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MATRIX PROPERTIES ASSOCIATED WITH DISCRETE CONSERVATION IN FLOW SIMULATIONS

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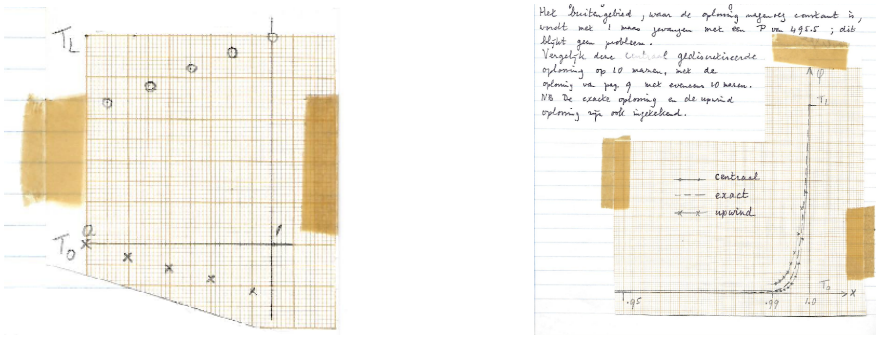
Abstract. Supraconservative discretization methods are studied which conserve primary (mass, momentum and internal energy) as well as secondary (total energy) invariants. In particular, the coefficient matrices which are related to such conservation properties are analyzed. This analysis holds for any discretization method with a volume-consistent scaling.

1 HISTORY

1.1 Recollections of the first author

My first encounter with energy-preserving discretizations, although I did not realize it then, occurred in February 1985, when I was teaching my very first class on CFD at the Technical University in Delft. I had told the students about the challenges when solving a convection-diffusion equation at large Péclet numbers (= small k):

$$x \in [0,1]: \quad \partial_x \phi - k\, \partial_{xx} \phi = 0, \quad \phi(0) = 0,\ \phi(1) = 1. \tag{1}$$

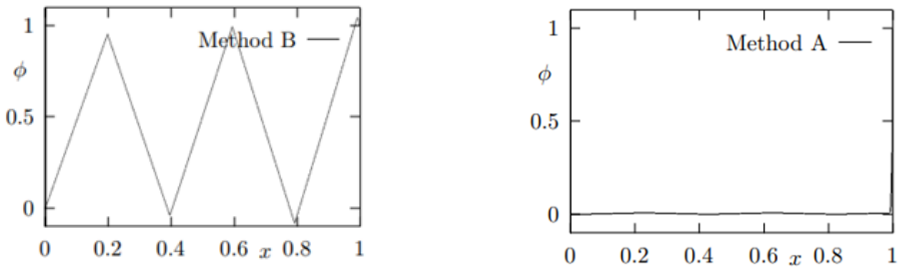


(a) Uniform grid. (b) Non-uniform grid.

Figure 1: February 1985: my first encounter. In those days, graphs were hand-drawn using french curves to draw smooth interpolants, and 'glued' in the hand-written lecture notes by adhesive tape.

I had shown that on a grid which is too coarse to resolve the boundary layer, central discretization yields a wildly-oscillating solution with odd-even decoupling (Fig. 1a). Then I showed my students that the oscillations disappear when the boundary layer is resolved, while at the same time outside the layer the grid cells still can be much coarser. Figure 1b shows this 1985 solution for $k = 0.002$ with one large grid cell ($h = 0.99$) outside the boundary layer, and 9 small cells ($h = 0.001$) inside. Indeed, the refined grid led to a smooth solution, but ...

One year later we had a brand-new, refrigerator-sized, graphical terminal, so I could make more professional plots. Unfortunaltely, I could not find my pile of (Hollerith) punch cards anymore, and I had to recode my algorithm. But how often I checked and re-checked my derivations of the discretization formulas, all I saw on the screen were wiggles (Fig. 2a). The day that I had to lecture about these discretizations for the second time was getting nearer - what did I tell my students last year? Fake science?



(a) Lagrangian discretization.

(b) The simplest discretization.

Figure 2: February 1986: improved graphics for a non-uniform grid. (a) The traditional Lagrangian approach shows nothing but wiggles. (b) The simplest possible discretization shows the desired smooth solution.

With only one week left to go, I tried to reset my mind to the state it would have had one year earlier. And then I realized that everything had to be done at the very last moment; a familiar feeling when you give a course for the first time. I just did not have the time to derive the 'classical' Lagrangian discretization, based on polynomial interpolation. I had only time to use the simplest possible discretization: $\partial_x \phi_i \approx \frac{1}{2}(\phi_{i+1} - \phi_{i-1})/h$! After recoding it, the smooth solution from the year before appeared on the screen (Fig. 2b). I felt a great relief...

