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[7-A-01] Kinetic-energy and entropy preserving (KEEP) scheme with logarithmic mean approximations for improved entropy conservation

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Keywords: Non-dissipative schemes , Entropy conservation , Pressure equilibrium, Compressible flows

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Kinetic-energy and entropy preserving (KEEP) scheme with logarithmic mean approximations for improved entropy conservation

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Abstract: This study seeks the logarithmic mean approximations in the numerical fluxes for the kinetic-energy and entropy preserving (KEEP) schemes that enhances the entropy conservation property while maintaining the pressure equilibrium. The present analyses show that the geometric mean serves as a better approximation of the logarithmic mean than other mean values. We propose asymptotic expansions of the logarithmic mean based on the geometric mean, and the improved entropy conservation property of the proposed spatial discretization is validated theoretically and numerically.

Keywords: Non-dissipative schemes, Entropy conservation, Pressure equilibrium, Compressible flows.

1 Introduction

The use of non-dissipative and stable numerical schemes is crucial for high-fidelity flow computations. While the kinetic energy preserving (KEP) schemes [1, 2] are widely recognized as such schemes, the kinetic-energy and entropy preserving (KEEP) schemes [3, 4] have been proposed and significantly improve numerical robustness for compressible flows simulations compared to the KEP schemes.

In addition to the entropy conservation [5, 6], the pressure equilibrium preserving (PEP) [7] is an important flow physics for high robustness of a numerical scheme for compressible flows. In this context, for example, asymptotically entropy conservative (AEC) schemes have been proposed by De Michele & Coppola [8] using the arithmetic and harmonic means for the approximation of the logarithmic mean in the mass and internal-energy fluxes, respectively, so that the derived spatial discretization satisfies the PEP. Their work motivated us to analyze the PEP and entropy conservation properties simultaneously to enhance the entropy conservation property of the KEEP schemes while maintaining the PEP.

The objective of this study is to improve the entropy conservation property of the KEEP schemes by theoretically deriving suitable logarithmic mean approximations while maintaining the PEP property. For this purpose, we investigate the entropy conservation property for different logarithmic mean approximations that satisfies the PEP. Given the results of the present analyses, we propose a new class of the KEEP schemes using asymptotic expansions of the logarithmic mean based on the geometric mean. The present analyses are validated by the numerical experiments for the one-dimensional (1D) density wave advection and for the three-dimensional (3D) compressible inviscid Taylor–Green vortex. More details of the present analyses are presented in Ref. [9].

2 Governing Equations and Spatial Discretization

The governing equations are the following Euler equations for the inviscid compressible flows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p \delta_{ij}}{\partial x_j} = 0, \tag{2}$$

$$\frac{\partial E}{\partial t} + \frac{\partial \rho e u_j}{\partial x_j} + \frac{\partial \rho k u_j}{\partial x_j} + \frac{\partial p u_j}{\partial x_j} = 0, \tag{3}$$

where ρ is the density, u_i is the velocity component in the i direction, p is the static pressure, δ_{ij} is Kronecker's delta, and the total energy E is given by the sum of the kinetic energy ρk and the internal energy ρe, i.e.,

$$E = \rho k + \rho e = \rho \frac{u_i u_i}{2} + \frac{p}{\gamma - 1}, \tag{4}$$

where $\gamma = 1.4$ is the specific heat ratio.

In this study, we consider the governing equations in Eqs. (1)–(3) in the spatially discretized form with half-point numerical fluxes as

$$\left.\frac{\partial \rho}{\partial t}\right|_m = -\mathcal{D}_j|_m(C_j), \tag{5}$$

$$\left.\frac{\partial \rho u_i}{\partial t}\right|_m = -\mathcal{D}_j|_m(M_{ij}) - \mathcal{D}_j|_m(\Pi_{ij}), \tag{6}$$

$$\left.\frac{\partial E}{\partial t}\right|_m = -\mathcal{D}_j|_m(I_j) - \mathcal{D}_j|_m(K_j) - \mathcal{D}_j|_m(P_j), \tag{7}$$

where

$$C_j \equiv \rho u_j, \quad M_{ij} \equiv \rho u_i u_j, \quad \Pi_{ij} \equiv p\delta_{ij}, \tag{8}$$

$$I_j \equiv \rho e u_j, \quad K_j \equiv \rho k u_j, \quad P_j \equiv p u_j. \tag{9}$$

$\mathcal{D}_j|_m$ is a flux-difference operator in the j direction defined as

$$\mathcal{D}_j|_m(F_j) \equiv \frac{F_j|_{m+\frac{1}{2}} - F_j|_{m-\frac{1}{2}}}{\Delta x_j}, \tag{10}$$

where $m \pm 1/2$ denotes the midpoint between grid points m and $m \pm 1$, and F_j is an arbitrary numerical flux in the j direction.

