# ASYMPTOTICALLY ENTROPY CONSERVATIVE DISCRETIZATION OF CONVECTIVE TERMS IN COMPRESSIBLE EULER EQUATIONS

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## Abstract

A new class of Asymptotically Entropy Conservative schemes is proposed for the numerical simulation of compressible (shock-free) turbulent flows. These schemes consist of a suitable spatial discretization of the convective terms in the Euler equations, which retains at the discrete level many important properties of the continuous formulation, resulting in enhanced reliability and robustness of the overall numerical method. In addition to the Kinetic Energy Preserving property, the formulation guarantees the preservation of pressure equilibrium in the case of uniform pressure and velocity distributions, and arbitrarily reduces the spurious production of entropy. The main feature of the proposed schemes is that, in contrast to existing Entropy Conservative schemes, which are based on the evaluation of costly transcendental functions, they are based on the specification of numerical fluxes involving only algebraic operations, resulting in an efficient and economical procedure. Numerical tests on a highly controlled one-dimensional problem, as well as on more realistic turbulent three-dimensional cases, are shown, together with a cost-efficiency study.

## 1 Introduction

Numerical simulation of turbulent compressible flows is a very active research topic in fluid dynamics and aerospace engineering. The coexistence of several physical phenomena related to compressibility effects (i.e. acoustics, shock waves, etc.) adds tough challenges to the already complex phenomenology of turbulent flows. This reflects not only in a difficulty in the interpretation and understanding of the physical mechanisms but also in the design of accurate and robust numerical methods. The advent of high-performance computing facilities has increased the interest in the numerical investigation of this type of flow, and has pushed the numerical community towards the design of more reliable and fast discretization procedures.

Modern numerical methods for compressible flows are usually required to satisfy some physics-compatible constraints which typically amount to the discrete enforcement of the induced balance of suitably selected secondary quantities.

Kinetic Energy Preserving (KEP) methods are probably the most famous example. They are numerical discretization procedures able to guarantee that the divergence structure of the convective terms in the induced kinetic-energy equation is discretely preserved. KEP methods are well known to improve the robustness of the simulations and have been explored quite extensively in recent years (Coppola et al. (2019a)). The enforcement of the KEP property requires that the mass and momentum equations are discretized in a coordinated manner, without any constraint on the energy equation. As shown in Coppola et al. (2019b), in the context of Finite Difference (FD) methods based on the direct discretization of advective or divergence forms of the convective terms in the Euler equations, KEP schemes can be specified as members of a one-parameter family of locally conservative schemes. This means that one can formulate a locally-conservative, KEP formulation with a certain latitude, which can be used to enforce additional constraints. From the Finite Volume (FV) point of view, for which the method is defined by the specification of numerical fluxes, KEP schemes require a specific form of the momentum flux, leaving the mass flux as a degree of freedom (Jameson (2008) and Veldman (2019)).

Alongside KEP, also Entropy Conservative (EC) schemes have been extensively studied starting from the pioneering papers by Tadmor (1987) and Tadmor (2003). Entropy conservation requires that mass and energy equations are coordinately discretized to induce a conservative structure of the convective terms in the discrete entropy equation; i.e. the overall method can guarantee a correct balance of entropy: an important additional property for both the reliability and robustness of the overall procedure. EC schemes have been almost exclusively introduced in the context of FV methods, and typically require the specification of nonlinear fluxes involving the evaluation of transcendental functions, which are more expensive than the classical algebraic fluxes associated with FD discretizations. Moreover, popular EC fluxes are based on the logarithmic mean of density and internal energy, with additional issues associated with division by zero in the case of uniform spatial distribution of the variables.

Finally, Pressure Equilibrium Preserving (PEP)

discretizations are numerical procedures able to preserve the property that an initial condition with a constant distribution of pressure $p$ and velocity $u$ induces time derivatives $\partial_t p$ and $\partial_t u$ everywhere zero: the evolution of density waves is correctly reproduced by the discretization (Shima et al. (2021) and Ranocha and Gassner (2022)). This last condition can be enforced by treating the convective terms for the energy equation in such a way that the induced discrete pressure equation has in turn convective terms in conservation form.

