initial condition).



(a) Grid refinement study. Dashed lines: 4thorder central discretization, solid lines: 2nd-order central discretization.

(b) Evolution of linear and quadratic invariants (2nd-order central discretization,  $N_x = N_y = 40$ ).

Figure 1: 2nd- and 4th-order central discretizations of the Euler equations on uniform meshes for the advection of a circular isentropic vortex.

#### 4.3 Uniform grids

In this section, we report a preliminary test on a formulation in which classical central schemes (2nd- and 4th-order) on a uniform mesh are employed. The global invariants of

the system have been normalized with respect to the initial value according to

$$\langle f(t) \rangle = \frac{\overline{f}(t) - \overline{f}(0)}{\overline{f}(0)},\tag{13}$$

where the overbar indicates spatial integration over the domain. In this particular case of central schemes on uniform meshes, the duality relations are trivially satisfied, as all the derivative operators are naturally skew symmetric and the discretization preserves (globally and locally) linear invariants. Moreover, the discretization preserves also quadratic invariants, since convective terms are discretized by using Eq. (10) with  $\xi = 1/2$ .

Fig. 1(a) (calculated at the final time T = 0.3) confirms the expected scaling of the discretizations for all the variables, whereas Fig. 1(b) illustrates a typical situation for a locally-conservative, energy-preserving discretization of the Euler equations. The linear invariants  $\overline{\rho}, \overline{\rho u}$  and  $\overline{\rho e_{\text{tot}}}$  are preserved to machine accuracy, whereas the global kinetic energy  $\overline{K} = \frac{1}{2} \overline{u \cdot u}$  has very small variations around its initial value, although it does not remain constant, even for energy-preserving discretizations, because of the non-conservative pressure term.

#### 4.4 Non-uniform grids



Figure 2: Mapping functions and associated grid for the case  $N_x = N_y = 40$ .

The analysis of the energy-preserving discretizations on non-uniform meshes is conducted by considering a Cartesian grid stretched along x and y according to the mapping

$$x = \frac{\sigma \left(2\sigma^2 - 3\sigma + s_x\right)}{s_x - 1}$$

and its akin version along y. This mapping is used by sampling  $\sigma$  uniformly between 0 and 1 and results in a grid for x which has a refinement region around the centre of the

domain for values of s > 1.5. In our tests we used the slightly different streching factors for x and y given by  $s_x = 1.7$  and  $s_y = 1.9$ . The mapping functions and the associated grid for the case  $N_x = N_y = 40$  are depicted in Fig. 2.



(a) Grid refinement study for various choice of  $\mathfrak{H}$ . Dashed:  $\mathfrak{H} = \text{diag}(\mathfrak{D} \mathsf{x})$ ; solid and dotted: local grid sizes.

(b) Evolution of linear and quadratic invariants (4th-order central discretization,  $N_x = N_y = 40$ ).

Figure 3: 4th-order central discretization of Euler equations on non-uniform meshes for the advection of a circular isentropic vortex.

In Fig. 3 a convergence study of the classical central 4th-order discretization on the non-uniform mesh is reported for different choices of the control volumes. For the correct preservation of the nominal order of accuracy of the discretization on non-uniform grids, the control volumes  $\mathfrak{H}$  have to be chosen according to  $\mathfrak{H} = \operatorname{diag}(\mathfrak{D} \mathsf{x})$  (cf. [1]). This case is represented by dashed lines in Fig. 3(a). The choice of control volumes according to  $h_{2\mathrm{nd-order}} = (x_{i+1} - x_{i-1})/2$  or  $h_{1\mathrm{st-order}} = (x_{i+1} - x_i)$  deteriorates the convergence rate of the method to 2nd or 1st-order, respectively (solid and dotted lines in Fig. 3(a)). Fig. 3(b)) reports the evolution of linear and quadratic invariants for the case of the 4th-order central discretization with  $\mathfrak{H} = \operatorname{diag}(\mathfrak{D} \mathsf{x})$ . The plot shows that also in the case of a non-uniform mesh the central discretization does preserve linear and quadratic invariants and that the formal order of accuracy is also preserved.