3 Improvement of Entropy Conservation of KEEP Schemes with PEP Property

In this section, the analyses of the PEP and entropy conservation properties of the KEEP schemes presented in Ref. [9] are briefly described.

3.1 Entropy Conservation Error of the KEEP Schemes

According to Tamaki *et al.* [4], the entropy conservation error ε_j of the KEEP schemes are given by the following equation:

$$\varepsilon_j|_{m+\frac{1}{2}} = \left(\frac{1}{e|_{m+1}} - \frac{1}{e|_m}\right) I_j|_{m+\frac{1}{2}} + (\gamma - 1)\left(\rho|_{m+1} - \rho|_m\right) \bar{u}_j|_{m+\frac{1}{2}} + \left(s|_{m+1} - s|_m\right) C_j|_{m+\frac{1}{2}}, \tag{11}$$

where $s \equiv \log p - \gamma \log \rho$ is the entropy, and $\bar{\phi}|_{m+1/2} \equiv \left(\phi|_{m+1} + \phi|_m\right)/2$ is the arithmetic mean. The entropy is exactly conserved if the following mass and internal-energy fluxes are used:

$$C_j|_{m+\frac{1}{2}} = \bar{\rho}^{\log}|_{m+\frac{1}{2}} \bar{u}_j|_{m+\frac{1}{2}}, \tag{12}$$

$$I_j|_{m+\frac{1}{2}} = C_j|_{m+\frac{1}{2}} \left(\overline{1/e}^{\log}|_{m+\frac{1}{2}}\right)^{-1}, \tag{13}$$

where $\bar{(\cdot)}|_{m+1/2}$ is the logarithmic mean defined as

$$\bar{\phi}^{\log}|_{m+\frac{1}{2}} \equiv \frac{\phi|_{m+1} - \phi|_m}{\log \phi|_{m+1} - \log \phi|_m}. \tag{14}$$

Note that the mass and internal-energy fluxes in Eqs. (12) and (13) are consistent with the entropy conservative (EC) fluxes derived by Chandrashekar [10] and Ranocha & Gassner [11]. However, the definition of the logarithmic mean in Eq. (14) needs a local treatment to avoid division by zero, leading to a less straightforward implementation. Thus, some approximations of the logarithmic mean consisting of simple algebraic operations are commonly used. This study considers the following means as the candidates for the logarithmic mean approximation:

1. the arithmetic mean

$$\bar{\phi}^{A}|_{m+\frac{1}{2}} = \bar{\phi}|_{m+\frac{1}{2}} = \frac{\phi|_m + \phi|_{m+1}}{2}, \tag{15}$$

2. the geometric mean

$$\bar{\phi}^{G}|_{m+\frac{1}{2}} \equiv \sqrt{\phi|_m \phi|_{m+1}}, \tag{16}$$

   and

3. the harmonic mean

$$\bar{\phi}^{H}|_{m+\frac{1}{2}} \equiv 2\left(\frac{1}{\phi|_m} + \frac{1}{\phi|_{m+1}}\right)^{-1}. \tag{17}$$

3.2 Logarithmic Mean Approximations with PEP Property

A numerical method preserves the PEP property if an initial condition with constant distributions of pressure and velocity induces their time derivatives everywhere zero: the solution evolves as a density wave. The PEP property of the KEEP schemes can be investigated through the following pressure evolution equation derived by Shima *et al.* [7]:

$$\left.\frac{\partial p}{\partial t}\right|_m = -(\gamma - 1)\mathcal{D}_j|_m(I_j) + p|_m \mathcal{D}_j|_m(u_j). \tag{18}$$

The right-hand side (RHS) of this equation needs to be zero for the PEP property under the initial conditions of constant velocity and pressure. By applying the general PEP condition for approximate EC fluxes derived in Ref. [9], the following combination of mass and internal-energy fluxes, corresponding to each logarithmic mean approximation listed in Sec. 3.1 holds the PEP property:

1. If we use the arithmetic mean for the logarithmic mean approximations,

$$\begin{cases} C_j|_{m+\frac{1}{2}} = \bar{\rho}^{A}|_{m+\frac{1}{2}} \bar{u}_j|_{m+\frac{1}{2}}, \\ I_j|_{m+\frac{1}{2}} = C_j|_{m+\frac{1}{2}} \bar{e}^{H}|_{m+\frac{1}{2}}. \end{cases} \tag{19}$$

   This flux pair is consistent with the AEC$^{(0)}$ scheme proposed by De Michele & Coppola [8].