## 2 Existing KEP schemes

The satisfaction of the conditions required for a numerical scheme to be simultaneously KEP, EC and PEP is quite a difficult task. No method based on a classical FD discretization of the advective or divergence forms of the convective terms is known to exactly satisfy the requirements to be KEP, EC and PEP. When central schemes are adopted, FD discretizations can be expressed as a difference of numerical fluxes, which are based on bilinear or trilinear interpolations (Pirozzoli (2010), Coppola et al. (2019b), and Coppola and Veldman (2023)). Since these formulations cannot satisfy the conditions for KEP, EC and PEP schemes, one should turn to more general nonlinear fluxes.

Among the formulations based on non-algebraic fluxes, the recent scheme by Ranocha and Gassner (2022) is here selected because it is able to satisfy all the required conditions by using the logarithmic mean as an interpolator in the mass and internal energy equations. In fact, it can be expressed by specifying the (two-point, second-order) convective fluxes for mass, momentum, and internal energy as:

$$\begin{aligned} \mathcal{F}_\rho &= \overline{\rho}^{\log}\,\overline{u}, \\ \mathcal{F}_{\rho u} &= \mathcal{F}_\rho\,\overline{u}, \\ \mathcal{F}_{\rho e} &= \mathcal{F}_\rho\,\left[\overline{(1/e)}^{\log}\right]^{-1}, \end{aligned} \tag{1}$$

where the fluxes are expressed in a one-dimensional setting, the three-dimensional extension being obtained by adding analogous contributions along the other directions. In Eq. (1) $\mathcal{F}$ is the 'right' flux $\mathcal{F}^{i+1/2}$, where we assume that in a semidiscretized framework the convective convective evolution of a generic variable $\rho\phi$ at node $x_i$ is governed by the locally conservative 'difference of fluxes' formula $\partial \rho_i \phi_i / \partial t = -\left(\mathcal{F}_{\rho\phi}^{i+1/2} - \mathcal{F}_{\rho\phi}^{i-1/2}\right)/h$. In the specification of the flux functions $\overline{\phi} = (\phi_i + \phi_{i+1})/2$ is the arithmetic mean and $\overline{\phi}^{\log} = \delta\phi_i / \delta \log \phi_i$ is the logarithmic mean, where $\delta\psi_i = \psi_{i+1} - \psi_i$. Density, velocity and pressure are denoted by $\rho, u$ and $p$, respectively, whereas $e$ is the internal energy per unit mass. Perfect gas model is assumed, for which $p = (\gamma - 1)\,\rho e$, where $\gamma = 1.4$ is the ratio of specific heats. The physical entropy is given by $s = \log(p/\rho^\gamma)$.

Note that in Eq. (1) only the convective fluxes are considered. The total flux for momentum should also include a pressure term, which is typically discretized as $\overline{p}$, whereas the internal energy equation has a pressure term in nonconservative form. Moreover, the original version of the Ranocha flux was formulated in terms of fluxes for mass, momentum and total energy, in place of internal energy. However, since the kinetic-energy part of the flux was assumed exactly as the one induced by the discretization of mass and momentum (Coppola and Veldman (2023)), i.e. $\mathcal{F}_{\rho u^2/2} = \mathcal{F}_\rho\, u_i u_{i+1}/2$, for exact time integration the total energy flux can be equivalently formulated as a flux for internal energy (see De Michele and Coppola (2023) for further details).