We now know that this simple discretization behaves fundamentally different on non-uniform grids [1] as it discretely preserves energy. Grid resolution is not sufficient to produce accurate results. Several years later, after having moved to the University of Groningen, together with Roel Verstappen the use of such discretizations for solving the Navier–Stokes equations was further developed [2–4]. And the rest is history, as people say...

1.2 Short general history

The history of energy-preserving discretizations goes back further in time. Already in the early days of CFD, around 1960, when studying long-time numerical weather prediction, a skew-symmetric discretization of convection was related to discrete energy conservation [5–8]. Espe-

cially, Bryan's little-known two-page paper [6] deserves mentioning, as it presents a cell-centered finite-volume method *avant la lettre*, including a mathematical proof of energy preservation.

Although first mistrusted because of its local truncation error on non-uniform grids, inspite of Manteuffel's proof of 2nd-order accuracy [9], in the 1990s skew-symmetric discretization and energy preservation was gradually attracting more attention of finite-difference and finite-volume methods. For instance, [10] studied the convective, divergence and skew-symmetric forms of the equations for incompressible flow on uniform grids. Studies on non-uniform rectilinear grids include [2,3,11], for curvilinear grids see e.g. [12,13], and (staggered and collocated) unstructured grids are treated in [14, 15]. Convective skew-symmetry also features in the SBP method [16]. Recently, also the finite-element community has recognized the favorable properties of discrete energy preservation [17, 18].

Also for compressible flow much effort has been put in finding split forms and finite-volume formulations of the flow equations that lead to additional conservation properties [19, 20]. Analytically all formulations are equivalent, but after discretization this equivalence is partly lost and differences appear in the induced discrete invariants. In the current paper the above discretizations are studied in terms of their matrix properties, as developed in [21].

A construction of energy-preserving time integration methods has been presented in [22]. But in practice, within the stability limits, the time integration errors are small with respect to the errors stemming from the space discretization [4]. So, here we will not dig deeper into this aspect of supraconservative discretization methods, and in our theoretical considerations we assume exact time integration. A more extensive historical account can be found in [23].

Applications A major application of energy-preserving discretization is the numerical simulation of turbulence. Turbulent flow features a subtle balance between advective energy production and diffusive energy dissipation [24, 25]. It is important that this balance is not disturbed by other physical and numerical effects, e.g. by numerical diffusion from upwind-biased convective discretization [26, 27]. It is essential that stability is only controlled by the physical diffusion of the flow as provided by the molecular viscosity. For turbulent flow, this usually is only a very limited amount, and the slightest numerical imperfections can make the discrete system unstable or overly stable, therewith destroying the physical character of the numerical solution. The numerical challenge is to maneuver in this narrow zone necessary for an accurate description of turbulence. The text below will give some ideas and guide lines for analyzing this zone.

2 CONSERVATION

2.1 Analytic

The equations for fluid flow fit in the general conservation-law framework

$$\partial_t(\rho\psi) + \nabla\cdot\mathcal{F}(\psi) = 0 \quad \Leftrightarrow \quad \int_{\Omega_h} \partial_t(\rho\psi)\,\mathrm{d}\Omega_h + \int_{\Gamma_h} \mathcal{F}(\psi)\cdot\boldsymbol{n}\,\mathrm{d}\Gamma_h = 0, \tag{2a,b}$$

for any control volume Ω_h with boundary Γ_h, thus expressing the conservation of the primary invariant $\rho\psi$. Often the flux is given by $\mathcal{F}(\psi) = \boldsymbol{m}\psi$, where $\boldsymbol{m} \equiv \rho\boldsymbol{u}$ is the mass flux. When

combining the conservation laws for mass ($\psi = 1$), momentum ($\psi = \boldsymbol{u}$) and internal energy ($\psi = e$) an analytic relation for the evolution of total energy $E_{\text{total}} \equiv \frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u} + e$ can be derived [23]:

