Supraconservative finite-volume methods for the Euler equations of subsonic compressible flow

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SUPRA-CONSERVATIVE FINITE-VOLUME METHODS FOR THE EULER EQUATIONS OF SUBSONIC COMPRESSIBLE FLOW

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Abstract. It has been found advantageous for finite-volume discretizations of flow equations to possess additional (secondary) invariants, next to the (primary) invariants from the constituting conservation laws. The paper presents general (necessary and sufficient) requirements for a method to convectively preserve discrete kinetic energy. The key ingredient is a close discrete consistency between the convective term in the momentum equation and the terms in the other conservation equations (mass, internal energy). As examples, the Euler equations for subsonic (in)compressible flow are discretized with such supra-conservative finite-volume methods on structured as well as unstructured grids.

Key words. CFD, conservation laws, finite-volume method, supra-conservative discretization

AMS subject classifications. 65M08, 65M12, 76G25

1. Introduction.

1.1. Background. The equations describing fluid dynamics can be expressed as conservation laws in terms of primary variables: mass, momentum and (internal) energy. In the absence of dissipative mechanisms, according to Noether's theorem [5,80], they possess a number of invariants induced by the symmetries of the Hamiltonian/Lagrangian structure. Next to the (obvious) primary invariants expressed by the explicit conservation laws, other secondary invariants exist [21, 86, 116]. Preserving (globally and/or locally) one or more of these analytical invariants in a discrete setting has proven quite useful over the years, but is not obvious to realize, e.g. [91]. Gradually, experience is built up about which additional discrete invariants are worthwhile to preserve, and about the way to achieve this. In this paper, we analyze the steps that can lead to simultaneous discrete conservation of several of these (primary and secondary) invariants.

In particular, we consider the Euler equations for subsonic (in)compressible flow. These will be formulated as conservation laws in terms of the primary variables mass density ρ, momentum per unit mass $\boldsymbol{u}$, and internal energy per unit mass e:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{m} = 0\,; \tag{1.1a}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{m} \otimes \boldsymbol{u}) = -\nabla p\,; \tag{1.1b}$$

$$\frac{\partial \rho e}{\partial t} + \nabla(\boldsymbol{m} e) = -p\, \nabla \cdot \boldsymbol{u}\,. \tag{1.1c}$$

Here, $\boldsymbol{m} \equiv \rho \boldsymbol{u}$ denotes the mass flux and p the pressure. The set of equations is closed by an equation of state which relates p, ρ and e (for the limit of incompressible flow, see Appendix A).

The introduction of the mass flux $\boldsymbol{m}$ will help to distinguish between the two appearances of $\boldsymbol{u}$ in the momentum equation: one as transporting velocity, the other as transported quantity. We will also see that the particular value of $\boldsymbol{m}$ is relevant only at two places in the analysis: in the derivation of the pressure Poisson equation

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(Sect. 4.2) and in the limit between compressible and incompressible flow (Sect. 5.3). All other considerations in this paper hold for *any* vector field $\boldsymbol{m}$. Note that the time derivative in (1.1b) contains the product of the density ρ and the velocity $\boldsymbol{u}$ (together making the momentum per unit volume), and not the mass flux $\boldsymbol{m}$ (which nevertheless has the same value). The mathematical reason behind this will become clear in the sequel, when studying the evolution of kinetic energy (see also [132, Sect. 7]).

The equations are solved on a (two- or three-dimensional) domain Ω with appropriate initial and boundary conditions. For convenience, we will assume either homogeneous boundary conditions or periodic ones, such that we do not have to bother with terms along the boundaries. Physically, this means that in this paper external influences on the flow field are excluded.

The equations (1.1) have been written in conservation form, immediately revealing the primary invariants. As main invariants, next to mass and linear momentum, also angular momentum, mean kinetic energy, helicity and circulation (Kelvin) are (globally) preserved [72,75,86]. Furthermore, in two dimensions, enstrophy and other integrals of the vorticity are invariant. In [2, 21, 25, 116] methods are presented to construct even more invariants.

The convection term in the momentum equation (1.1b) can be written in various formulations. For incompressible flow, next to the conservative form $\nabla(\boldsymbol{u} \otimes \boldsymbol{u})$, one has the convective form $\boldsymbol{u} \cdot \nabla \boldsymbol{u}$, the skew-symmetric form $\frac{1}{2}\boldsymbol{u} \cdot \nabla \boldsymbol{u} + \frac{1}{2}\nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u})$, the rotational form $(\nabla \times \boldsymbol{u}) \times \boldsymbol{u} + \frac{1}{2}\nabla(\boldsymbol{u} \cdot \boldsymbol{u})$, the closely related velocity-vorticity(-helicity) formulations [51,82,83] and the streamfunction-vorticity formulation [3]. For compressible flow, with even more freedom in formulating the equations, Coppola et al. [27, 28] have analyzed a large family of variants.

Analytically all formulations are equivalent, because of the equation for mass conservation (1.1a), and they possess the same invariants. But after discretization this equivalence is partly lost, and differences appear in the induced discrete invariants. Depending upon the desired discrete invariant, e.g. kinetic energy or helicity, a different analytical formulation can be chosen as a starting point. The present paper intends to study how this loss of discrete equivalence can be reduced. In particular it is shown how discrete energy can be conserved, as this property directly improves numerical stability; for incompressible flow stability is even guaranteed. Recently, Edoh et al. [34] have shown in detail how other means of achieving numerical stability, such as artificial dissipation and solution-filtering, result in (nonphysical) inaccuracies of the numerical solution.

1.2. History - incompressible flow. Around 1960, in long-time numerical weather prediction [3,13,67,94,95], the (possibly negative) influence of the discretization of the non-linear convective term on numerical stability (in those days coined non-linear instability) was already discussed. In particular, Arakawa [3], working in 2D, advocated the use of the streamfunction-vorticity formulation of the flow equations, which he shows to discretely conserve mean kinetic energy and enstrophy.

Building on the staggered-grid formulation by Harlow and Welch [50], Piacsek and Williams [96] promoted the discretization of the skew-symmetric convective formulation, as it directly leads to discrete global energy conservation and its numerical stability. Several years later, Horiuti [54] and Zang [152] were among the first to systematically explore the rotational form of the equations. Later, Perot et al. [90, 153] stressed how on unstructured grids using the rotational form, next to global conservation of kinetic energy and circulation, also local conservation can be achieved.

Finite-element methods. In search for more 'useful' secondary invariants, in a finite-element setting Layton et al. [63] compared several formulations of the equations, but they did not include the conservation form (1.1) which is our starting point. As a follow-up, Rebholz and colleagues [23, 24, 29] further extended the quest for finite-element methods with enhanced conservation properties, again motivated by accurate long-time integration [8]. Also, Lehmkuhl et al. [65] advocate the use of low-dissipative and conservative finite-element schemes. In general, the geometrical flexibility of a finite-element discretization can be combined with the conservation properties of a finite-volume formulation. This led to a number of closely-related methods [6, 148], like the discontinuous Galerkin method [26], the spectral volume method [125, 126] and the energy-stable flux reconstruction method [20, 55, 147, 149].

Mimetic methods. Inspired by the work of Samarskii in the 1970s, the support operator method was developed in which basic analytical relations between the main operators of calculus (div, grad and curl) were preserved [111, 118]. Later, this approach was renamed by Hyman and Shashkov [56] as a mimetic finite-difference method. A broad overview of these methods is given by Lipnikov et al. [68]. Links with differential geometry and algebraic topology were made in the language of discrete exterior calculus, e.g. [11, 19, 31, 35, 52]. Note that in the latter language the mass flux $\boldsymbol{m}$ is a 2-form, whereas the velocity $\boldsymbol{u}$ is a 1-form, again making the distinction between $\boldsymbol{m}$ and $\rho\boldsymbol{u}$. Explanations for non-specialists of this, highly mathematical, approach can be found in [36, 93]. These methods have been applied mainly in diffusion-dominated flow problems, see the overview paper by Perot [92], but a few convection-dominated studies can be mentioned [30, 45, 76].