Eq. (1) will be compared to the more standard KEP scheme formulated by using only arithmetic means:

$$\begin{aligned} \mathcal{F}_\rho &= \overline{\rho}\,\overline{u}, \\ \mathcal{F}_{\rho u} &= \mathcal{F}_\rho\,\overline{u}, \\ \mathcal{F}_{\rho e} &= \mathcal{F}_\rho\,\overline{e}. \end{aligned} \tag{2}$$

This scheme can be obtained as a FD discretization of the fully triple splitting of the convective terms in mass, momentum, and internal energy, as considered by Kennedy and Gruber (2008) and Pirozzoli (2010), and for this reason, it has been termed KGP($\rho e$) in Coppola et al. (2019b). For exact time integration, it can be equivalently expressed as a set of fluxes for mass, momentum and total energy $\rho E$ by using the kinetic-energy convective flux induced by the discretization of mass and momentum, as for the Ranocha flux. In this form it is equivalent to the KEEP scheme by Kuya et al. (2018). The method defined by Eq. (2) has been analyzed in several publications in recent years (Kuya et al. (2018), Coppola et al. (2019b), Tamaki et al. (2022), and De Michele and Coppola (2023)) and is known to exhibit excellent entropy conservation properties, although strictly speaking it is not EC.

The scheme defined by Eq. (2) is also not PEP, and its use in simple density wave tests shows spurious perturbations of the uniform pressure and velocity distributions. An exemplary KEP and PEP scheme is expressed by the fluxes:

$$\begin{aligned} \mathcal{F}_\rho &= \overline{\rho}\,\overline{u}, \\ \mathcal{F}_{\rho u} &= \mathcal{F}_\rho\,\overline{u}, \\ \mathcal{F}_{\rho e} &= \overline{u}\,\overline{\rho e}. \end{aligned} \tag{3}$$

This method is known in the literature (Shima et al. (2021)) as $\text{KEEP}_{\text{PE}}$ and has been proposed as an exemplary PEP (and KEP) method. However, being based on arithmetic means, it is not EC, as can be easily seen in standard test cases (De Michele and Coppola (2023)).

## 3 Numerical efficiency of KEP schemes

| Flux | KEP | PEP | EC | Iter. time (sec) | Rel. Diff. |
|---|---|---|---|---|---|
| Ranocha, (Eq. (1)) | ✓ | ✓ | ✓ | $8.3836 \times 10^{-3}$ | – |
| KGP($\rho e$), (Eq. (2)) | ✓ | × | × | $6.0735 \times 10^{-3}$ | $-27.6\%$ |
| $\text{KEEP}_{\text{PE}}$, (Eq. (3)) | ✓ | ✓ | × | $5.9882 \times 10^{-3}$ | $-28.6\%$ |

Table 1: Conservation properties and performances of the selected schemes

Tab. 1 (first three columns) summarizes the conservation properties of the schemes illustrated in the previous section. It is readily seen that the Ranocha flux is the most complete scheme in terms of structural properties. To the our best knowledge, it is the only scheme possessing KEP, PEP and EC properties, which has also a mass flux that does not depend on pressure (Ranocha and Gassner (2022)). On the other hand, the schemes defined by the fluxes in Eq. (2) and Eq. (3) probably constitute the best performing ones, in terms of robustness and computational burden, within the class of fluxes based on bilinear or trilinear interpolations, which can be also expressed as a classical FD discretizations of the divergence and advective forms of the convective terms.

The nice conservation properties of the Ranocha formulation come with an increased computational cost, due to the evaluation of the logarithmic mean. To quantify this drawback, we implemented the three schemes here considered in the open-source code STREAmS-2 (Bernardini et al. (2023)), which is a GPU parallel, high-order compressible flow solver, and performed a numerical simulation of the inviscid 3D Taylor Green Vortex (TGV) test at Mach number 0.085. The simulation was carried out on a $32^3$ uniform grid with the 6th order version of the spatial fluxes and a classical 4th order Runge-Kutta method (RK4) at CFL = 0.1. Calculations were made on the Marconi100 machine at the Italian CINECA consortium, on which the simulations were performed using one node with 4 GPUs. The performance results are summarized in the last two columns of Tab. 1, from which we infer that the increase in computational cost due to the evaluation of the logarithmic mean is around $28\%$ on the computation of the inviscid part of the solver, as compared to standard formulations.