$$
\begin{aligned}
\frac{\partial}{\partial t}(\rho E_{\text{tot}}) &= -\tfrac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\frac{\partial}{\partial t}\rho \;+\; \boldsymbol{u}\cdot\frac{\partial}{\partial t}(\rho\boldsymbol{u}) \;+\; \frac{\partial}{\partial t}(\rho e) \\
&\qquad\qquad \overbrace{\qquad\qquad}^{\text{mass}} \qquad\qquad \overbrace{\qquad\qquad\qquad\qquad}^{\text{momentum}} \qquad\qquad \overbrace{\qquad\qquad}^{\text{internal energy}} \\
&= \tfrac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\nabla\cdot\boldsymbol{m} - \mathsf{u}\cdot\Big\{\nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u}) + \nabla p\Big\} - \Big\{\nabla\cdot(\boldsymbol{m}e) + p\nabla\cdot\boldsymbol{u}\Big\} \\
&= \underbrace{\boldsymbol{u}\cdot\Big\{\tfrac{1}{2}(\nabla\cdot\boldsymbol{m})\boldsymbol{u} - \nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u})\Big\}}_{\text{Property 1}} - \nabla\cdot(\boldsymbol{m}e) - \underbrace{\Big\{\boldsymbol{u}\cdot\nabla p + p\nabla\cdot\boldsymbol{u}\Big\}}_{\text{Property 2}} \\
&= \underbrace{-\nabla\cdot(\tfrac{1}{2}\boldsymbol{m}\boldsymbol{u}^2) - \nabla\cdot(\boldsymbol{m}e)}_{\text{Property 3}} - \nabla\cdot(p\boldsymbol{u}) \\
&= -\nabla\cdot(\boldsymbol{m}E_{\text{total}}) - \nabla\cdot(p\boldsymbol{u})\,.
\end{aligned}
$$

The colors denote from which conservation law a certain term originates. When two colors meet, it requires a consistency between the confluent terms, which is not obvious to hold after discretization. The confluence we want to study in this paper is indicated by Property 1. We refer to [23, 28, 29] for the other two properties, which involve the (blue) thermodynamic terms.

By integrating over the domain, Property 1 implies

$$
\int_\Omega \boldsymbol{u}\cdot\underbrace{\Big\{\tfrac{1}{2}(\nabla\cdot\boldsymbol{m})\boldsymbol{u} - \nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u})\Big\}}_{\mathcal{K}\boldsymbol{u}}\,\mathrm{d}\Omega = \int_\Omega \nabla\cdot(\tfrac{1}{2}\boldsymbol{m}\boldsymbol{u}^2)\,\mathrm{d}\Omega \quad \forall \boldsymbol{m}, \boldsymbol{u}. \tag{3}
$$

which is equivalent to

$$
\int_\Omega \boldsymbol{u}\cdot\mathcal{K}\boldsymbol{u}\,\mathrm{d}\Omega = 0 \quad \forall\,\text{real } \boldsymbol{u} \quad \leftrightarrow \quad \mathcal{K} \text{ is skew symmetric.} \tag{4}
$$

2.2 Discrete

The idea is now to mimic the above analysis in the discrete setting. Hereto, we first formulate the conservation equations in a general finite-volume format:

$$
\int_{\Omega_h}\frac{\partial\rho\psi}{\partial t}\,\mathrm{d}\Omega_h + \int_{\Gamma_h}(\mathsf{m}\cdot\boldsymbol{n})\psi\,\mathrm{d}\Gamma_h = \ldots, \quad \psi\in\{1,\mathsf{u},e\}.
$$

The equations are solved on a domain Ω with appropriate initial and boundary conditions. In order not to be bothered by the boundaries, we will consider periodic boundary conditions. Physically, this means that external influences on the flow field are excluded. In particular, we denote the discrete mass and momentum equations and the discrete operators in the following way:

$$
\text{mass} \quad \mathfrak{H}\frac{\partial\rho}{\partial t} + \mathfrak{D}_{\text{mass}}\,\mathsf{m} = 0\,; \qquad \text{momentum} \quad \mathfrak{H}\frac{\partial\rho\mathsf{u}}{\partial t} + \mathfrak{C}_{\text{mom}}\,\mathsf{u} = -\mathfrak{G}_{\text{mom}}\,p\,. \tag{5}
$$

The symbol $\mathfrak{H}$ denotes the size of the control volumes Ω_h, such that a summation of the first term leads to an approximate volume integral of the time derivative. An equation scaled this way is said to possess a *volume-consistent* scaling [30]. Combining both equations, and summing the result over the domain, leads to a discrete expression for the total amount of energy:

$$\begin{aligned}\frac{\partial}{\partial t}\sum_{\Omega_h}\mathfrak{H}\,\rho E_{\text{total}} \;&=\; -\sum_{\Omega_h}\mathsf{u}\cdot\overbrace{\left(\mathfrak{C}_{\text{mom}}-\tfrac{1}{2}\,\mathfrak{D}_{\text{mass}}\mathsf{m}\right)}^{\mathfrak{K}}\mathsf{u}\\ &\quad -\sum_{\Omega_h}(\mathsf{u}\cdot\mathfrak{G}_{\text{mom}}\,p+\text{other thermodynamic terms}).\end{aligned}$$

The requirement we are interested in is the necessary and suffcient condition for preservation of discrete kinetic energy:

$$\text{Discrete Requirement 1:}\quad \mathfrak{K}\equiv\mathfrak{C}_{\text{mom}}-\tfrac{1}{2}\,\mathfrak{D}_{\text{mass}}\mathsf{m}\ \text{ is skew-symmetric.}\tag{6}$$

Observe that this requirement poses a strong relation between the diagonal of the discrete convective operator $\mathfrak{C}_{\text{mom}}$ and the transport term for discrete mass conservation $\mathfrak{D}_{\text{mass}}\,\mathsf{m}$ [30].