Finite-difference methods. An extensive overview of finite-difference options for the incompressible flow equations has been presented by Morinishi [78]. He discusses the discretization of the convective, divergence and skew-symmetric forms on uniform grids. A generalization of his approach to non-uniform grids was presented by Vasilyev [139] and Ham et al. [49]. As a curvilinear case, the energy-preserving formulation in cylindrical coordinates was studied in [40, 79, 87]; a more general approach for structured curvilinear staggered grids has been proposed in [138]. Discrete skew-symmetry of the convective terms also features in the summation-by-parts (SBP) method introduced by Strand [123] and Olsson [84, 85], and generalized in [74, 81, 127, 128]. Next to these approaches to globally preserve discrete energy, also ideas to preserve helicity [69, 100, 116] and angular momentum [44] have been proposed.

Finite-volume methods. Around the same time, similar considerations for finite-volume discretizations were discussed. Starting from the conservation laws behind the equations given in Eq. (1.1), conservation of the primary variables is 'automatic' in this approach. In the 1990s, inspired by [143], by means of a symmetry-preserving approach Verstappen and Veldman [144] were among the first to combine discrete mass, momentum and energy conservation for incompressible flow on non-uniform, staggered Cartesian grids. They emphasized the need for, counter-intuitive, geometry-independent interpolations for the fluxes. Higher-order finite-volume versions followed soon [145, 146, 150]. Early generalizations to unstructured staggered grids have been presented by Perot et al. [90, 153]. Later, Trias et al. included collocated grids [60, 115, 133, 134].

1.3. History - compressible flow. Extensions to the equations for compressible flow have also been presented. Often, but not always, starting from the conservative formulation and discretized with a finite-volume approach. Also here, early use of skew-symmetric forms can be mentioned, such as the formulations by Feiereisen et al. [37], Tadmor [130] and Blaisdell et al. [9]. These, non-conservative, analytical forms are better combined with a finite-difference discretization, although some of them can be recast into a finite-volume discretization [28, 49]. Consistency between the individual discrete equations was found beneficial for stability [14, 18, 70, 97, 99]. Even as early as 1967, Richtmyer and Morton [103, p. 142] in their study of the Burgers equation already noticed that some discretizations conserve an energy norm "thus ensuring stability".

The use of entropy variables can be profitable, see e.g. [15, 22, 43, 53, 89, 113, 129, 151], but often discrete momentum conservation is lost. The latter papers were mainly concerned with the numerical treatment of shock wave discontinuities, where monotonicity and TVD properties are relevant (e.g. [7, 98]). In contrast, and complementary, our interest is in the treatment of the relatively smooth (but possibly turbulent) part of the flow; hence our restriction to subsonic flow. Yet, due to the absence of numerical diffusion, our approach will not interfere with the, necessarily, dissipative character of numerical shock treatment.

In this paper, we would like to retain all primary conservation properties and to extend them with additional secondary conservation. Some finite-volume studies in this vein can be mentioned already, e.g. those by Ducros et al. [33], Jameson [58], Kok [62], Morinishi [77] and Rozema [108]. We will highlight the general principles behind these spatial discretization methods.

Time integration. Finally, after the above summary of spatial discretization developments, we should mention the efforts to let the time integration preserve invariants. In particular, symplectic methods [114], like the implicit midpoint rule, preserve kinetic energy. Such methods for incompressible flow have been studied, e.g., by Sanderse [112] and Capuano et al. [16]; thusfar, only implicit methods with these conservation properties have been found. It appears that energy-preserving time integration for compressible flow requires the introduction of the square root of the density $\sqrt{\rho}$ [46, 77, 108, 124]. Following the use of these 'square-root variables' in the time-integration method, spatial discretization studies were carried out based on the same variables; see e.g. Reiss et al. [12, 101, 102], Rozema et al. [105, 107, 110] and Cadieux et al. [15]. In particular, Rozema's square-root formulation can preserve not only primary (mass, momentum and internal energy) and secondary (kinetic and total energy) invariants through spatial and temporal discretization, but it additionally allows for a compressible formulation of regularization turbulence models [108, 109]. A wider overview of energy-preserving time-integration methods for compressible flow can be found in [27].

Similar ideas in adjacent areas. Next to the above developments in the realm of discrete-grid methods, similar energy-preserving ideas have been proposed for other discretization paradigms like spectral methods [10, 42, 88] and SPH methods [39]. Moreover, other application areas can be mentioned where energy conservation and similar properties are advantageous, like geophysical fluid dynamics [4, 32, 131] and multi-phase flow [41, 57, 135, 140]. The literature shows that preserving these desirable conservation properties usually goes at the expense of mass and/or momentum conservation. Also for the shallow-water equations discrete energy conservation is actively pursued [119, 121, 136], sometimes in conjunction with one other discrete invariant, e.g. enstrophy [120, 122]. Only a few exceptions with more than one discretely conserved invariant, viz. mass and momentum, have been presented [137, 138].

1.4. Supra-conservative discretization. The general idea behind many of the above methods is that they want to discretely conserve *more* (secondary) invariants then just the (primary) ones directly featuring in the conservation laws. Therefore, these methods are coined *supra-conservative* [142]. To achieve this property requires sufficient compatibility between the discrete operators in the equations of motion: not only div, grad and curl, but also composite operators. Below, we will discuss the details of such a discrete compatibility for (stretched) structured and unstructured computational grids with staggered as well as collocated positioning of the unknowns.

Most of the above studies have been based on the properties of the analytical formulations, which are then 'hopefully' retained after discretization. In our discussion we will start, as advocated in [141], from the discrete finite-volume formulation of the basic equations (1.1), and never return to the analytical formulation. In this way we make sure that discrete conservation of the primary invariants is guaranteed from the start. Then, at the discrete level, the freedom left in the formulation will be used to generate additional properties like secondary invariants.

Outline. In the paper we focus in particular on the (secondary) conservation of energy in finite-volume methods. Necessary and sufficient criteria hereto will be derived. We restrict ourselves to subsonic flow (i.e. no shock waves) and stick to the conservative formulation in primitive variables. In Sections 2 and 3 the derivation steps are discussed that are required to obtain energy conservation, first in the analytic case, thereafter mimicked in the discrete setting. Section 4 works out a supra-conservative method for incompressible flow discretized on a structured, staggered grid. In Section 5 the approach is generalized to compressible flow on an unstructured, collocated grid. Finally, the common line in the approach will be discussed in Section 6, followed by a section with conclusions.

2. Conservation of energy - analytic. The theoretical study of the invariants of the Euler flow equations thus far has mainly focused on the incompressible special case of the formulation as given in (1.1); here we treat the general case of compressible flow. As the flow equations are formulated in conservation form they 'automatically' conserve mass, momentum and internal energy. Analysis shows that, as mentioned above, they additionally convectively preserve kinetic energy and total energy. The analytic derivation of this property is relevant for the discrete discussion in the sequel. We give it here as a starting point and guide line, as we want to mimic it step-by-step in the discretization.