2. If the geometric mean is used for the logarithmic mean approximations,

$$\begin{cases} C_j|_{m+\frac{1}{2}} = \bar{\rho}^{G}|_{m+\frac{1}{2}} \bar{u}_j|_{m+\frac{1}{2}}, \\ I_j|_{m+\frac{1}{2}} = C_j|_{m+\frac{1}{2}} \bar{e}^{G}|_{m+\frac{1}{2}}. \end{cases} \tag{20}$$

   This flux pair is consistent with the finite-volume method proposed by Rozema *et al.* [12].

3. If the harmonic mean is used for the logarithmic mean approximations,

$$\begin{cases} C_j|_{m+\frac{1}{2}} = \bar{\rho}^{H}|_{m+\frac{1}{2}} \bar{u}_j|_{m+\frac{1}{2}}, \\ I_j|_{m+\frac{1}{2}} = C_j|_{m+\frac{1}{2}} \bar{e}^{A}|_{m+\frac{1}{2}}. \end{cases} \tag{21}$$

3.3 Analysis of Entropy Conservation Error for Different Logarithmic Mean Approximations

To facilitate the discussions below, we introduce the following normalized difference value:

$$\hat{\phi}|_{m+\frac{1}{2}} \equiv \frac{\phi|_{m+1} - \phi|_m}{2\bar{\phi}|_{m+\frac{1}{2}}}. \tag{22}$$

In this section, we briefly present the results of the evaluation of the entropy conservation error for each PEP flux pair derived in Sec. 3.2 in terms of the leading term of the small value of $\hat{\rho}|_{m+1/2}$ and $\hat{e}|_{m+1/2}$. Hereafter, the subscript $(\cdot)|_{m+1/2}$ for the normalized difference is omitted for simplicity.

1. For the flux pair in Eq. (19) based on the arithmetic mean, the leading term of the entropy conservation error is estimated as

$$\varepsilon_j|_{m+\frac{1}{2}} \approx -\frac{2}{3}\bar{\rho}|_{m+\frac{1}{2}}\bar{u}_j|_{m+\frac{1}{2}}\left[(\gamma-1)\hat{\rho}^3 - \hat{e}^3\right]. \tag{23}$$

2. If the flux pair in Eq. (20) based on the geometric mean is used, then

$$\varepsilon_j|_{m+\frac{1}{2}} \approx \frac{1}{3}\bar{\rho}|_{m+\frac{1}{2}}\bar{u}_j|_{m+\frac{1}{2}}\left[(\gamma-1)\hat{\rho}^3 - \hat{e}^3\right]. \tag{24}$$

3. If the flux pair in Eq. (21) based on the harmonic mean is used, then

$$\varepsilon_j|_{m+\frac{1}{2}} \approx -\frac{4}{3}\bar{\rho}|_{m+\frac{1}{2}}\bar{u}_j|_{m+\frac{1}{2}}\left[(\gamma-1)\hat{\rho}^3 - \hat{e}^3\right]. \tag{25}$$

Hence, the flux pair based on the geometric mean induces the smallest entropy conservation error of the candidates considered in this study while retaining the PEP property.

3.4 Proposed Asymptotic Expansion of the Logarithmic Mean Based on the Geometric Mean

The propose asymptotic expansion of the logarithmic mean based on the geometric mean is derived by the similar approach to that based on the arithmetic mean. The asymptotic expansion based on the arithmetic mean [8] is given as:

$$\bar{\rho}^{\log} \approx \bar{\rho}^{A}\left(\sum_{n=0}^{N}\frac{\hat{\rho}^{2n}}{2n+1}\right)^{-1}, \tag{26}$$

$$\left(\overline{1/e}^{\log}\right)^{-1} \approx \bar{e}^{H}\sum_{n=0}^{N}\frac{\hat{e}^{2n}}{2n+1}, \tag{27}$$

where N is the prescribed finite truncation order. These polynomials in Eqs. (26) and (27) can be derived from the ratio of the arithmetic mean to the logarithmic mean and the general PEP condition [9].