It follows that *global energy conservation* is equivalent to the *skew symmetry* of $\mathfrak{K}$. In that case the convective terms in the equations (5) do globally conserve the secondary invariant kinetic energy, next to the primary invariants mass ρ and momentum $\rho\phi$. A discretization with secondary conservation properties is called *supraconservative* [30].

3 GLOBAL AND LOCAL CONSERVATION

3.1 Global conservation

A finite-volume discretization of a general conservation law (2) can be formulated as

$$\int_{\mathfrak{H}}\frac{\mathrm{d}\psi}{\mathrm{d}t}\,\mathrm{d}\mathfrak{H}+\int_{\Gamma_{\mathfrak{H}}}\boldsymbol{n}\cdot\mathsf{f}(\psi)\,\mathrm{d}\Gamma_{\mathfrak{H}}=0\quad\leftrightarrow\quad\mathfrak{H}\frac{\mathrm{d}\psi}{\mathrm{d}t}+\mathfrak{D}\mathsf{f}(\psi)=0,$$

where $\mathfrak{D}$ is a general derivative matrix, i.e. all of its row sums vanish.

Because of the volume-consistent scaling, global conservation can be found by adding the separate equations per control volume. In the discrete case this corresponds with a multiplication by the vector $\mathbf{1}=(1,1,...,1)^{\mathsf{T}}$ consisting of only ones:

$$\int_{\Omega}\frac{\partial\psi}{\partial t}\,\mathrm{d}\Omega=0\leftrightarrow\mathbf{1}^{\mathsf{T}}\mathfrak{H}\frac{\mathrm{d}\psi}{\mathrm{d}t}=0\quad\Leftrightarrow\quad\mathbf{1}^{\mathsf{T}}\mathfrak{D}\mathsf{f}(\psi)=0\quad\forall\,\mathsf{f}(\psi)\quad\Leftrightarrow\quad\mathbf{1}^{\mathsf{T}}\mathfrak{D}=\mathbf{0}^{\mathsf{T}}.$$

This means that *global conservation* is equivalent with *vanishing column sums.*

3.2 Local conservation

Discrete *local conservation* entails that the discretization can be expressed as a difference of fluxes, as in a finite-volume discretization. The latter approach obviously creates local and

global conservation, but the opposite is also true. To show this, we need some more notation, in particular a discrete shift operator. In one dimension, this operator shifts the grid index as $\mathsf{E}(\psi)|_i = \psi_{i+1}$, and a derivative operator can be written as[1]

$$\mathfrak{D} = \mathsf{I} - \mathsf{E}^{-1} \quad \leftrightarrow \quad \mathfrak{H}\frac{\mathrm{d}\psi}{\mathrm{d}t} + (\mathsf{I} - \mathsf{E}^{-1})\mathsf{f}(\psi) = 0.$$

It can be proven [21] that a matrix $\mathfrak{D} = \sum_{k=-L}^{L} \mathrm{diag}(\mathsf{a}_k)\mathsf{E}^k$ allows a flux decomposition

$$\mathfrak{D} = (\mathsf{I} - \mathsf{E}^{-1})\mathfrak{F} \quad \text{with} \quad \mathfrak{F} = \sum_{k=-L}^{L}\sum_{h=k}^{L} \mathrm{diag}(\mathsf{E}^{k-h}\mathsf{a}_h)\mathsf{E}^k \tag{7a,b}$$

if and only if all of its column sums vanish. This shows that for periodic problems the concepts of global and local conservation are equivalent. It also implies that any globally conservative discretization (finite differences, finite elements, etc.) can be written as a finite-volume method, with (7b) giving the corresponding fluxes.

4 CONSERVATION PROPERTIES OF SPLIT FORMS

4.1 Split forms

In what follows, we will discuss several discretizations for the conservation equations for mass and momentum based on their split forms [19, 20]. For the mass transport operator we study

$$\mathcal{D}_{\mathrm{mass}}\boldsymbol{m} = \xi\,\nabla\cdot(\rho\boldsymbol{u}) + (1-\xi)[\boldsymbol{u}\cdot\nabla\rho + \rho\nabla\cdot\boldsymbol{u}]. \tag{8}$$

The convective term in the momentum equation is written in split form as

$$\begin{aligned}\mathcal{C}_{\mathrm{mom}}\phi =& \alpha\nabla\cdot(\rho\boldsymbol{u}\phi) + \beta\big[\rho\boldsymbol{u}\cdot\nabla\phi + \phi\nabla\cdot(\rho\boldsymbol{u})\big] + \\ & \gamma\big[\boldsymbol{u}\cdot\nabla(\rho\phi) + \rho\phi\nabla\cdot\boldsymbol{u}\big] + \delta\big[\rho\nabla\cdot(\boldsymbol{u}\phi) + \boldsymbol{u}\cdot\phi\nabla\rho\big]\end{aligned} \tag{9}$$

with $\alpha+\beta+\gamma+\delta = 1$, where we allow for different discretizations of the ∇-operators.