$$
\begin{aligned}
\frac{\partial}{\partial t}(\rho E_{\text{tot}}) &= -\tfrac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\frac{\partial}{\partial t}\rho \quad + \quad \boldsymbol{u}\cdot\frac{\partial}{\partial t}(\rho\boldsymbol{u}) \quad + \quad \frac{\partial}{\partial t}(\rho e) \\
\text{(2.1a)} \quad &= \overbrace{\tfrac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\nabla\cdot\boldsymbol{m}}^{\text{mass (1.1a)}} - \boldsymbol{u}\cdot\overbrace{\left\{\nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u}) + \nabla p\right\}}^{\text{momentum (1.1b)}} - \overbrace{\left\{\nabla\cdot(\boldsymbol{m}e) + p\nabla\cdot\boldsymbol{u}\right\}}^{\text{internal energy (1.1c)}} \\
\text{(2.1b)} \quad &= \underbrace{\boldsymbol{u}\cdot\left\{\tfrac{1}{2}(\nabla\cdot\boldsymbol{m})\boldsymbol{u} - \nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u})\right\}}_{\text{Property 2.1}} - \nabla\cdot(\boldsymbol{m}e) - \underbrace{\left\{\boldsymbol{u}\cdot\nabla p + p\nabla\cdot\boldsymbol{u}\right\}}_{\text{Property 2.2}} \\
\text{(2.1c)} \quad &= \underbrace{-\nabla\cdot(\tfrac{1}{2}\boldsymbol{m}\boldsymbol{u}^2) - \nabla\cdot(\boldsymbol{m}e)}_{\text{Property 2.3}} \quad - \nabla\cdot(p\boldsymbol{u}) \\
\text{(2.1d)} \quad &= -\nabla\cdot(\boldsymbol{m}E_{\text{tot}}) \quad - \nabla\cdot(p\boldsymbol{u}).
\end{aligned}
$$

From the primary conservation laws one can deduce secondary conservation laws for kinetic energy $\rho E_{\text{kin}} \equiv \frac{1}{2}\rho\boldsymbol{u}^2$ and total energy $\rho E_{\text{tot}} \equiv \rho(E_{\text{kin}} + e)$. The evolution of the total energy can be calculated analytically as a weighted combination of the primary conservation laws (1.1a), (1.1b) and (1.1c). Equation (2.1) schematically shows how the derivation of the energy evolution proceeds. The divergence forms in the last two lines (2.1c) and (2.1d) not only induce global energy conservation but also local conservation. It is stressed that this derivation holds for *any* $\boldsymbol{m}$: its explicit value $\rho\boldsymbol{u}$ is not used.

The derivation in (2.1) reveals, by means of a background shading, how terms from the separate primary conservation laws have to be combined, requiring a certain level of compatibility. Analytically this is not an issue, but in a discrete setting it is not straightforward, and this will be the focal point in the presentation to follow.

In the last two steps, from (2.1b) to (2.1c) and from (2.1c) to (2.1d), three analytic properties between the operators are essential (although trivial at first sight). We will discuss these steps in detail, making a distinction between the various appearances of the ∇-operator. Hereto, hopefully self-explaining, subscripts have been added to the operators to indicate in which conservation law they are featuring.

PROPERTY 2.1 ((2.1b)$\rightarrow$(2.1c)). *The convection operator for momentum conservation* $\nabla_{\text{mom\_conv}}$ *together with the divergence operator of mass conservation* ∇_{mass} *form a convective divergence expression with operator* $\nabla_{\text{toten\_conv}}$. *This requires that (for any* $\boldsymbol{m}$*) the operator*

$$\mathcal{A} : \boldsymbol{u} \rightarrow \nabla_{\text{mom\_conv}} \cdot (\boldsymbol{m} \otimes \boldsymbol{u}) - \tfrac{1}{2}(\nabla_{\text{mass\_div}} \cdot \boldsymbol{m})\boldsymbol{u} \quad \textit{is skew symmetric.} \tag{2.2}$$

Explanation. First, let the L_2-inner product for real-valued functions be defined through $\big((\phi, \psi)\big) \equiv \int_\Omega \phi\psi \, \mathrm{d}\Omega$. Then, if an expression $\phi\mathcal{A}\phi$ can be rewritten as $\phi\mathcal{A}\phi \equiv \nabla\mathcal{B}(\phi)$ for some function $\mathcal{B}$, then (for all real-valued ϕ) $\big((\phi, \mathcal{A}\phi)\big) = \int_\Omega \phi\mathcal{A}\phi \, \mathrm{d}\Omega = \int_\Omega \nabla\mathcal{B}(\phi) \, \mathrm{d}\Omega = 0$ because of Gauss' theorem and our assumption that the outer boundaries of Ω do not contribute. That means that $\mathcal{A}$ is skew-symmetric with respect to this L_2-inner product. Indeed, we can rewrite (for any $\boldsymbol{m}$ and ϕ) $\nabla \cdot (\boldsymbol{m}\phi) - \frac{1}{2}(\nabla \cdot \boldsymbol{m})\phi \equiv \frac{1}{2}\nabla \cdot (\boldsymbol{m}\phi) + \frac{1}{2}(\boldsymbol{m} \cdot \nabla)\phi$, which reveals the skew-symmetry as an operator acting on ϕ. ∎

PROPERTY 2.2 ((2.1b)$\rightarrow$(2.1c)). *The gradient operator* $\nabla_{\text{mom\_grad}}$ *acting on the pressure is the negative transpose, with respect to the* L_2*-inner product, of the divergence operator* $\nabla_{\text{inten\_div}}$ *in the dilatation term of the internal energy equation:*

$$\big((\boldsymbol{u}, \nabla_{\text{mom\_grad}}\, p)\big) = -\big((\nabla_{\text{inten\_div}} \cdot \boldsymbol{u}, p)\big) \; \textit{for all } \boldsymbol{u} \textit{ and } p. \tag{2.3}$$

In short hand, this property can be written as

$$\nabla_{\text{mom\_grad}} = -\nabla^T_{\text{inten\_div}} \; (= -\nabla^T_{\text{mass}}) \,. \tag{2.4}$$

Between parentheses the incompressible limit is given, when the conservation law for internal energy degenerates into the continuity equation [47, 61]; see also Appendix A.

PROPERTY 2.3 ((2.1c)$\rightarrow$(2.1d)). *The divergence operator* $\nabla_{\text{inten\_conv}}$ *in the convective term of the internal energy equation is the same as the divergence operator* $\nabla_{\text{mom\_conv}}$ *from Property 2.1 in the momentum equation:*

$$\nabla_{\text{inten\_conv}} = \nabla_{\text{mom\_conv}} \quad (\equiv \nabla_{\text{toten\_conv}}) \,.$$

This property allows to combine both convective terms into one term describing convection of total energy.

The above properties reveal that there is a close relation between the operators from the individual conservation laws. It is our intention to transfer these analytic properties towards the discrete setting. This will then give guide lines for the design of the supra-conservative discretization schemes.

3. Conservation of energy - discrete.

The discretization will be carried out with finite-volume methods. Therefore, first the governing equations are reformulated as conservation laws (for an arbitrary control volume Ω_h with boundary Γ_h):

$$\int_{\Omega_h} \frac{\partial \rho}{\partial t}\, \mathrm{d}\Omega_h + \int_{\Gamma_h} \boldsymbol{m}\cdot\boldsymbol{n}\, \mathrm{d}\Gamma_h = 0\,, \tag{3.1a}$$

$$\int_{\Omega_h} \frac{\partial \rho \boldsymbol{u}}{\partial t}\, \mathrm{d}\Omega_h + \int_{\Gamma_h} (\boldsymbol{m}\cdot\boldsymbol{n})\boldsymbol{u}\, \mathrm{d}\Gamma_h = -\int_{\Gamma_h} p\,\boldsymbol{n}\, \mathrm{d}\Gamma_h\,, \tag{3.1b}$$

$$\int_{\Omega_h} \frac{\partial \rho e}{\partial t}\, \mathrm{d}\Omega_h + \int_{\Gamma_h} (\boldsymbol{m}\cdot\boldsymbol{n})e\, \mathrm{d}\Gamma_h = -\int_{\Omega_h} p\nabla\cdot\boldsymbol{u}\, \mathrm{d}\Omega_h\,. \tag{3.1c}$$

Note that Ω_h is a generic notation for a control volume. For a collocated grid these will be the same for each conserved variable, while on a staggered grid for the individual variables different control volumes are usually pertinent.