A similar approach leads to the asymptotic expansions based on the geometric mean as follows:

$$\begin{aligned}\bar{\rho}^{\log} &= \bar{\rho}^{G}\left\{\left[\sum_{n=0}^{\infty}(-1)^n\binom{1/2}{n}\hat{\rho}^{2n}\right]\sum_{n=0}^{\infty}\frac{\hat{\rho}^{2n}}{2n+1}\right\}^{-1} && (28)\\ &= \bar{\rho}^{G}\left(1-\frac{1}{6}\hat{\rho}^2-\frac{11}{120}\hat{\rho}^4-\dots\right)^{-1}, && (29)\\ \left(\overline{1/e}^{\log}\right)^{-1} &= \left[\sum_{n=0}^{\infty}(-1)^n\binom{1/2}{n}\hat{e}^{2n}\right]\sum_{n=0}^{\infty}\frac{\hat{e}^{2n}}{2n+1} && (30)\\ &= \bar{e}^{G}\left(1-\frac{1}{6}\hat{e}^{2n}-\frac{11}{120}\hat{e}^4-\dots\right). && (31)\end{aligned}$$

Here,

$$\binom{\alpha}{n} \equiv \frac{\alpha(\alpha-1)(\alpha-2)\dots(\alpha-n+1)}{n!}$$

denotes the binomial coefficient.

Considering the present theoretical analyses, a new class of mass and internal-energy fluxes based on the geometric mean is proposed:

$$C_j|_{m+\frac{1}{2}} = \bar{\rho}^G|_{m+\frac{1}{2}} \bar{u}_j|_{m+\frac{1}{2}} \left(1 - \frac{1}{6}\hat{\rho}^2 - \frac{11}{120}\hat{\rho}^4 - \dots\right)^{-1}, \tag{32}$$

$$I_j|_{m+\frac{1}{2}} = C_j|_{m+\frac{1}{2}} \left(1 - \frac{1}{6}\hat{e}^2 - \frac{11}{120}\hat{e}^4 - \dots\right), \tag{33}$$

where the summation are truncated at a finite order N. Combined with the KEEP's numerical fluxes for the momentum, kinetic energy, and pressure terms [3], the proposed spatial discretization is called the KEEP-G$^{(N)}$ scheme.

4 Numerical Experiments

In this section, we compare the PEP and entropy conservation properties of the following numerical schemes: the KEEP$^{(N)}$ [4], the KEEP-PE [7], the AEC$^{(N)}$ [8], and the proposed KEEP-G$^{(N)}$ schemes. The truncation order N for the asymptotic expansions is set to zero and one for each scheme.

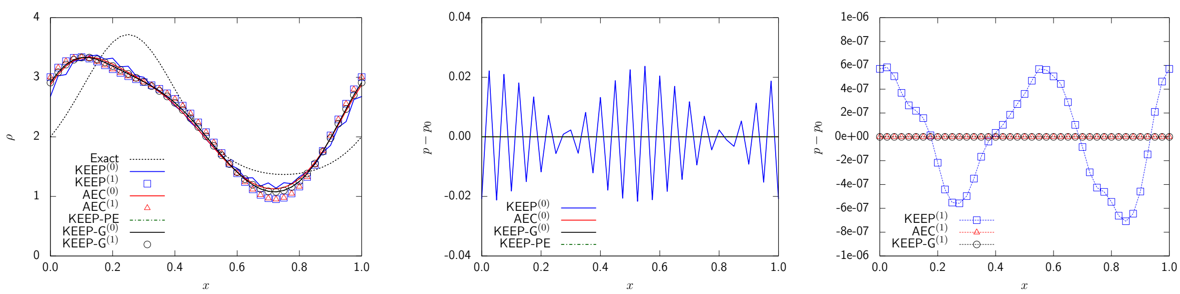
4.1 1D Density Wave Advection

We consider the following initial flow conditions defined in the 1D computational domain $[0, 1]$ with periodic boundary conditions:

$$\rho_0 = 1 + \exp\left[\sin(2\pi x)\right], \quad u_0 = 1, \quad p_0 = 1. \tag{34}$$

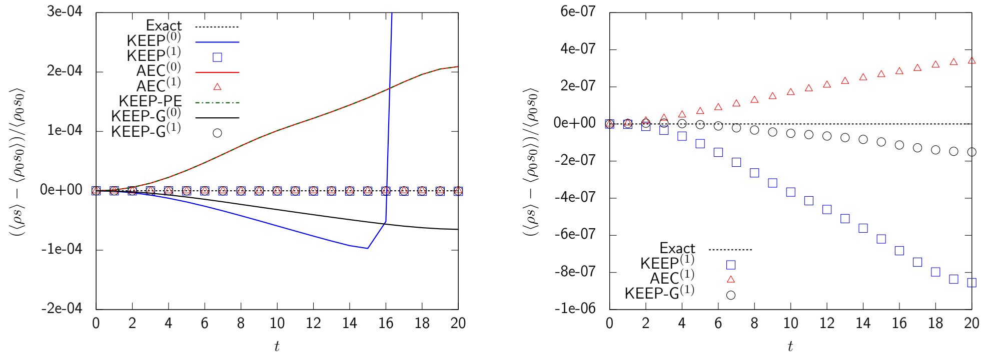
The computation is performed on 61 equidistant grid points, and the classical four-stage fourth-order Runge–Kutta (RK4) scheme is used for the time integration with the Courant-Friedrichs-Lewy (CFL) number approximately 0.01.