4.2 Conservation of mass

The split forms we study for the mass equation are given by (8). Here, we discuss the extreme cases $\xi = 1$ and $\xi = 0$:

- The case $\xi = 1$ corresponds with the divergence form (mass flux $\boldsymbol{m} = \rho\boldsymbol{u}$)

  $$\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{m} = 0 \quad \overset{\text{discrete}}{\longrightarrow} \quad \mathfrak{H}\frac{\mathrm{d}\rho}{\mathrm{d}t} + \mathfrak{D}^{\rho\mathsf{u}}\mathsf{m} = \mathbf{0}.$$

  Global mass conservation amounts to $\mathbf{1}^{\mathsf{T}}\mathfrak{D}^{\rho\mathsf{u}} = \mathbf{0}$ and the finite-volume discretization reads $\mathfrak{D}^{\rho\mathsf{u}}\mathsf{m} = (\mathsf{I} - \mathsf{E}^{-1})\mathsf{m}^{\mathsf{fv}}$.

[1] Use will be made of 1D matrix-vector notation as introduced by Coppola et al. [20]; see Appendix A.

- The case $\xi = 0$ corresponds with the advective form of the transport term

$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \rho = 0 \quad \overset{\text{discrete}}{\longrightarrow} \quad \mathfrak{H} \frac{\mathrm{d}\mathsf{\rho}}{\mathrm{d}t} + \mathsf{R}\mathfrak{D}^{\mathsf{u}}\mathsf{u} + \mathsf{U}\mathfrak{D}^{\rho}\mathsf{\rho} = \mathbf{0}.$$

  Discrete global conservation requires

$$\mathbf{1}^{\mathsf{T}}(\mathsf{R}\mathfrak{D}^{\mathsf{u}}\mathsf{u} + \mathsf{U}\mathfrak{D}^{\rho}\mathsf{\rho}) = 0 \quad \forall\ \mathsf{u}, \mathsf{\rho} \quad \Longleftrightarrow \quad \mathfrak{D}^{\rho} = -(\mathfrak{D}^{\mathsf{u}})^{\mathsf{T}}, \tag{10}$$

  where we recognize the familiar duality between gradient and divergence operators.

In both cases, all *column* and *row* sums vanish.

The next table gives some examples of the above discretizations, showing the discrete mass fluxes:

	ξ	mass flux $m_{i+1/2}$
Feiereisen [31]; Kok [32]; Kuya [33]	1	$\frac{1}{2}(\rho_{i+1}u_{i+1} + \rho_i u_i)$
Kennedy–Gruber [34]; Pirozzoli [35]; Kuya [33]; Singh [36]	$\frac{1}{2}$	$\frac{1}{4}(\rho_{i+1} + \rho_i)(u_{i+1} + u_i)$
Coppola [19]	0	$\frac{1}{2}(\rho_i u_{i+1} + \rho_{i+1} u_i)$

4.3 Conservation of momentum

The discretizations of the momentum transport equation have the generic form

$$\mathfrak{H} \frac{\mathrm{d}\mathsf{R}\mathsf{\phi}}{\mathrm{d}t} + \mathfrak{C}_{\mathrm{mom}}\mathsf{\phi} = 0, \tag{11}$$

while global conservation boils down to vanishing column sums of the matrix $\mathfrak{C}_{\mathrm{mom}}$. For the various split forms (9), this condition puts constraints on the discretization of the individual terms, as we will now see.

We will study momentum discretizations of the following form

$$\begin{aligned}\mathfrak{C}_{\mathrm{mom}} = \alpha \mathfrak{D}^{\rho\mathsf{u}}\mathsf{R}\mathsf{U} + \beta\big[\mathsf{R}\mathsf{U}\mathfrak{D}^{0} + \mathrm{diag}(\mathfrak{D}^{\rho\mathsf{u}}\mathsf{R}\mathsf{u})\big] + \\ + \gamma\big[\mathsf{U}\mathfrak{D}^{\rho}\mathsf{R} + \mathrm{diag}(\mathsf{R}\mathfrak{D}^{u}\mathsf{u})\big] + \delta\big[\mathsf{R}\mathfrak{D}^{u}\mathsf{U} + \mathrm{diag}(\mathsf{U}\mathfrak{D}^{\rho}\mathsf{\rho})\big].\end{aligned}$$