The considerations exposed for the case of central schemes on non-uniform meshes are now contrasted with the analysis of a discretization based on Lagrangian interpolation, i.e. based on maximum order of accuracy schemes on non-uniform meshes. This discretization is used here because it conducts to derivative matrices which in general do not satisfy the duality relations (8) (they are not skew-symmetric) nor they have the vanishing row and column sums property, leading to a discretization which does not preserve linear invariants nor kinetic energy.



(a) Grid refinement study. Dashed lines: 4thorder central discretization, solid lines: 2nd-order central discretization.



(b) Evolution of linear and quadratic invariants (2nd-order Lagrangian discretization,  $N_x = N_y = 40$ ).

**Figure 4**: Discretization of the Euler equations based on Lagrange interpolation derivatives on non-uniform meshes for the advection of a circular isentropic vortex.

Both 2nd- and 4th-order Lagrangian derivative schemes have been implemented on the stretched grid considered. Fig. 4 reports the usual grid refinement study and the plot of the evolution of linear and quadratic invariants. The grid refinement study confirms the correct scaling of the discretizations. However, the evolution of linear invariants is significantly spoiled by the non-conservative discretization, confirming the theoretical predictions. Also, global kinetic energy evolution shows variations two orders of magnitude greater than in the case of the kinetic-energy preserving (KEP) formulation, which is a symptom of the lacking of conservation of quadratic invariants. The comparison between the velocity profiles obtained with the two formulations (not reported here) shows a substantial equivalence on accuracy. However, the stability is different, as for the Lagrangian derivatives the simulation diverges for  $T \simeq 1$  for the 4th-order scheme, whereas the analogous central discretization is stable up to  $T \simeq 14$ .

### 4.5 Dual-sided discretization

As a final example we now consider a dual-sided upwind-type discretization, based on the duality relations derived above, which is locally conservative and kinetic energy preserving. This test serves also as an example of a KEP formulation in which the derivative schemes are selected pointwise, leading to a formulation in which the scaled derivative matrices are not skew symmetric, nor Toeplitz, even on uniform meshes. A suitable definition of the local schemes guarantees that the resulting derivative matrices have vanishing column sums and satisfy the duality relations (8), giving a formulation which preserves, globally and locally, linear and quadratic invariants. The main feature of the dual-sided discretization is that the convective terms are discretized with an 'upwind-downwind' approach based on the local velocity. The procedure starts with the definition of upwind-based derivative matrices  $\mathfrak{D}_{upw}^{\rho u}$ , along x and y, satisfying vanishing column sums. Note that a straightforward treatment within the finitedifference framework, in which the numerical derivative at a point  $x_i$  is selected based on an upwind principle, would lead to a derivative matrix which in general does not satisfy the vanishing column sum property, with consequent lack of conservation of linear (and quadratic) invariants. However, since our theory shows that all the derivative matrices having vanishing column sums can be decomposed as the difference of flux vectors, we start from the definition of local 'upwind' fluxes, from which a derivative operator could be defined.

To illustrate this discretization we need here to briefly recall the definition of a basic matrix operator which is used in [1] to derive all the results illustrated in Sec. 3 (for a complete treatment see [1]). In particular, we need here the definition of the *shift* matrix  $\mathsf{E}$  which is characterized by the property that for any vector  $\mathsf{m}$  the *i*th component of  $\mathsf{Em}$  is given by the (i + 1)th component of  $\mathsf{m}$ :  $(\mathsf{Em})_i = (\mathsf{m})_{i+1}$  (a circulant convention is adopted for boundary entries of  $\mathsf{m}$ ). This property naturally extends also to positive and negative powers of  $\mathsf{E}$ :  $(\mathsf{E}^k\mathsf{m})_i = (\mathsf{m})_{i+k}$ . With this operator, the basic decomposition theorem estabilishing the possibility of decomposing matrices with vanishing column sums as a 'difference of fluxes' operator is expressed by the relation  $\mathfrak{D} = (\mathsf{I} - \mathsf{E}^{-1})\mathfrak{F}$  where  $\mathfrak{F}$  is a suitable interpolation operator.