The discretized versions of (3.1a)-(3.1c) in all grid volumes will be collected in matrix-vector notation and abbreviated as

$$\mathfrak{H}\frac{\partial \rho}{\partial t} + \mathfrak{D}_{\text{mass}}\,\boldsymbol{m} = 0\,, \tag{3.2a}$$

$$\mathfrak{H}\frac{\partial \rho\boldsymbol{u}}{\partial t} + \mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\,\boldsymbol{u} = -\mathfrak{G}_{\text{mom}}\,p\,, \tag{3.2b}$$

$$\mathfrak{H}\frac{\partial \rho e}{\partial t} + \mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}\,e = -p\,\mathfrak{D}_{\text{inten}}\,\boldsymbol{u}\,. \tag{3.2c}$$

Here $\mathfrak{H}$ denotes a diagonal matrix operator containing the sizes of the control volumes Ω_h. The dependent variables are now discrete (vector) grid functions, but we will use the same (lower case) symbols as in the continuous case. The $\mathfrak{Fraktur}$-font operators denote *volume-consistent* [18, 71, 142] discrete approximations of the continuous differential operators, with subscripts to identify in which equation they are being used:

- $\mathfrak{D}_{\text{mass}}$ is a discrete divergence matrix operator acting on the mass flux vector $\boldsymbol{m}$ in (3.1a). With the grid vector $\mathfrak{D}_{\text{mass}}\,\boldsymbol{m}$, a diagonal grid matrix $\text{diag}(\mathfrak{D}_{\text{mass}}\boldsymbol{m})$ can be formed.
- $\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}$ is a discrete grid operator, acting on $\boldsymbol{u}$, for the convective term in the momentum equation (3.1b). Its coefficients depend on the mass flux $\boldsymbol{m}$.
- $\mathfrak{G}_{\text{mom}}$ is a discrete gradient operator in (3.1b) acting on the pressure p.
- $\mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}$ is a discrete grid operator, acting on e and dependent on $\boldsymbol{m}$, for the convective term in the conservation law for internal energy (3.1c).
- $\mathfrak{D}_{\text{inten}}$ is a discrete divergence operator acting on the velocity $\boldsymbol{u}$ in (3.1c).

Note that with the above finite-volume scaling, the sizes $\mathfrak{H}$ of the control volumes are included in the operators, i.e. the scaling in (3.2) is volume consistent [18, 71, 142]. In fact, analytic and discrete operators are related like $\text{div} \leftrightarrow \mathfrak{H}^{-1}\,\mathfrak{D}_{\text{mass}}$. This may look a bit awkward, but it fits naturally in the finite-volume setting, and the symmetry properties of the discrete differential operators will come out more directly. The alternative would have been a scaling of the above operators by $\mathfrak{H}^{-1}$, which then would fit naturally in a finite-difference setting. Both notation choices have their pros and cons; in this paper we opt for the finite-volume related option.

With the notation from (3.2), and similar to Eq. (2.1), the discrete (finite-volume) evolution of total energy can be formulated locally as

$$\begin{aligned}\mathfrak{H}\frac{\partial \rho E_{\text{total}}}{\partial t} &= \tfrac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\,\mathfrak{D}_{\text{mass}}\boldsymbol{m} - \boldsymbol{u}\cdot\left(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\,\boldsymbol{u} + \mathfrak{G}_{\text{mom}}\,p\right) - \mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}e - p\,\mathfrak{D}_{\text{inten}}\boldsymbol{u}\\ &= \boldsymbol{u}\cdot\left(\tfrac{1}{2}\text{diag}(\mathfrak{D}_{\text{mass}}\,\boldsymbol{m}) - \mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\right)\boldsymbol{u} - \left(\boldsymbol{u}\cdot\mathfrak{G}_{\text{mom}}\,p + p\,\mathfrak{D}_{\text{inten}}\boldsymbol{u}\right) - \mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}\,e. \qquad (3.3)\end{aligned}$$

The last line in (3.3) corresponds with line (2.1b) in the analytic derivation. From here, we would like to make the steps to (2.1c) and (2.1d) in this discrete version too. Therefore, let us find out which relations between the discrete operators have to be satisfied.

The evolution of the total amount of energy can be found by summing (3.3) over all grid cells (effectuated by multiplying with the grid vector 1^T consisting of only ones):

$$\begin{aligned}1^T\mathfrak{H}\,\frac{\partial \rho E_{\text{total}}}{\partial t} &= -1^T\boldsymbol{u}\cdot\left(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}} - \tfrac{1}{2}\text{diag}(\mathfrak{D}_{\text{mass}}\,\boldsymbol{m})\right)\boldsymbol{u}\\ &\quad - 1^T\left(\boldsymbol{u}\cdot\mathfrak{G}_{\text{mom}}\,p + p\,\mathfrak{D}_{\text{inten}}\boldsymbol{u}\right) - 1^T\mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}\,e\,. \qquad (3.4)\end{aligned}$$

Because of the finite-volume scaling of (3.2), the left-hand side forms a consistent approximation of the total amount of energy in the domain: it reflects a midpoint quadrature rule. Other formulations are possible, as in the higher-order methods of Verstappen and Veldman [145, 146] which are related to Simpson's quadrature rule. This volume-consistent [18, 71, 142] scaling property motivated us to 'hide' the size of the control volumes into the definition of the discrete operators.

The first two summations in the right-hand side of (3.4) can be interpreted as inner products in the space of scalar and vector-valued grid functions. The symmetry properties that we will discuss below are with respect to these inner products. From here the requirements for discrete energy conservation can be derived. We will see in the sequel that this requires a certain amount of compatibility between the discrete operators.

REQUIREMENT 3.1 (Compare Property 2.1). *The first summation in the right-hand side of (3.4) should vanish, i.e. the matrix operator between the first pair of brackets should satisfy*

$$\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}} - \tfrac{1}{2}\,\text{diag}(\mathfrak{D}_{\text{mass}}\,\boldsymbol{m}) \quad \textit{is skew-symmetric.} \qquad (3.5)$$

This necessary and sufficient condition for global discrete convective energy conservation has thus far been mentioned only a few times, e.g. by Kok [62], Morinishi [77], Van 't Hof et al. [137,138], and implicitly by Chandrashekar [22, Sect. 3]. It provides a relation between the diagonal of $\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}$ and discrete mass conservation $\mathfrak{D}_{\text{mass}}\,\boldsymbol{m}$. The examples in Sect. 4 and 5 indicate that when starting from a finite-volume discretization one also has local energy conservation. It would be interesting to investigate which conditions govern local secondary conservation in the general case [27, 28, 90].

REQUIREMENT 3.2 (Compare Property 2.2). *In order for the second sum in the right-hand side of (3.4) to vanish, the (pressure) gradient and the dilatational divergence should be each other's negative transpose:*

$$\mathfrak{G}_{\text{mom}} = -\mathfrak{D}^T_{\text{inten}}\ (= -\mathfrak{D}^T_{\text{mass}})\,. \qquad (3.6)$$

This is a necessary and sufficient condition to ensure that the pressure does not contribute to the global total energy. In this way, the two operators $\mathfrak{D}_{\text{inten}}$ and $\mathfrak{G}_{\text{mom}}$ combine into a meaningful discrete divergence expression for $\nabla(p\boldsymbol{u})$ in the virtual evolution of total energy. Alternatively, if we would have started in (1.1c) with a conservation law for total energy, then to achieve a physically meaningful exchange between internal and kinetic energy a similar consistency condition between the pressure gradient and the latter divergence would be required.

In (3.6), the right-hand side between parentheses corresponds with the incompressible limit, in which the equation for internal energy degenerates into the continuity equation [47, 61]. Also, it leads to a symmetric negative-definite Laplacian in the often used pressure Poisson equation.

The final requirements concern the discretization of the equation for internal energy. First of all, for discrete energy conservation it is necessary that it is conservative. As an additional property, for low Mach numbers [47,61] we would like the discretization for compressible flow to approach a discretization for incompressible flow. This requires further consistency between the discrete operators; see Appendix A.