It is not difficult to see that discrete momentum conservation, i.e. $\mathfrak{C}_{\mathrm{mom}}$ has vanishing column sums, holds if and only if

$$\mathbf{1}^{T}\mathfrak{C}_{\mathrm{mom}} = \mathbf{0} \quad \Leftrightarrow \quad \mathfrak{D}^{0} = -(\mathfrak{D}^{\rho\mathsf{u}})^{\mathsf{T}} \ \wedge\ \mathfrak{D}^{\rho} = -(\mathfrak{D}^{u})^{\mathsf{T}}. \tag{12}$$

The second duality condition we have seen before in Eq. (10) when studying mass conservation of the advective form of mass transport. The duality conditions (12) imply that all four derivative matrices $\mathfrak{D}^{(\cdot)}$ must have vanishing row as well as column sums. But there are no special conditions (yet) on the weights $\alpha,\ \beta,\ \gamma$ and δ.

4.4 Conservation of energy - general

The discrete global evolution of the quadratic invariant kinetic energy in Eq. (6) can be re-formulated as

$$\mathfrak{H}\frac{\mathrm{d}}{\mathrm{d}t}\left(\tfrac{1}{2}\mathsf{R}\Phi\phi\right) = \mathfrak{H}\left(\Phi\frac{\mathrm{d}\mathsf{R}\phi}{\mathrm{d}t} - \tfrac{1}{2}\Phi^2\frac{\mathrm{d}\rho}{\mathrm{d}t}\right) = -\Phi\left(\mathfrak{C}_{\mathrm{mom}} - \tfrac{1}{2}\,\mathrm{diag}(\mathcal{D}_{\mathrm{mass}}\mathsf{m})\right)\phi.$$

As before, iIt follows that discrete global energy conservation is guaranteed if and only if [23,30]

$$\mathfrak{K} \equiv \mathfrak{C}_{\mathrm{mom}} - \tfrac{1}{2}\,\mathrm{diag}(\mathfrak{D}_{\mathrm{mass}}\mathsf{m}) \;\text{ is skew symmetric.} \tag{13}$$

This shows once more that outside its diagonal a discrete convective operator $\mathfrak{C}_{\mathrm{mom}}$ must be skew-symmetric, while at its diagonal a discrete mass transport term $\mathfrak{D}_{\mathrm{mass}}\mathsf{m}$ must be recognized. This will link the mass and momentum fluxes from the mass and momentum equations, respectively, which upto this moment were fully free to choose.

Condition (13) for energy preservation can be rewritten as the vanishing of the symmetric part of $\mathfrak{K}$, which in case of momentum conservation, i.e. $\mathbf{1}^T\mathfrak{C}_{\mathrm{mom}} = \mathbf{0}$, can be regrouped as

$$\mathfrak{C}_{\mathrm{mom}} + \mathfrak{C}_{\mathrm{mom}}^T = \mathrm{diag}(\mathfrak{D}_{\mathrm{mass}}\mathsf{m}) \quad\Rightarrow\quad \mathfrak{D}_{\mathrm{mass}}\mathsf{m} = \mathfrak{C}_{\mathrm{mom}}\mathbf{1}. \tag{14a,b}$$

It shows that the discrete mass equation, including the discrete mass transport, is uniquely defined as soon as the discrete momentum equation is given. Further, $\mathbf{1}^T\mathfrak{D}_{\mathrm{mass}}\mathsf{m} = (\mathbf{1}^T\mathfrak{C}_{\mathrm{mom}})\mathbf{1} = 0$. Thus, for any type of discretization, the combination of momentum and energy conservation implies mass conservation.

4.5 Conservation of energy - split forms

The finite-difference discretization of the general split form (9) leads to an operator $\mathfrak{K}$ given by

$$\begin{aligned}\mathfrak{K} = {} & \alpha\,\mathfrak{D}^{\rho u}\mathsf{R}\mathsf{U} + \beta\,\mathsf{R}\mathsf{U}\mathfrak{D}^{0} + \gamma\,\mathsf{U}\mathfrak{D}^{\rho}\mathsf{R} + \delta\,\mathsf{R}\mathfrak{D}^{u}\mathsf{U} + (\beta - \tfrac{1}{2}\xi)\,\mathrm{diag}(\mathfrak{D}^{\rho u}\mathsf{R}u) \\ & + \left(\gamma - \tfrac{1}{2}(1-\xi)\right)\mathrm{diag}(\mathsf{R}\mathfrak{D}^{u}\mathsf{u}) + \left(\delta - \tfrac{1}{2}(1-\xi)\right)\mathrm{diag}(\mathsf{U}\mathfrak{D}^{\rho}\rho).\end{aligned}$$

The diagonal of $\mathfrak{K}$ vanishes if and only if

$$\alpha = \beta = \tfrac{1}{2}\xi \quad\wedge\quad \gamma = \delta = \tfrac{1}{2}(1-\xi).$$

Outside its diagonal the matrix $\mathfrak{K}$ is skew-symmetric under the familiar duality conditions

$$\mathfrak{D}^{0} = -(\mathfrak{D}^{\rho u})^{\mathsf{T}} \;\wedge\; \mathfrak{D}^{\rho} = -(\mathfrak{D}^{u})^{\mathsf{T}}.$$

We conclude that analytically the energy-preserving split forms form a one-parameter family parametrized by ξ. Moreover, the discrete derivative operators still contain some freedom, as will be explained in Sec. 5.2.

