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Short note

A general condition for kinetic-energy preserving discretization of flow transport equations

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1. Energy conservation and skew symmetry

The convective term in the (in)compressible flow equations can be written in a variety of analytic formulations. For already half a century, these have been explored as a basis for numerical discretization methods [1–6]. All formulations can be transformed into each other by combining them with the continuity equation (expressing conservation of mass). Thus, analytically, all formulations possess the same invariants. Experience over the years has shown that it can be beneficial for the discretized forms to also possess several of these invariants.

In particular, it appears advantageous to extend the primary (linear) invariants mass and momentum with the secondary (quadratic) invariant kinetic energy. Indeed, often the latter invariant has been added to a (conservative) finite-volume setting [7–15]. But, just as often, it has been introduced in a (non-conservative) finite-difference setting [3–6,16–21], giving the secondary conservation of kinetic energy priority over the primary conservation of mass and momentum. An alternative is to reformulate the equations of motion into so-called square-root variables [22–25] which, in a natural way, conserve both primary and secondary invariants.

As a 'reward', for incompressible flow conserved kinetic energy guarantees stability of the semi-discretized problem without the use of any numerical diffusion. To achieve this requires a close discrete consistency between the convective term and the continuity equation. The present short note will focus on this consistency by studying a simplified form of the general flow equations.

Analytic Consider a conservation law for a quantity ϕ which is transported by a flow with mass density ρ and mass fluxes $\boldsymbol{m}$ (which may be an arbitrary vector field):

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$$\frac{\partial\rho}{\partial t}+\mathcal{D}_{\text{mass}}\boldsymbol{m}\equiv\frac{\partial\rho}{\partial t}+\nabla\boldsymbol{\cdot}\boldsymbol{m}=0\,;\qquad \frac{\partial\rho\phi}{\partial t}+\mathcal{C}^{\boldsymbol{m}}_{\text{mom}}\phi\equiv\frac{\partial\rho\phi}{\partial t}+\nabla\boldsymbol{\cdot}(\boldsymbol{m}\phi)=0\,. \tag{1}$$

It is assumed that these equations hold in a domain with periodic and/or homogeneous boundary conditions, in order not to be bothered by boundary influences. The latter can be handled as in the closely-related summation-by-parts method [26].

The local evolution of 'energy' $\frac{1}{2}\rho\phi^2$ can be inferred from the above equations as

$$\frac{\partial}{\partial t}(\tfrac{1}{2}\rho\phi^2)=\phi\frac{\partial\rho\phi}{\partial t}-\tfrac{1}{2}\phi^2\frac{\partial\rho}{\partial t}=-\phi\,\mathcal{C}^{\boldsymbol{m}}_{\text{mom}}\phi+\tfrac{1}{2}\phi^2 d^{\boldsymbol{m}}_{\text{mass}}\equiv-\phi\mathcal{A}\phi\,, \tag{2}$$

where $d^{\boldsymbol{m}}_{\text{mass}}\equiv\mathcal{D}_{\text{mass}}\boldsymbol{m}$. The operator $\mathcal{A}$ is defined as

$$\mathcal{A}:\phi\mapsto(\mathcal{C}^{\boldsymbol{m}}_{\text{mom}}-\tfrac{1}{2}d^{\boldsymbol{m}}_{\text{mass}})\phi=\nabla\boldsymbol{\cdot}(\boldsymbol{m}\phi)-\tfrac{1}{2}(\nabla\boldsymbol{\cdot}\boldsymbol{m})\phi\,. \tag{3}$$

By integrating the evolution (2) over the whole domain, it immediately follows that energy conservation (integrated left-hand side equal to zero) is equivalent to the skew symmetry of $\mathcal{A}$ (integrated right-hand side equal to zero). As analytically the operator $\mathcal{A}$ indeed is skew-symmetric for all choices of the mass flux $\boldsymbol{m}$, the equations (1) do conserve kinetic energy. This property has been used by Coppola et al. [18,19] to design a large family of kinetic-energy preserving discretizations, based on *analytic* considerations. In contrast, here this issue will be considered from a *discrete* point of view.

Semi-discrete After this analytical introduction, let us proceed with a semi-discretization of equations (1):

$$^h\Omega\frac{\mathrm{d}\rho}{\mathrm{d}t}+{}^hd^{\boldsymbol{m}}_{\text{mass}}=0\,;\qquad {}^h\Omega\frac{\mathrm{d}\rho\phi}{\mathrm{d}t}+{}^hC^{\boldsymbol{m}}_{\text{mom}}\phi=0\,. \tag{4}$$

In a finite-volume setting, $^h\Omega$ is a diagonal matrix containing the sizes of the computational grid cells. Further, $^hd^{\boldsymbol{m}}_{\text{mass}}\equiv{}^hD_{\text{mass}}\boldsymbol{m}$ is a grid vector containing the values of the discrete divergence $\nabla\cdot\boldsymbol{m}$ in the grid points, whereas $^hC^{\boldsymbol{m}}_{\text{mom}}$ is a grid matrix representing the discrete convection operator from (1).