Requirement 3.3 (Compare Property 2.3).
A: Vanishing of the last sum in the right-hand side (3.4) requires

$$\mathfrak{C}^{\boldsymbol{m}}_{\text{inten}} \textit{ is telescoping (like a finite-volume operator).} \tag{3.7}$$

B: To combine the momentum and internal-energy equations into a unified equation for total energy, the respective discrete convective operators should be the same:

$$\mathfrak{C}^{\boldsymbol{m}}_{\text{inten}} = \mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\,. \tag{3.8}$$

C: A smooth discrete transition from compressible flow to incompressible flow requires that the divergence operators in (3.1c) are consistent (in the incompressible limit) with the divergence operator in (3.1a):

$$\mathfrak{D}_{\text{inten}} = \mathfrak{D}_{\text{mass}} \quad \vee \quad \mathfrak{C}^{\boldsymbol{m}}_{\text{inten}} \to \rho_0 \mathfrak{D}_{\text{mass}}\boldsymbol{u} \tag{3.9}$$

(ρ_0 is the incompressible density).

While being sufficient, it is noted that these conditions are not strictly necessary to achieve global conservation of total energy. Also note that in view of the relations (3.8) and (3.5), the conditions in (3.9) will usually be satisfied.

The above requirements suggest to introduce the following definition of symmetry-preserving operators for (in)compressible flow:

Definition 3.4 (symmetry-preserving). *The triple of discrete finite-volume operators for the incompressible Euler equations $\{\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}, \mathfrak{D}_{\text{mass}}, \mathfrak{G}_{\text{mom}}\}$, where $\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}$ is a discrete convection operator, $\mathfrak{D}_{\text{mass}}$ a discrete divergence and $\mathfrak{G}_{\text{mom}}$ a discrete gradient, is called* symmetry-preserving *when Requirements 3.1 and 3.2 hold. For compressible flow, a convection operator $\mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}$ and a dilatation operator $\mathfrak{D}_{\text{inten}}$ for the internal-energy equation should be added, for which Requirement 3.3 holds.*

With this definition, we can summarize our main result as:

Theorem 3.5. *A (volume-consistent) finite-volume discretization of the Euler equations (1.1) for (in)compressible flow is supra-conservative with respect to global discrete energy if it is symmetry-preserving in the sense of Definition 3.4. Hereto Requirements 3.1 and 3.2 are not only sufficient but also necessary.*

The above requirements guide the way to construct finite-volume triples/quartets which all additionally conserve discrete kinetic energy. These triples/quartets cannot be chosen freely. In particular, the choice for the discretization of the convective term $\mathfrak{C}^{\boldsymbol{m}}_{\mathrm{mom}}$ induces *all* other discretizations:

1. Through Requirement 3.1 the discretization of the conservation of mass $\mathfrak{D}_{\mathrm{mass}}$ is determined.
2. Requirement 3.2 then determines the discrete pressure gradient $\mathfrak{G}_{\mathrm{mom}}$ in the conservation of momentum, and the dilatational divergence $\mathfrak{D}_{\mathrm{inten}}$ in the conservation of internal energy.
3. Finally, Requirement 3.3 determines the discrete convective term $\mathfrak{C}^{\boldsymbol{m}}_{\mathrm{inten}}$ in the conservation of internal energy.

On staggered grids, where the individual unknowns are located at different positions, the above requirements may involve some form of interpolation; we will come back to this later. In the next sections we will work out the above requirements for some specific situations involving a finite-volume discretization.

It is remarked that the above requirements have been derived starting from the symbolic discrete formulation in (3.2). The finite-volume origin led in a natural way to a scaling for which the summation in the left-hand side of (3.4) represents an approximate volume integral, i.e. the scaling is volume consistent. But no other properties of a finite-volume method have been used. As a consequence, all requirements for discrete energy conservation hold for any discretization that can be written in the volume-consistent form (3.2); its analytical 'provenance' is less relevant [132].

Finally, a diffusive term can be added, i.e. the extension to the Navier–Stokes equations can be made, independently of the above discretizations. Of course, one would want the discretization of the viscous stresses to lead to a consistent, symmetric negative-definite operator. But no further requirements have to be imposed as far as we are concerned here, as in this way diffusion will not interfere with the physics of convection. Perot [92] gives guide lines on how to achieve this on arbitrary grids.

4. Incompressible flow - staggered grid. As a first example, we will work out the above requirements when discretizing the equations (1.1) in the special case of incompressible flow on a staggered grid, as shown in Figure 1. The case of collocated grids will be discussed later on, when applied to the equations for compressible flow.

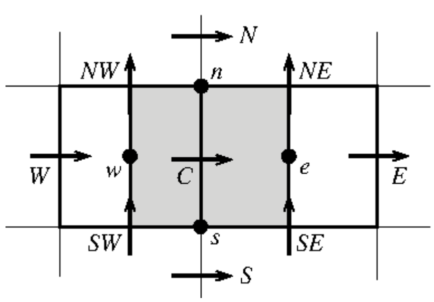

FIG. 1. *A staggered control volume for the conservation of x-momentum (shaded area), covering half of two adjacent control volumes (grid cells) for mass conservation.*

4.1. Conservation of mass. On a staggered grid, the velocity components are defined on the edges/faces of the computational cells. Also the momentum equation (3.1b) is discretized in those locations; see the shaded momentum control volume in Figure 1. The continuity equation (3.1a) is discretized in cell centers, with the grid cells as control volumes.

In the right-hand cell in Figure 1 (around the location e), the incompressible form of the conservative continuity equation (3.1a) can be discretized as

$$0 = \oint_{\Gamma_e} \boldsymbol{m}\cdot\boldsymbol{n}\ \mathrm{d}\Gamma = \int_{\Gamma_E} m^x\ \mathrm{d}\Gamma_E + \int_{\Gamma_{NE}} m^y\ \mathrm{d}\Gamma_{NE} - \ldots\ldots$$

$$\equiv \widetilde{m}^x_E + \widetilde{m}^y_{NE} - \widetilde{m}^x_C - \widetilde{m}^y_{SE} \equiv \mathfrak{D}_{\text{mass}}\,\boldsymbol{m}|_e\,. \tag{4.1}$$

Here, $\widetilde{m}$ denotes a mass flux integrated over an (infinitesimal) edge $\mathrm{d}\Gamma$ of the control volume, e.g. (but not necessarily) by a midpoint integration rule (like $\widetilde{m}^x_E \equiv m^x_E|\mathrm{d}\Gamma_E|$). Note that (4.1) puts no further restrictions on the choice of $\widetilde{m}$.

4.2. Conservation of momentum. Next, the discretization of the convective term and the pressure gradient on a staggered grid will be shown.