These results motivate the search for more economical (i.e. based on algebraic operations) formulations which are able to retain the nice conservation properties of the Ranocha flux. This task is accomplished by devising a class of Asymptotically Entropy Conservative (AEC) methods based on algebraic fluxes which, while retaining the classical KEP property, provide a hierarchy of approximations with increasingly accurate entropy-conservative properties. In contrast to existing asymptotic expansions approximating exact EC fluxes (Tamaki et al. (2022)), the proposed approach is able to retain the PEP property at each order of approximation. In line with the methods introduced in Sec. 2, the new method will be formulated by specifying the fluxes for mass, momentum, and internal energy, although it can be equivalently expressed by specifying the total energy flux.

## 4 Specification of AEC numerical fluxes

To overcome the disadvantage of the evaluation of transcendental functions in Eq. (1), it is possible to expand the logarithmic mean of a generic variable $\phi$ in a Taylor series in the small parameter $\delta\phi = \phi_{i+1} - \phi_i$. This approach was already used in Ismail and Roe (2009) to resolve the singularity of the logarithmic mean when uniform distribution of $\phi$ appears. Starting from a different perspective, a similar formulation is obtained also in Tamaki et al. (2022), who propose an asymptotically EC formulation that shares many similarities with the approach used here. However, our formal expansion of the logarithmic mean in density and internal energy fluxes leads to a different formulation, whose first-order approximation involves the *harmonic* mean for $e$ in place of the arithmetic mean.

We start by expressing the difference of logarithms for a generic quantity $\phi$ as

$$\delta \log \phi_i = \log\left(1 + \hat{\phi}_i\right) - \log\left(1 - \hat{\phi}_i\right) \qquad (4)$$

with $\hat{\phi}_i = \delta\phi_i / 2\overline{\phi_i}$. Since the quantity $|\hat{\phi}|$ is always less than one for a positive $\phi$, it is possible to use the Taylor series expansion for the logarithm and obtain

$$\delta \log \phi = \left(\frac{\delta\phi}{\overline{\phi}}\right) \sum_{n=0}^{\infty} \frac{\hat{\phi}^{2n}}{2n+1}. \qquad (5)$$

Applying this substitution to $\delta \log \rho$ and $\delta \log e$ in the logarithmic means $\overline{\rho}^{\log}$ and $\overline{e^{-1}}^{\log} = -(\delta \log e)/(\delta e^{-1})$ in Eq. (1) and truncating the sum to finite $N$, we obtain the class of AEC fluxes

$$\begin{aligned} \mathcal{F}_\rho &= \overline{\rho}\,\overline{u}\left(\sum_{n=0}^{N} \frac{\hat{\rho}^{2n}}{2n+1}\right)^{-1}, \\ \mathcal{F}_{\rho u} &= \mathcal{F}_\rho\,\overline{u}\,, \\ \mathcal{F}_{\rho e} &= \mathcal{F}_\rho\,\overline{e}^{H} \sum_{n=0}^{N} \frac{\hat{e}^{2n}}{2n+1}. \end{aligned} \qquad (6)$$

where $\overline{e}^{H} = e_i e_{i+1}/\overline{e}$ is the *harmonic* mean of $e$. Note that this expansion differs from that adopted by

Tamaki et al. (2022), denoted as KEEP$^{(n)}$, which in our notation reads:

$$\begin{aligned}
\mathcal{F}_\rho &= \overline{\rho}\,\overline{u}\left(\sum_{n=0}^{N}\frac{\hat{\rho}^{2n}}{2n+1}\right)^{-1},\\
\mathcal{F}_{\rho u} &= \mathcal{F}_\rho\,\overline{u}\,,\\
\mathcal{F}_{\rho e} &= \mathcal{F}_\rho\,\overline{e}\left(\sum_{n=0}^{N}\hat{e}^{2n}\right)^{-1}\sum_{n=0}^{N}\frac{\hat{e}^{2n}}{2n+1},
\end{aligned} \tag{7}$$

since the asymptotic expansion is applied to $\delta \log e$ in the internal energy flux, but not to $\delta e^{-1}$. In fact, it leads to the appearance of the harmonic mean in place of the arithmetic mean in the internal energy flux. Eq. (6) reduces to the formulation

$$\begin{aligned}
\mathcal{F}_\rho &= \overline{\rho}\,\overline{u},\\
\mathcal{F}_{\rho u} &= \mathcal{F}_\rho\,\overline{u},\\
\mathcal{F}_{\rho e} &= \mathcal{F}_\rho\,\overline{e}^{H}
\end{aligned} \tag{8}$$

in the first-order case $N = 0$, and to Eq. (1) for $N \to \infty$. One additional property of the class of schemes in Eq. (6) is that it is always PEP, no matter the value of $N$, as long as it is chosen consistently for density and internal energy expansions.