Similar to (2), with the notation from (4), the evolution of discrete energy can be written as

$$^h\Omega\frac{\mathrm{d}}{\mathrm{d}t}(\tfrac{1}{2}\rho\phi^2)={}^h\Omega\left(\phi\frac{\mathrm{d}\rho\phi}{\mathrm{d}t}-\tfrac{1}{2}\phi^2\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)=-\phi\left({}^hC^{\boldsymbol{m}}_{\text{mom}}-\tfrac{1}{2}{}^hd^{\boldsymbol{m}}_{\text{mass}}I\right)\phi, \tag{5}$$

where $^hd^{\boldsymbol{m}}_{\text{mass}}I\equiv\text{diag}({}^hd^{\boldsymbol{m}}_{\text{mass}})$ is a diagonal matrix. The final step is a summation of (5) over all grid cells. In the left-hand side this should result in a discrete approximation of the evolution of the total amount of kinetic energy, i.e. integrated over the whole flow domain. This then determines the scaling in (4): the (possibly non-diagonal) matrix $^h\Omega$ must contain information about the individual grid cell volumes, herewith inducing a discrete norm. We might call such a scaling *volume consistent* [27]. While being natural in a finite-volume setting, it may require some (unusual) scaling when other discretization methods (finite differences, finite elements, ...) are used. After summation, the right-hand side of (5) forms an inner product. When the latter vanishes for all (real) ϕ, the (real) matrix operator involved is skew symmetric. Combining both sides of (5), it can be concluded that with a volume-consistent scaling, the semi-discretization (4) conserves kinetic energy, in the norm induced by $^h\Omega$, if and only if the discrete operator

$$^hA:\phi\mapsto({}^hC^{\boldsymbol{m}}_{\text{mom}}-\tfrac{1}{2}{}^hd^{\boldsymbol{m}}_{\text{mass}}I)\,\phi\quad\text{is skew-symmetric.} \tag{6}$$

As argued above, during the last decades discrete energy conservation has been pursued frequently. Yet, only a few times this condition has been mentioned explicitly [11,12,28]. The important message is that the requirement (6) for discrete energy conservation closely links the discrete operators for momentum and mass conservation. In particular, when the discrete momentum operator has been chosen there is no freedom left for the discretization of the mass operator: it is fixed by the diagonal of the discrete convective term.

The next section will show how this works out when a finite-volume discretization is applied, ensuring that also mass and momentum are conserved discretely. It is left to the interested readers to figure out whether or not a discretization of their favorite analytic form exists which possesses the above property.

2. Example: finite-volume discretization on an unstructured grid

On a (structured or unstructured) collocated grid, as used commonly for compressible flow, all flow variables are defined in nodal points located at 'cell centers', with a liberal interpretation of the meaning of 'center' (centroid, circumcenter, ...); Fig. 1. First, attention is focused to the symmetry properties of the discrete operators, starting with the momentum equation.

With reference to Fig. 1, in a finite-volume method the discrete divergence term in the equation for momentum conservation (4b) can be written as

$$^hC^{\boldsymbol{m}}_{\text{mom}}\,\phi|_C\equiv\sum_{f\in\mathcal{F}_C}(\boldsymbol{m}_f\boldsymbol{\cdot}\boldsymbol{n}_f)\phi_f\,,$$

where the summation is over the faces f of the volume around the node C, together constituting the set $\mathcal{F}_C$. Skew symmetry (6) off and on the diagonal now determines several details.

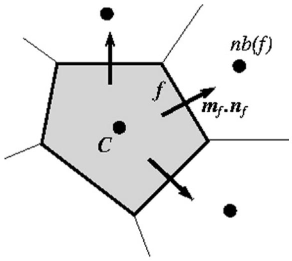

Fig. 1. Unstructured control volume for the conservation equations (1).

Off-diagonal In order for the above expression to be skew-symmetric outside the diagonal, it is necessary that the flux ϕ_f is expressed as a symmetric expression in ϕ_C and $\phi_{nb(f)}$ (here $nb(f)$ denotes the neighboring grid cell sharing the face f). The only way to achieve this is by means of an equal-weighted ($\frac{1}{2}$-$\frac{1}{2}$) interpolation between the adjacent nodal points

$$\phi_f = \tfrac{1}{2}(\phi_C + \phi_{nb(f)})\,.$$

This interpolation has to be used *irrespective of the geometric configuration*.