Convection. In the u-component of the momentum equation (3.1b), the discrete convective contribution from the shaded control volume in Figure 1 reads approximately

$$\int_{\Gamma_h} (\boldsymbol{m}\cdot\boldsymbol{n})u\ \mathrm{d}\Gamma_h \approx u_e \int_{\Gamma_e} \boldsymbol{m}\cdot\boldsymbol{n}\ \mathrm{d}\Gamma_e + u_n \int_{\Gamma_n} \boldsymbol{m}\cdot\boldsymbol{n}\ \mathrm{d}\Gamma_n + \ldots$$

$$= \widetilde{m}^x_e\, u_e + \widetilde{m}^y_n\, u_n - \widetilde{m}^x_w\, u_w - \widetilde{m}^y_s\, u_s \equiv \mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\,\boldsymbol{u}|_C\,, \tag{4.2}$$

which defines the convection operator $\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}$ from (3.2b). To achieve symmetry in the coefficient matrix, it is necessary that the u-fluxes are chosen according to an equal-weighted ($\frac{1}{2}$-$\frac{1}{2}$) interpolation between the faces of the continuity cells, even if the faces of the momentum control volume are not located in the cell centers:

$$u_e = \tfrac{1}{2}(u_E + u_C), \quad u_n = \tfrac{1}{2}(u_N + u_C), \text{ etc.} \tag{4.3}$$

Then substitution of (4.3) into (4.2) yields

$$\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\, u|_C = \tfrac{1}{2}[\widetilde{m}^x_e(u_E + u_C) + \widetilde{m}^y_n(u_N + u_C) - \widetilde{m}^x_w(u_W + u_C) - \widetilde{m}^y_s(u_S + u_C)]$$

$$= \tfrac{1}{2}[\widetilde{m}^x_e u_E - \widetilde{m}^x_w u_W + \widetilde{m}^y_n u_N - \widetilde{m}^y_s u_S] + \tfrac{1}{2}[\widetilde{m}^x_e - \widetilde{m}^x_w + \widetilde{m}^y_n - \widetilde{m}^y_s]u_C\,.$$

It is clear that the coefficients of the neighboring grid points are skew symmetric due to the equal-weighted interpolation in (4.3). Whether the central coefficient (of u_C) vanishes is as yet unclear, and will be examined next.

In the diagonal coefficient $\text{diag}(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}})|_C \equiv \frac{1}{2}[\widetilde{m}^x_e - \widetilde{m}^x_w + \widetilde{m}^y_n - \widetilde{m}^y_s]$ we recognize a discrete divergence operator over a momentum control volume, but not yet immediately the one from the discrete continuity equation given in (4.1). Skew symmetry (3.5) requires $\text{diag}(\mathfrak{C}^{\boldsymbol{u}}_{\text{mom}}) - \frac{1}{2}\,\mathfrak{D}_{\text{mass}}\,\boldsymbol{m} = 0$. This is now a requirement for the construction of $\mathfrak{D}_{\text{mass}}$, which herewith becomes related to the diagonal entries given by $\text{diag}(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}})$ (though it will require some interpolations between the staggered grid positions). The requirement can be satisfied by interpolating the mass fluxes $\widetilde{m}$ with equal weights, similar to the velocity components, i.e. we define

$$\widetilde{m}^x_e = \tfrac{1}{2}(\widetilde{m}^x_E + \widetilde{m}^x_C), \quad \widetilde{m}^y_n = \tfrac{1}{2}(\widetilde{m}^y_{NE} + \widetilde{m}^y_{NW}), \text{ etc.} \tag{4.4}$$

For this choice of the mass fluxes, the central coefficient becomes

$$\text{diag}(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}})|_C = \tfrac{1}{4}[\widetilde{m}^x_E - \widetilde{m}^x_W + \widetilde{m}^y_{NE} + \widetilde{m}^y_{NW} - \widetilde{m}^y_{SE} - \widetilde{m}^y_{SW}]\,,$$

which equals $\frac{1}{4}\times$[mass conservation of right- + left-hand cell]. As a result

$$\operatorname{diag}(\mathfrak{C}^{\boldsymbol{m}}_{\mathrm{mom}})|_C = \tfrac{1}{4}(\mathfrak{D}_{\mathrm{mass}}\boldsymbol{m}|_e + \mathfrak{D}_{\mathrm{mass}}\boldsymbol{m}|_w) = 0\,, \tag{4.5}$$

i.e. the diagonal of the convective operator vanishes. Thus, we have achieved our goal Requirement 3.1 of skew symmetry. It is remarked that the choice (4.4) is not unique, as demonstrated in [137, Sect. 3.1].

The above guarantees global conservation of kinetic energy. Substitution of $\mathfrak{C}^{\boldsymbol{m}}_{\mathrm{mom}}$ in (3.3) shows that energy is also conserved locally, with energy fluxes given by $\frac{1}{2}\widetilde{m}^x_e u_C u_E$, etc.

Pressure gradient. Finally, we have to consider the contribution of the pressure to the evolution of kinetic energy. The pressure is defined in cell centers, e.g. the points w and e in Figure 1. The contribution to the x-momentum equation (3.1b) can be approximated as (with $\boldsymbol{e}_x$ denoting the unit vector in x-direction)

$$\oint_{\Gamma_h} p\,\boldsymbol{n}\;\mathrm{d}\Gamma \approx \int_e p_e\boldsymbol{e}_x\;\mathrm{d}\Gamma_e - \int_w p_w\boldsymbol{e}_x\;\mathrm{d}\Gamma_w \equiv \mathfrak{G}_{\mathrm{mom}\,x}\,p\,, \tag{4.6}$$

which defines the x-component of the discrete pressure gradient $\mathfrak{G}_{\mathrm{mom}}$. Its coefficients are equal to the size of the corresponding faces, similar to the discrete approximation of the continuity equation in (4.1), with coefficients equal to the local size of the face dΓ. Noting that the grid is rectangular, it follows that the discrete pressure gradient and the discrete divergence satisfy Requirement 3.2.

The pressure can be computed by requiring that the solution of the discrete momentum equation (3.2b) satisfies the discrete constraint (3.2a). I.e., there must hold

$$0 = \frac{\partial}{\partial t}\mathfrak{D}_{\mathrm{mass}}\,\boldsymbol{m} \overset{(*)}{=} \mathfrak{D}_{\mathrm{mass}}\,\frac{\partial \rho\boldsymbol{u}}{\partial t} = -\mathfrak{D}_{\mathrm{mass}}\,\mathfrak{H}^{-1}\left(\mathfrak{C}^{\boldsymbol{m}}_{\mathrm{mom}}\,\boldsymbol{u} + \mathfrak{G}_{\mathrm{mom}}\,p\right)\,, \tag{4.7}$$

which defines the Poisson equation for the pressure. Note that the discrete Poisson operator is symmetric negative definite, due to Requirement 3.2. Also, note that the step (*) in (4.7) is one of only two places in this paper where the equality between $\boldsymbol{m}$ and $\rho\boldsymbol{u}$ is needed.

5. Compressible flow - collocated grid. On a structured collocated grid, as used commonly for compressible flow, all flow variables are defined in 'cell centers' with a liberal interpretation of the meaning of 'center' (centroid, circumcenter, ...); see Figure 2 (*left*). E.g., positioning the faces halfway the locations where the flow variables are defined (known as a Voronoi grid) is a valid option, as in Figure 2 (*right*) of an unstructured grid. No choice between the 'center-options' will be made in this paper; we merely focus on the symmetry properties of the discrete operators.

5.1. Conservation of mass. With reference to Figure 2, it is natural to choose the finite-volume form of the divergence term in the equation for mass conservation (3.2a) as

$$\mathfrak{D}_{\mathrm{mass}}\,\boldsymbol{m}|_C \equiv \widetilde{m}^x_e + \widetilde{m}^y_n - \widetilde{m}^x_w - \widetilde{m}^y_s = \sum_{f\in\mathcal{F}_C} \widetilde{\boldsymbol{m}}_f\cdot\boldsymbol{n}_f\,. \tag{5.1}$$

The right-hand side is formulated in a general notation for arbitrarily-shaped control volumes. The summation is over the faces f of the volume around C, together constituting the set $\mathcal{F}_C$, and $\boldsymbol{n}_f$ is an outward-pointing normal.