With this notation, a locally conservative 'upwind' derivative matrix  $\mathfrak{D}_{upw}^{\rho u}$  can be directly defined through the relation

$$\mathfrak{D}_{upw}^{\rho u} \mathsf{R} u = \left(\mathsf{I} - \mathsf{E}^{-1}\right) \mathsf{m}_{upw}.$$
(14)

where  $\mathsf{m}_{upw}$  is a consistent mass-flux vector whose *i*th component is obtained by interpolating the values of  $\rho u$  at  $x_{i+1/2}$  using values at neighboring points. To specify  $\mathsf{m}_{upw}$  with a locally 'upwind' character, we firstly define the *backward* and *forward* fluxes as

$$\mathbf{m}_{\rm bkw} = \left(\frac{3}{2}\mathsf{I} - \frac{1}{2}\mathsf{E}^{-1}\right)\mathsf{Rw}, \qquad \mathbf{m}_{\rm frw} = \left(\frac{3}{2}\mathsf{E} - \frac{1}{2}\mathsf{E}^{2}\right)\mathsf{Rw}, \tag{15}$$

where w is either u or v. Their definition comes from the fact that simple calculations show:

$$\left(\mathsf{I} - \mathsf{E}^{-1}\right)\mathsf{m}_{\mathrm{bkw}} = \mathfrak{D}_{\mathrm{bkw}}\mathsf{Rw}, \qquad \left(\mathsf{I} - \mathsf{E}^{-1}\right)\mathsf{m}_{\mathrm{frw}} = \mathfrak{D}_{\mathrm{frw}}\mathsf{Rw}, \tag{16}$$

where  $\mathfrak{D}_{bkw} = \left(\frac{3}{2}\mathsf{I} - 2\mathsf{E}^{-1} + \frac{1}{2}\mathsf{E}^{-2}\right)$  and  $\mathfrak{D}_{frw}\left(-\frac{3}{2}\mathsf{I} + 2\mathsf{E} - \frac{1}{2}\mathsf{E}^{2}\right)$  (with  $\mathfrak{D}_{bkw} = -\mathfrak{D}_{frw}^{T}$ ) are the classical (Toeplitz) backward and forward derivative matrices with second-order accuracy on uniform meshes. The total flux  $\mathsf{m}_{upw}$  is then constructed as:

$$\mathbf{m}_{\rm upw} = \Lambda^+ \mathbf{m}_{\rm bkw} + \Lambda^- \mathbf{m}_{\rm frw},\tag{17}$$

where  $\Lambda^{\pm} = \text{diag}(\lambda^{\pm})$  and  $\lambda_i^{\pm} = \frac{1}{2}(w_{i+1/2} \pm |w_{i+1/2}|)/w_{i+1/2}$ . With these definitions, each component of the flux  $\mathbf{m}_{\text{upw}}$  is selected as a backward or forward flux depending on the local velocity component  $w_{i+1/2}$ . This implicitly defines the matrix  $\mathfrak{D}^{\rho u}$  as:

$$\mathfrak{D}^{\mathsf{pu}} = \left(\mathsf{I} - \mathsf{E}^{-1}\right) \left[ \Lambda^+ \left( \frac{3}{2} \mathsf{I} - \frac{1}{2} \mathsf{E}^{-1} \right) + \Lambda^- \left( \frac{3}{2} \mathsf{E} - \frac{1}{2} \mathsf{E}^2 \right) \right].$$



Figure 5: Discretization of the Euler equations based on the dual-sided procedure on uniform mesh for the advection of a circular isentropic vortex.

The matrix  $\mathfrak{D}^{\rho u}$  is a second-order, first-derivative matrix which is not skew symmetric, nor Toeplitz, but has vanishing column sums. As such,  $\mathfrak{D}^{\rho u}$  is globally and locally conservative and its transpose is still a first-derivative matrix with vanishing column sums. The procedure is completed by specifying  $\mathfrak{D}^0$  satisfying the duality relation  $\mathfrak{D}^0 = -\mathfrak{D}^{\rho u T}$ and by using Eq. (10) with  $\xi = 1$ . As concerns the convective terms, the previous discussion defines a pointwise-dependent, finite-difference discretization which is a dual-sided upwind-based, second-order, locally-conservative and KEP method. We emphasize here once again that the adoption of an upwind-based procedure for the definition of the divergence operator in the mass equation does not affect the conservation of kinetic energy, provided that the gradient terms in momentum and total energy equations are discretized according to the duality relations. The proposed procedure should not be confused with an upwind discretization of the full system of equations, which does not preserve kinetic energy; it is equivalent to the choice of a particular (upwind-based) consistent mass flux, which constitute the main degree of freedom within the family of locally conservative and KEP methods discussed (cf. [1])