5 Choice of fluxes

5.1 Finite volume

The fluxes in the momentum equation are given by $\boldsymbol{m}\phi$, and choices have to be made how these are constructed from the values in the neighboring grid points. When one chooses $(m\phi) = \frac{1}{2}[(m\phi)_{i+1} + (m\phi)_i]$ then the discretization of the first derivative becomes

$$(m\phi)_{i+1/2} \equiv \tfrac{1}{2}[(m\phi)_i + (m\phi)_{i+1}] \quad \rightarrow \quad h\frac{\partial}{\partial x}(m\phi) \approx (m\phi)_{i+1} - (m\phi)_{i-1},$$

which equals a central-difference discretization. Observe that the convective coefficient matrix has a zero diagonal, hence it can never cancel the mass flux from the mass equation (except in the incompressible case where the convective diagonal should vanish).

An alternative option is to choose

$$(m\phi)_{i+1/2} \equiv m_{i+1/2}\phi_{i+1/2} = \tfrac{1}{2}m_{i+1/2}(\phi_i + \phi_{i+1}) \;\longrightarrow$$
$$h\frac{\partial}{\partial x}(m\phi) \approx \tfrac{1}{2}m_{i+1/2}\phi_{i+1} + \tfrac{1}{2}(m_{i+1/2} - m_{i-1/2})\phi_i - \tfrac{1}{2}m_{i-1/2}\phi_{i-1}.$$

The mass flux $m_{i+1/2}$ is still free, but it is essential that the flux of the transported quantity ϕ is chosen as an equally-weighted interpolation (irrespective of the position of the face):

$$\phi_{i+1/2} = \tfrac{1}{2}(\phi_{i+1} + \phi_i) \quad \longleftrightarrow \quad \boldsymbol{\phi}_f \equiv \tfrac{1}{2}(\mathsf{I} + \mathsf{E})\boldsymbol{\phi}, \tag{15}$$

Only with this choice the convective coefficient matrix becomes skew-symmetric outside its diagonal. At the diagonal we recognize the derivative of the mass flux, and the condition (13) for discrete energy conservation is satisfied.

In matrix-vector notation the convective operator reads

$$\mathfrak{C}^{\mathrm{fv}}_{\mathrm{mom}} = \tfrac{1}{2}(\mathsf{I} - \mathsf{E}^{-1})\mathsf{M}^{\mathrm{fv}}_f(\mathsf{I} + \mathsf{E}) = \tfrac{1}{2}(\mathsf{M}^{\mathrm{fv}}_f\mathsf{E} - \mathsf{E}^{-1}\mathsf{M}^{\mathrm{fv}}_f) + \tfrac{1}{2}\,\mathrm{diag}\big((\mathsf{I} - \mathsf{E}^{-1})\mathsf{m}^{\mathrm{fv}}_f\big),$$

where the first term shows its skew-symmetry, while the second term contains the derivative of the mass fluxes. Indeed, for the above choice (15) of the fluxes, the corresponding operator $\mathfrak{K}$ satisfies the condition (13) for energy preservation. When one pursues higher-order discretization, more complex combinations of m and ϕ in the neighboring grid points are required [21].

As a special case, with the above choice (15), at the face $i+1/2$ the energy flux has the form $\big(\frac{1}{2}\rho u\phi^2\big)_{i+1/2} = \frac{1}{2}m_{i+1/2}\phi_i\phi_{i+1}$. This choice for the kinetic energy flux equals the one used in e.g. [22, Eq. (6)], [37, Section 4.7(1)] and [33, Eqs. (32, 33)].

The mass flux $m_{i\pm1/2} = (\rho u)_{i\pm1/2} \leftrightarrow \mathsf{M}^{\mathrm{fv}}_f$ may be chosen arbitrary without loosing (local and global) discrete energy conservation, as long as it is done consistently over both conservation equations. For two-point fluxes $m_{i+1/2} = (\rho u)_{i+1/2}$, four coefficients of $\rho_{i,i+1}$ and $u_{i,i+1}$ are available, of which flux consistency leaves three degrees of freedom.