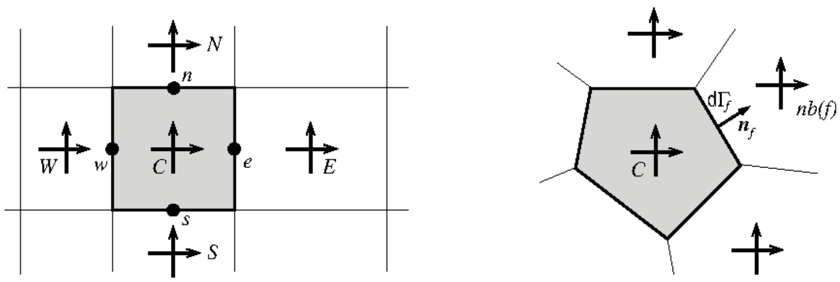

FIG. 2. *Control volumes for collocated grids: (left) structured with* $\boldsymbol{u}$*-locations halfway faces (= cell-centered); and (right) unstructured with faces halfway* $\boldsymbol{u}$*-locations (= face- or vertex-centered).*

5.2. Conservation of momentum.

Convection. With similar notation, the discrete convective contribution to the momentum equation reads

$$\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}\, \boldsymbol{u}|_C \equiv \widetilde{m}^x_e \boldsymbol{u}_e + \widetilde{m}^y_n \boldsymbol{u}_n - \widetilde{m}^x_w \boldsymbol{u}_w - \widetilde{m}^y_s \boldsymbol{u}_s = \sum_{f\in\mathcal{F}_C} (\widetilde{\boldsymbol{m}}_f \cdot \boldsymbol{n}_f)\boldsymbol{u}_f\,. \tag{5.2}$$

To compute the fluxes at the cell edges, again an equal-weighted ($\frac{1}{2}$-$\frac{1}{2}$) interpolation for the velocity component u should be applied:

$$\boldsymbol{u}_f = \tfrac{1}{2}(\boldsymbol{u}_C + \boldsymbol{u}_{nb(f)})\,, \tag{5.3}$$

where $nb(f)$ denotes the neighboring grid cell sharing the face f. As a direct consequence, the coefficients in the convective contribution are skew-symmetric outside the diagonal. The $\frac{1}{2}$-$\frac{1}{2}$ interpolation is essential here, even when the faces are not half-way between the cell centers. Jameson, in the early 1980s [59], interprets the values in the cell 'centers' as averages over the cells, after which a $\frac{1}{2}$-$\frac{1}{2}$ averaging at the separating face is natural. The 'reward' is discrete energy conservation [58], whereas the location of the cell center turns out to be not very critical. Jameson's approach has become one of the most widely used CFD methods in the aircraft industry [1].

The interesting part is the coefficient on the diagonal of $\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}$. With the above interpolation (5.3), the central coefficient in the convection operator (5.2) becomes

$$\text{diag}(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}) = \tfrac{1}{2} \sum_{f\in\mathcal{F}_C} (\widetilde{\boldsymbol{m}}_f \cdot \boldsymbol{n}_f) \overset{(5.1)}{=} \tfrac{1}{2}\mathfrak{D}_{\text{mass}}\boldsymbol{m}\,.$$

Hence the vector $\text{diag}(\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}}) - \frac{1}{2}\mathfrak{D}_{\text{mass}}\boldsymbol{m}$ vanishes. In fact, the latter requirement determines the choice of $\mathfrak{D}_{\text{mass}}$. The 'freedom' we felt while choosing the discrete divergence operator for mass conservation as in (5.1) is just an illusion: if one insists on energy conservation, given (5.2) and (5.3), there is no other choice possible! Anyhow, the above discretization, (5.1)+(5.2) with interpolation (5.3), satisfies the main Requirement 3.1 for global energy conservation: $\mathfrak{C}^{\boldsymbol{m}}_{\text{mom}} - \frac{1}{2}\text{diag}(\mathfrak{D}_{\text{mass}}\,\boldsymbol{m})$ is skew symmetric, for *all* choices of the mass fluxes $\widetilde{\boldsymbol{m}}$. Also, we have local conservation with a kinetic energy flux given by $\frac{1}{2}(\widetilde{\boldsymbol{m}}_f \cdot \boldsymbol{n}_f)(\boldsymbol{u}_C \cdot \boldsymbol{u}_{nb(f)})$.

Some freedom is left in the choice for the mass fluxes [110]). E.g., there is room to use geometry information to interpolate from the values of $\boldsymbol{m}$ in the cell centers to the values of $\widetilde{\boldsymbol{m}}$ at the faces. It would be interesting to explore this interpolation freedom on (highly) irregular grids.

Pressure gradient. A natural choice for the finite-volume form of the pressure gradient is

$$\mathfrak{G}_{\mathrm{mom}}\, p|_C \equiv (\widetilde{p}_e - \widetilde{p}_w)\boldsymbol{e}_x + (\widetilde{p}_n - \widetilde{p}_s)\boldsymbol{e}_y = \sum_{f\in\mathcal{F}_C} \widetilde{p}_f \boldsymbol{n}_f\,.$$

Once more using equal-weighted interpolation, as in (4.3), we define the pressure 'fluxes' as

$$\widetilde{p}_f = \tfrac{1}{2}(p_C + p_{nb(f)})\,|\mathrm{d}\Gamma_f|\,.$$

The gradient operator can now be rewritten as

$$\mathfrak{G}_{\mathrm{mom}}\, p|_C = \sum_{f\in\mathcal{F}_C} \tfrac{1}{2}|\mathrm{d}\Gamma_f|\,\boldsymbol{n}_f\, p_{nb(f)}\,, \tag{5.4}$$

where the (central) coefficient of p_C vanishes because $\sum_{f\in\mathcal{F}_C}|\mathrm{d}\Gamma_f|\,\boldsymbol{n}_f = 0$.

Remark. For collocated grids, in the incompressible limit the stencil of the pressure Poisson equation (4.7) is prone to odd-even decoupling due to Requirement 3.2, which is needed to maintain perfect discrete energy conservation. To resolve this issue, provided all details are filled in correctly, the corresponding checkerboard mode can be filtered out, as done, e.g., by Ham et al. [48] and Shashank et al. [117].

5.3. Conservation of internal energy. Similar to the definition of $\mathfrak{D}_{\mathrm{mass}}$ in (5.1), the discrete divergence operator $\mathfrak{D}_{\mathrm{inten}}$ in the dilatation term of the energy equation is defined as

$$\mathfrak{D}_{\mathrm{inten}}\, \boldsymbol{u}|_C \equiv \widetilde{u}^x_e + \widetilde{u}^y_n - \widetilde{u}^x_w - \widetilde{u}^y_s = \sum_{f\in\mathcal{F}_C} \widetilde{\boldsymbol{u}}_f \cdot \boldsymbol{n}_f\,.$$

Again, equal-weighted ($\frac{1}{2}$-$\frac{1}{2}$) interpolation is used to define the face fluxes:

$$\widetilde{\boldsymbol{u}}_f = \tfrac{1}{2}(\boldsymbol{u}_C + \boldsymbol{u}_{nb(f)})\,|\mathrm{d}\Gamma_f|\,.$$

The divergence operator can now be rewritten as

$$\mathfrak{D}_{\mathrm{inten}}\, \boldsymbol{u}|_C = \sum_{f\in\mathcal{F}_C} \tfrac{1}{2}|\mathrm{d}\Gamma_f|\,\boldsymbol{n}_f \cdot \boldsymbol{u}_{nb(f)}\,, \tag{5.5}$$

where the (central) coefficient of $\boldsymbol{u}_C$ has vanished as in (5.4).

Looking at the evaluation of (5.5) in the neighboring cell, the coefficient of $\boldsymbol{u}_C$ in the neighboring divergence operator is $\frac{1}{2}|\mathrm{d}\Gamma_f|\boldsymbol{n}_{nb(f)}$, with $\boldsymbol{n}_{nb(f)}$ pointing from the neighboring cell towards C. This generates a minus sign when compared to the coefficient of $p_{nb(f)}$ in the gradient operator (5.4) in C. Thus, $\mathfrak{D}_{\mathrm{mass}} = \mathfrak{D}_{\mathrm{inten}}$ and $\mathfrak{G}_{\mathrm{mom}}$ are each other's negative transpose, as imposed by Requirement 3.2.