In order for a scheme to be PEP, the conditions on the fluxes are that for constant $u = U$ and $p = P$ the momentum flux (convective plus pressure) reduces to $\mathcal{F}_\rho\,U$ + const (in which the constant is only function of $U$ and $P$) and that the internal energy flux is equal to a constant dependent on only $U$ and $P$ (Ranocha and Gassner (2022)). These conditions are satisfied by our formulation, as it can be easily verified, since $\overline{e}^{H} = P/[(\overline{\rho}\,(\gamma-1)]$ and $\hat{e} = -\hat{\rho}$, so Eq. (6) results in the convective internal energy flux

$$\mathcal{F}_{\rho e} = \frac{UP}{\gamma - 1} \tag{9}$$

which proves the PEP property for the fluxes in Eq. (6). The same condition is not satisfied by the fluxes defined by the formulations in Eq. (2) and (7) which, in fact, are not PEP.

## 5 Numerical results

In this section, two test cases are presented to assess the accuracy and robustness of the proposed formulation and to compare it with existing KEP schemes. In the first test, we consider a 1D steady shock wave case, which allows the evaluation of the entropy-preserving capabilities in the presence of discontinuities. In the second one, we simulate a classical inviscid Taylor-Green vortex to test the proposed fluxes in a three-dimensional case in which an initially smooth flow experiences distortion and instability, with the eventual formation of small unresolved scales.

For the stationary shock wave test, we used the same parameters as in Tamaki et al. (2022). The values

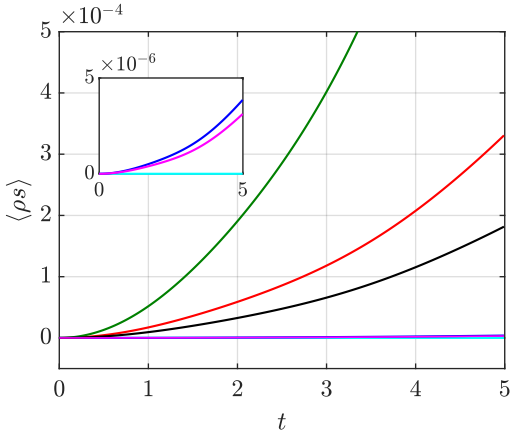


Figure 1: Time evolution of entropy integral for the stationary shock wave for different numerical fluxes. For the meaning of the colors see text.

of $\rho$, $u$ and $p$ upstream and downstream of the wave are derived from the Rankine-Hugoniot relations so that the shock speed is zero. The domain has size $L = 100$ and is discretized with 101 nodes. Periodic boundary conditions have been imposed to avoid the influence of the boundaries on entropy conservation. The schemes are compared by considering the temporal evolution of the quantity $\langle \rho s \rangle$, which is the normalized global entropy production $(\widetilde{\rho s} - \widetilde{\rho_0 s_0})/(\widetilde{\rho_0 s_0})$, with $\rho_0 s_0$ being the initial value and the $\widetilde{\ }$ sign indicating integration over the domain. Figure 1 shows that the scheme defined in Eq. (8) using the harmonic mean (black line) exhibits some improvement in entropy conservation when compared with the KEEP$_{\text{PE}}$ scheme defined in Eq. (2) (green line) and with the KGP($\rho e$) (Eq. (2), red line). The schemes based on asymptotic expansions defined in Eq. (6) and (7) show improved conservation properties, as expected. Even in the case $N = 1$, we observe a marked decrease in spurious entropy production for both AEC$^{(1)}$ (Eq. (6)) and KEEP$^{(1)}$ (Eq. (7)) schemes, denoted with magenta and blue lines, respectively. The EC scheme of Ranocha (Eq. (1)) is also shown, denoted with a cyan line. As expected, it has machine-zero production of entropy.