In Fig. 5(a) the usual grid convergence study is proposed, whereas in Fig. 5(b) the evolution of linear and quadratic invariants is reported. The grid convergence analysis shows that the global procedure is able to reproduce the correct 2nd-order scaling on all the variables. The evolution of linear invariants also shows a perfect conservation of linear invariants and small variations in the global kinetic energy of the system. The procedure shows enhanced stability properties, also for very long simulations, although the accuracy is not as good as for the other methods based on central schemes. However, it is remarked that this lastly proposed procedure is not optimized in any way as concerns accuracy.

It is proposed just as a first example of a general application of the developed theory to the system of Euler equations. The investigation of more advanced and convenient discretizations based on the generalized family of KEP methods discussed here is a topic for future research.

## REFERENCES

- [1] G. Coppola and A.E.P. Veldman, Global and local conservation of mass, momentum and kinetic energy in the simulation of compressible flow. J. Comput. Phys., under review.
- [2] A.E.P. Veldman and G. Coppola Matrix properties associated with discrete conservation in flow simulations. The 8th European Congress on Computational Methods in Applied Sciences and Engineering. ECCOMAS Congress 2022. 5–9 June 2022, Oslo, Norway
- [3] F. Ducros, F. Laporte, T. Souleres, V. Guinot, P. Moinat, and B. Caruelle, High-order fluxes for conservative skew-symmetric-like schemes in structured meshes: application to compressible flows, J. Comput. Phys. (2000) Vol. 161:114–139.
- [4] S. Pirozzoli, Generalized conservative approximations of split convective derivative operators, J. Comput. Phys. (2010) Vol. 229:7180–7190.
- [5] S. Pirozzoli, Stabilized non-dissipative approximations of Euler equations in generalized curvilinear coordinates J. Comput. Phys. (2011) Vol. 230:2997–3014.
- [6] T.C. Fisher, M. H. Carpenter, J. Nordström, N.K. Yamaleev and C. Swanson, Discretely conservative finite-difference formulations for nonlinear conservation laws in split form: Theory and boundary conditions J. Comput. Phys. (2013) Vol. 234:353–375.
- [7] W.J. Feiereisen, W.C. Reynolds and J.H. Ferziger Numerical simulation of a compressible, homogeneous, turbulent shear flow, Report TF-13, Thermosciences Division, Mechanical Engineering, Stanford University (1981).
- [8] S. Pirozzoli, Numerical methods for high-speed flows Annu. Rev. Fluid Mech. (2011) Vol. 43:163-194.
- [9] G. Coppola, F. Capuano and L. de Luca, Discrete energy-conservation properties in the numerical solution of the Navier–Stokes equations. *Appl. Mech. Rev.*, (2019) Vol. 71:010803-1–010803-19.
- [10] G. Coppola, F. Capuano, S. Pirozzoli and L. de Luca, Numerically stable formulations of convective terms for turbulent compressible flows J. Comput. Phys. (2019) Vol. 382:86–104.
- [11] C. De Michele and G. Coppola An assessment of various discretizations of the energy equation in compressible flows. The 8th European Congress on Computational Methods in Applied Sciences and Engineering. ECCOMAS Congress 2022. 5–9 June 2022, Oslo, Norway.
- [12] C. De Michele and G. Coppola Numerical treatment of the energy equation in compressible flows simulations *Comput. Fluids*, under review.
- [13] A.E.P. Veldman, Supraconservative Finite-Volume Methods for the Euler Equations of Subsonic Compressible Flow SIAM Rev. (2021) Vol. 63:756-779.
- [14] J.C. Kok, A high-order low-dispersion symmetry-preserving finite-volume method for compressible flow on curvilinear grids J. Comput. Phys. (2009) Vol. 228:6811–6832.