The convective term in the equation for internal energy reads

$$\mathfrak{C}^{\boldsymbol{m}}_{\mathrm{inten}}\, e|_C \equiv \widetilde{m}^x_e e_e + \widetilde{m}^y_n e_n - \widetilde{m}^x_w e_w - \widetilde{m}^y_s e_s = \sum_{f\in\mathcal{F}_C} (\widetilde{\boldsymbol{m}}_f \cdot \boldsymbol{n}_f) e_f\,. \tag{5.6}$$

Substitution of (5.4), (5.5) and (5.6) in (3.3) shows that, next to global energy conservation, we also have local energy conservation, with a thermodynamic flux given by $[\frac{1}{2}(p_{nb(f)}\boldsymbol{u}_C + p_C\boldsymbol{u}_{nb(f)}) + \widetilde{\boldsymbol{m}}_f e_f]\cdot \boldsymbol{n}_f$.

In Appendix A, see also [47,61], it is shown that in the limit of compressible flow the internal energy e becomes a constant, say e_0. Also the density ρ approaches a constant ρ_0. Then the convective term from (5.6) becomes

$$\mathfrak{C}^{\boldsymbol{m}}_{\text{inten}}\, e|_C \approx \rho_0 e_0 \sum_{f\in\mathcal{F}_C} (\widetilde{\boldsymbol{u}}_f \cdot \boldsymbol{n}_f)\,,$$

where we used, for the second (and last) time in this paper, that $\boldsymbol{m} = \rho\boldsymbol{u}$. The above relation shows that in the incompressible limit the divergence operator in the convective term approaches the divergence $\mathfrak{D}_{\text{mass}} = \mathfrak{D}_{\text{inten}}$ from the continuity equation. Appendix A shows that this allows for a smooth transition from the compressible to the incompressible discretization.

6. Discussion. In the previous sections we have unraveled a strategy to derive supra-conservative finite-volume (semi-)discretizations for compressible Euler flow that possess additional discrete conservation properties as secondary invariants (like kinetic energy), assuming exact time integration. This paper focusses on the discrete conservation of energy, but, as mentioned in the Introduction, other secondary invariants could have been selected. More research is worthwhile to find out which invariants are best chosen for a given physical application; see e.g. [17]. Also, the subtle difference between global and local conservation deserves more attention [27,28,90].

Mimicking the analytic derivation, the key ingredient of energy-preserving discretizations is a close consistency between the discrete momentum equation and the discrete mass equation (Requirement 3.1). In particular, the diagonal of the discrete convection operator directly determines the discrete divergence in the mass equation and in the dilatation term of the internal energy equation (Requirement 3.3). Also, it determines the discrete pressure gradient (Requirement 3.2).

It is once more stressed, as Bryan [13] already did in 1966, that equal-weighted interpolations (for the velocity $\boldsymbol{u}$ and the mass flux $\boldsymbol{m}$) from cell centers to cell faces are essential to achieve the required compatibility, irrespective of any stretching of the grid! Note that the volume-consistent scaling does contain info about the cell sizes and hence the stretching, and also the mass fluxes provide some freedom to incorporate geometry information.

In our examples, the cell faces are located halfway the positions where $\boldsymbol{m}$ is defined for which an equal-weighted interpolation is natural. But also in other geometrical configurations the same interpolation has to be used, even when a linear unequal-weighted interpolation would seem more logical from an approximation point of view. We already noted that Jameson's [59] interpretation of this interpolation also points towards an equal weighting. The resulting skew-symmetry of the convective discretization turns out more important than local interpolation accuracy and the precise location of cell 'centers'. And, as Ham et al. [49] point out explicitly, on smooth grids (with a bounded ratio between the largest and the smallest grid cells) the respective truncation errors are all second order as usual. See Manteuffel and White [73] for a theoretical justification, and Felten and Lund [38] for practical experiences.

One 'reward' for this consistency in the discretization is the numerical stability of the semi-discretized equations without needing any numerical dissipation. This can be proven under the restriction that the density has a positive lower bound, as in the incompressible case. No rigorous proof has been found yet for the general compressible case, but in practice this appears to be mainly a theoretical issue. Another 'reward' is that subtleties in (eddy-viscosity) turbulence models are not masked by excessive numerical dissipation. Neither will emerging instabilities, like the transition from laminar to turbulent flow, be suppressed by an overdose of numerical artifacts [107]. In this non-interfering way, an energy-preserving discretization forms an excellent basis to combine with low-dissipation turbulence models [106,110].

Usually, this is the place to demonstrate the performance of such methods by showing results for a number of test cases. However, we think it is more convincing to point the reader to the original papers that are successfully using these methods. Many of these energy-preserving methods have been mentioned in the Introduction. Here, in Table 1, we restrict ourselves to a short overview of supra-conservative finite-volume methods for the Euler and/or Navier–Stokes equations. The table has been sorted according to the grid used (structured or unstructured) and the positioning of the unknowns (staggered or collocated). Also, higher-order (> 2) variants have been indicated, including the dispersion-relation preserving method by Kok [62].

Table 1
A sorted selection of supra-conservative finite-volume methods for the Euler/Navier–Stokes equations. The references marked $[\cdot]^*$ *use higher-order methods.*

flow	grid	staggered	collocated
incompressible	structured	[137], [138,144–146,150]*	[38]
	unstructured	[60,64,90,153]	[60,66,104,115,133]
compressible	structured	[77]	[28,33,58,124], [62,107,108]*

7. Conclusion. The paper describes general, necessary and sufficient, requirements for a (semi-)discretization method to conserve secondary invariants, in particular kinetic energy. The essential ingredient is a close consistency between the discrete convection term in the momentum equation, the discrete pressure gradient and the discrete divergences in the conservation laws for mass and for internal energy. When the discrete convection is chosen, the discretization of all other terms is fixed (with freedom left for the mass flux only).

As a general message, it is demonstrated how finite-volume methods can be designed such that, next to the primary invariants, they also conserve one or more secondary invariants, i.e., they can be called supra-conservative. The bottom-line is that the steps in the analytical derivations should be mirrored in the discrete setting. It is expected that this philosophy will be useful independent of the selected secondary invariants, and will lead to requirements, like the above, on the discretization scheme.

The specific requirements to realize discrete energy conservation hold for any discretization which can be put in the form (3.2) studied here. It is left to the readers to figure out whether or not their favorite discretization approach can be made to satisfy these requirements.

Appendix A. The incompressible limit.

One may also wish for a smooth transition of a discretization scheme between compressible and incompressible flow. We will pursue this limit following the scaling by Klein [61] and Guillard and Viozat [47]. These authors consider the following expansions for the flow variables in the incompressible limit $c^* \to \infty$ (ρ^*, u^* and c^*

are characteristic values for density, velocity and speed of sound, respectively):

$$\boldsymbol{u}/u^* = \boldsymbol{u}_0 + O(1/c^*)\,, \quad \rho/\rho^* = \rho_0 + O(1/c^*)\,,$$
$$p/\rho^* {c^*}^2 = p_0 + O(1/c^*)\,, \quad e/{c^*}^2 = e_0 + O(1/c^*)\,.$$

Substitution of these expansions in the equation for internal energy (1.1c) yields for the leading term of order ${c^*}^2$:

$$\frac{\partial \rho_0 e_0}{\partial t} + \nabla \cdot (\rho_0 e_0 \boldsymbol{u}_0) = -p_0 \nabla \cdot \boldsymbol{u}_0\,. \tag{A.1}$$

It can be shown that ρ_0, p_0 and e_0 are constant in space and time. Then this equation degenerates into

$$(\rho_0 e_0 + p_0) \nabla \cdot \boldsymbol{u}_0 = 0\,.$$

We recognize the continuity equation for incompressible flow. But we also see that this equation stems from both the convective term as well as the dilatation term in the equation for internal energy.

Therefore, if one would like the discrete version of the equations for compressible flow to smoothly approach the discrete equations for incompressible flow, then both discrete divergence operators in (A.1) must be the same, and equal to the divergence that describes conservation of mass. This is expressed in Requirement 3.3C.

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