Remark All three-point (finite-volume) discretizations conserving mass, momentum and energy fit in the framework

$$\nabla\cdot(\boldsymbol{m}\psi) \;\leftrightarrow\; (\mathsf{I} - \mathsf{E}^{-1})\mathsf{M}^{\mathrm{fv}}_f\boldsymbol{\psi} \quad \text{with} \quad \boldsymbol{\psi} \in \{\mathbf{1},\, \tfrac{1}{2}(\mathsf{I} + \mathsf{E})\boldsymbol{\phi},\, \tfrac{1}{2}\boldsymbol{\Phi}\mathsf{E}\boldsymbol{\phi}\}$$

5.2 Relation between finite-volume and finite-difference discretization

When we restrict ourselves to three-point stencils, it is not difficult to show the relation between energy-preserving split finite-difference discretizations and finite-volume methods.

In Sec.4.3 we have seen that the former form a one-dimensional analytic family, parametrized with ξ. We have also seen that the discretization schemes of the four discrete operators involved, have to satisfy two duality conditions (12), leaving two discrete operators free to choose. For three-point stencils they contain three coefficients each, which have to satisfy two conditions: *i)* as a derivative operator their row sum has to vanish; *ii)* the scaling of the discretization has to be volume-consistent. This leaves one free coefficient per operator (which can be used to give a directionally-biased flavor to the discretization). Hence, the energy-preserving discrete split forms form a three-parameter family.

Further, we have seen in Sec. 5.1 that the three-point finite-volume discretizations form a three-point family (in the choice of the mass flux). As might be expected, these families turn out to be the same, and a mapping (isomorphism) between them can explicitly be written down [21]. Whether all finite-volume discretizations can be written as a finite-difference discretization of a carefully chosen split form (more general than the current ones) is still an open question.

6 CONCLUSIONS

A general framework for supraconservative discretizations of transport equations has been presented, using discrete forms of the equations and assuming exact time integration. It allows a general, abstract study of the conservation properties of the equations, independent of the way in which these equations have been derived, and generalizes many studies on conservative split formulations [19, 20, 33, 35]. The emphasis is on the (primary and secondary) conservation properties of the advective (transport) terms, in particular we focus on kinetic energy.

We have shown that global conservation induces local conservation, corresponding with vanishing column sums of the discrete transport terms. It implies that any globally conservative discretization can be written as a finite-volume method.

For preservation of kinetic energy a necessary and sufficient condition is presented, which relates the discretization of mass transport to the discretization of convection. In particular, with a volume-consistent scaling, the convective coefficient matrix outside its diagonal should be skew-symmetric, whereas at the diagonal the mass flux from mass transport should be present. The flux of the transported quantity should be a $\frac{1}{2}$-$\frac{1}{2}$ interpolation between the adjacent nodes, irrespective of the position of the face. Yet, there is still a large freedom in the mass flux.

Conservation of split forms requires divergence-gradient type duality relations between the discrete differential operators. Skew-symmetric central discretizations satisfy this requirement, and so do dual-sided discretizations [21].

An interesting question, which has hardly been investigated thus far, is for which applications the preservation of (kinetic) energy is the best choice for a secondary invariant, and in which situations it would be advantageous to choose another secondary invariant (like angular momentum, enstrophy, helicity, etc.).

A Matrix-vector notation

Matrix-vector notation is used for a one-dimensional grid, but easily generalizable to more dimensions. Unknowns are represented by grid vectors and diagonal matrices, like

$$\mathsf{R} = \mathrm{diag}(\rho),\ \mathsf{U} = \mathrm{diag}(\mathsf{u}) \text{ and } \Phi = \mathrm{diag}(\phi).$$

The various realizations of the derivative operator $\mathfrak{D}$ are defined in terms of a circulant shift matrix E:

$$\mathsf{E} \equiv \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix} \quad \text{for which} \quad \mathsf{E}^{-1} = \mathsf{E}^{\mathrm{T}} \quad \text{and} \quad \Phi\mathsf{E}^k = \mathsf{E}^k \mathrm{diag}(\mathsf{E}^{-k}\phi) \quad \forall k. \tag{16a-c}$$

With these building blocks, any matrix can be expressed as a weighted sum of powers of E:

$$\mathfrak{D} = \sum_{k=-L}^{L} \mathsf{A}_k \mathsf{E}^k, \quad \text{e.g.} \quad \mathfrak{D}^{\mathrm{central}}\phi \equiv \tfrac{1}{2}(\mathsf{E} - \mathsf{E}^{-1})\phi. \tag{17}$$

The A_k are diagonal matrices $\mathsf{A}_k = \mathrm{diag}(\mathsf{a}_k)$, built from suitably chosen vectors a_k. The components of a_k that are not used are assumed to be zero.

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