The instantaneous distributions of density and pressure error at $t = 13$ are shown in Fig. 1. It is seen that the KEEP-PE, AEC, and proposed schemes maintain the constant pressure distributions to machine precision. Thus, the PEP property of the proposed schemes is numerically demonstrated at each truncation order. From Fig. 2, showing the time histories of the entropy conservation error, it is observed that the KEEP-G schemes achieves the improvement of the entropy conservation property compared to the existing schemes.



(a) Density (b) Pressure error

Figure 1: Instantaneous (a) density and (b) pressure-error distributions at $t = 13$ for the 1D density wave advection.



(a) Overview (b) Close-up view

Figure 2: Time evolution of the entropy conservation error for the 1D density wave advection.

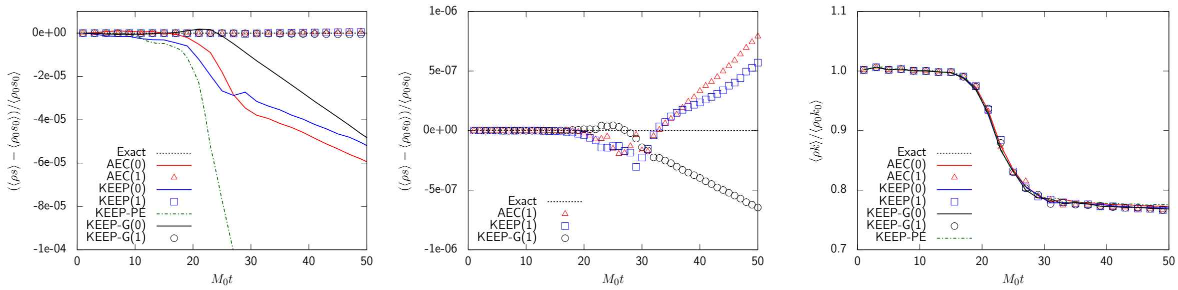
4.2 3D Compressible Inviscid Taylor–Green Vortex

The initial flow conditions for this test are

$$\begin{aligned}
\rho_0 &= 1, \\
u_0 &= M_0 \sin x \cos y \cos z, \\
v_0 &= -M_0 \cos x \sin y \cos z, \\
w_0 &= 0, \\
p_0 &= \gamma^{-1} + \frac{\rho_0 {M_0}^2}{16} \left(\cos 2x + \cos 2y\right) \left(\cos 2z + 2\right),
\end{aligned}$$

where the initial Mach number M_0 is 0.4 so that the compressibility effects are non-negligible. The triperiodic domain has side length 2π in all directions and is discretized using 64^3 equidistant grid points. The RK4 scheme is used for the time integration with the CFL number approximately 0.007.

The time evolution of the entropy conservation error and total kinetic energy is shown in Fig. 3. The histories of the total kinetic energy are comparable for all the schemes investigated in this study. It is seen that the KEEP-G$^{(0)}$ exhibits the better entropy conservation property than the AEC$^{(0)}$ and the KEEP$^{(0)}$, which is consistent with the present theoretical analyses. The entropy conservation property is further enhanced by increasing the truncation order of the asymptotic expansion of the logarithmic mean. It is observed that the deviation of the KEEP-G$^{(1)}$'s history of the entropy conservation error from the exact solution is later than those of the AEC$^{(1)}$ and the KEEP$^{(1)}$. The present numerical experiments demonstrate that the entropy conservation property is improved by the proposed schemes while maintaining the PEP.



(a) Entropy conservation error (b) Total kinetic energy

Figure 3: Time evolution of the (a) entropy conservation error and (b) total kinetic energy for the 3D compressible inviscid Taylor–Green vortex.

5 Conclusions

This study has analyzed the entropy conservation and pressure-equilibrium-preserving (PEP) properties of the kinetic-energy and entropy preserving (KEEP) schemes in the context of the approximation of the logarithmic mean in the mass and internal-energy fluxes. Given the analytical results, a new class of spatial discretization has been proposed using the asymptotic expansion of the logarithmic mean based on the geometric mean. The present theoretical analyses have been demonstrated by the numerical experiments for the one-dimensional density wave advection and for the three-dimensional compressible inviscid Taylor–Green vortex. See Ref. [9] for more details of the present study.

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