Diagonal The other requirement concerns the contribution on the diagonal: the coefficient of ϕ_C has to vanish. With the above symmetric interpolation, the diagonal term reads

$$\mathrm{diag}({}^h C^{\boldsymbol{m}}_{\mathrm{mom}})|_C = \tfrac{1}{2} \sum_{f \in \mathcal{F}_C} \boldsymbol{m}_f \cdot \boldsymbol{n}_f\,.$$

The skew-symmetry requirement (6) for the diagonal now fixes the discrete divergence operator ${}^h D_{\mathrm{mass}}$ as

$${}^h D_{\mathrm{mass}} \boldsymbol{m}|_C \equiv {}^h d^{\boldsymbol{m}}_{\mathrm{mass}}|_C = 2\,\mathrm{diag}({}^h C^{\boldsymbol{m}}_{\mathrm{mom}})|_C = \sum_{f \in \mathcal{F}_C} \boldsymbol{m}_f \cdot \boldsymbol{n}_f\,. \tag{7}$$

There is no freedom of choice left, but the outcome for the discrete mass operator is quite natural. Note that the above reasoning holds for any choice of the discrete mass fluxes $\boldsymbol{m}_f$, so the latter choice can be left outside the discussion (and leaves some freedom).

Observe how the grid-independent interpolation is essential, both on and off the diagonal, even when the cell faces are not half-way between the nodal points. Already in 1966, Bryan [29] advocated the use of this interpolation on irregular grids. Fifteen years later, in 1981, Jameson [30] interprets the values in the cell centers as averages over the cells, after which a simple averaging at the separating faces is a natural thing to do. My personal favorite would be a Voronoi grid, where the faces of the control volumes are half-way the nodal points. Then, again an equally-weighted interpolation is found to be natural. It becomes a matter of personal taste which choice of the grid and of the nodal 'cell centers' is preferred. Of course, the precise choice of nodal points and control volumes will effect the global discretization error, but conservation of discrete energy, and the corresponding numerical stability, is guaranteed.

A grid-independent interpolation might seem to lower the formal accuracy of a scheme. However, Manteuffel and White [31] have proven that such a scheme is still formally second-order accurate, as long as during grid refinement the ratio between the largest and the smallest grid cells remains bounded. In practice, this will be the case during most grid-refinement procedures, as explicitly shown by, e.g., Felten and Lund [32] when interpreting their calculations of turbulent flow.

3. Discussion

This short note has presented a necessary and sufficient condition for a semi-discretization of (conservative) flow transport equations to conserve kinetic energy additionally to any primary conserved variables. It has been argued that a consistent link, given by (6), between the discrete continuity equation and the discrete momentum equation is essential, necessitating grid-independent interpolations.

As the calculation of the mass flux $\boldsymbol{m}$ is not relevant for the foregoing discussion, the above reasoning holds for collocated as well as staggered grids. Also, the condition (6) for discrete energy conservation applies for any analytical formulation of the flow equations and any discretization method with volume-consistent scaling. When one also would like to conserve the primary invariants mass and momentum, one additionally has to require that the discretization is equivalent to a conservative one, i.e. it is telescoping like the above-discussed finite-volume method [18]. Such a discretization could be termed *supra-conservative*.

An obvious application is the simulation of (in)compressible flow, where $\phi = \mathbf{u}$ and $\boldsymbol{m} = \rho\mathbf{u}$. Condition (6) then is a generalization of the skew-symmetry requirement that is familiar from incompressible flow. For fluid flow equations, as a further requirement, the pressure gradient should be compatible with the continuity operator according to ${}^h G_{\mathrm{pres}} =$

$-{}^hD^T_{\text{mass}}$ (similar to $\nabla = -(\nabla\cdot)^T$). Shock-capturing schemes, which necessarily require an energy-dissipating mechanism, can be added without interference with the dissipation-free convective discretization. Further, diffusion should not interfere with convection and requires a symmetric negative-definite discretization. Finally, the step towards energy-conserving time integration, indicated by Sanderse [33] for incompressible flow and by Subbareddy and Candler [34] for compressible flow, can readily be added.

Philosophically, this way of discretization is based on non-interference and complementarity: each 'separate' physical ingredient of the flow should remain 'separate' after discretization. Experience over the years in flow simulations, as demonstrated by many of the indicated references, has shown that this discretization philosophy and its corresponding conservation properties is highly valuable for achieving numerical stability and accuracy.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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