The second test case has been simulated by implementing the schemes here discussed in the STREAmS-2 code with only some slight modifications on the time integration procedure. We took advantage of the high-order structure of the code to embed the two-point fluxes illustrated in the previous sections in the general procedure to obtain high-order versions of our fluxes. The initial conditions for the Taylor-Green vortex are

$$\begin{aligned}
\rho(x,y,z) &= 1\\
u(x,y,z) &= \sin(x)\cos(y)\cos(z)\\
v(x,y,z) &= -\cos(x)\sin(y)\cos(z)\\
w(x,y,z) &= 0\\
p(x,y,z) &= 10 + \frac{(\cos(2x)+\cos(2y))(\cos(2x)+2)-2}{16}
\end{aligned}$$

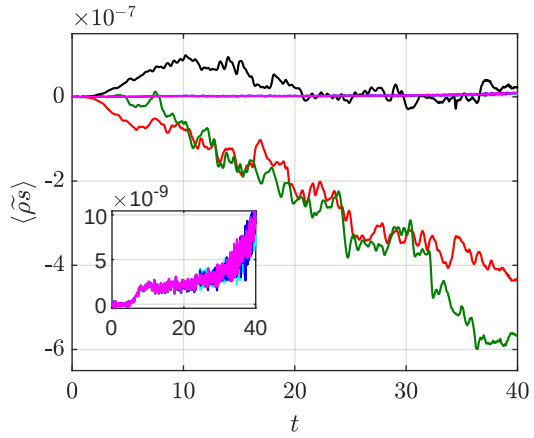


Figure 2: Time evolution of entropy integral for the inviscid Taylor-Green vortex test using different numerical fluxes. For the meaning of the colors see text.

with a pressure value corresponding to a Mach number $M \approx 0.26$. The triperiodic domain has side length $2\pi$ in all directions and is discretized using $32 \times 32 \times 32$ nodes. For the spatial discretization, the 6th-order version of the fluxes is used, whereas for time integration a standard RK4 procedure is used at CFL = 0.1, which is sufficiently small that linear invariants are exactly conserved to machine precision for all schemes. The time evolution of the entropy integral for this test is shown in Fig. 2 and it is in agreement with the previous results. The better performances from the novel scheme based on the harmonic mean of Eq. (8), when compared to $\text{KEEP}_{\text{PE}}$ and $\text{KGP}(\rho e)$ schemes, are more evident in this case. As in the previous test, an improvement can be obtained using an additional term in the expansions and $\text{KEEP}^{(1)}$ and $\text{AEP}^{(1)}$ are the schemes that more closely achieve a constant value for the entropy integral, exhibiting a behavior almost identical to that of the EC Ranocha scheme even for the lowest correction $N = 1$.

## 6 Conclusions

We proposed a new class of asymptotically entropy-preserving fluxes for the discretization of the convective terms in the compressible Euler equations with interesting properties. It provides a consistent asymptotic approximation of an existing entropy-preserving scheme based on the logarithmic mean, and it consists of economical algebraic fluxes based on the harmonic mean. Moreover, at all orders of approximation, the numerical fluxes have the pressure-equilibrium preservation property. The theoretical predictions are confirmed on two test cases, demonstrating good entropy conservation properties even in the presence of discontinuities. It was also shown that the error on entropy can be significantly reduced by using additional terms in the expansion of the AEC fluxes.

These results suggest that AEC fluxes could be good candidates for the discretization of compressible flow equations in high-performance solvers. Due to their algebraic form, they are less computationally expensive than the fluxes based on the logarithmic mean, while retaining many important properties. In fact, they guarantee the KEP and PEP properties, combined with arbitrarily small errors on entropy preservation.

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