On Entropy Conservation and Kinetic Energy Preservation Methods

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Abstract. The Tadmor-type entropy conservative method using the mathematical logarithmic entropy function and two forms of the Sjögreen & Yee entropy conservative methods using the Harten entropy function are examined for their nonlinear stability and accuracy in very long time integration of the Euler equations of compressible gas dynamics. Following the same procedure as Ranocha [6] these entropy conservative methods can be made kinetic energy preserving with minimum added computational effort. The focus of this work is to examine the nonlinear stability and accuracy of these newly introduced high order entropy conserving and kinetic energy preserving methods for very long time integration of selected test cases when compared with their original methods. Computed entropy, and kinetic energy errors for these methods are compared with the Ducros et al. and the Kennedy-Gruber-Pirozzoli skew-symmetric splittings.

1. Motivation and Objective
Numerical methods that are entropy conserving, momentum conserving and kinetic energy preserving are more desirable in computational physics simulations. Not all numerical method constructions possess all three of the properties. There are several constructions/definitions in the literature for a numerical method that preserves kinetic energy (to the order of the semi-discretization of central spatial methods) and conserves momentum. See Coppola et al. [2] for a generalization of the subject with different splittings and forms of the momentum and energy equations for the convection flux derivatives.

In this work we are mainly interested in high order central spatial numerical fluxes that are entropy conservative, and/or momentum conservative, and/or kinetic energy preserving for a standard form of the compressible Euler equations of conservation laws. See [26, 20, 21] for the form of the governing equations. A recent study by Gassner et al. [4] indicated that the design of kinetic energy preserving numerical fluxes by Jameson [8] and Chandraskekar [1] does not preserve kinetic energy. In [6] Ranocha presented analytical insights into kinetic energy preservation. An entropy conservative and kinetic energy preserving numerical flux was proposed by Ranocha for the Tadmor-type entropy conservative method using the mathematical logarithmic entropy function. His new approach to kinetic energy preservation was inspired by the incompressible Euler equations. Summation-by-parts operators were used for the construction of both finite difference and discontinuous Galerkin methods. The work of Ranocha is readily extended to the entropy conservative methods of Sjögreen and Yee [18, 21] using the logarithmic
and Harten entropy functions so that the resulting methods are entropy conserving and kinetic energy preserving. In the numerical test cases Grassner et al. and Ranocha concentrated on discontinuous Galerkin methods in the semi-discretized sense. Ranocha’s kinetic energy preserving construction was shown to improve accuracy over the Jameson numerical fluxes. It is not certain in what manner that the added kinetic energy preserving construction of Ranocha could affect the stability and accuracy of high order central finite difference methods. Here we assume high accuracy time discretizations are used with small time steps to avoid error contributed by non-entropy conserving time integrations.

The objective of this short paper is to examine these methods for two commonly used long time integration test cases. In all of the computations eighth-order central spatial finite difference methods are considered for comparison. No numerical dissipation is added to any of the considered eighth order central methods. Note that without the entropy conserving, or momentum conserving, or kinetic energy preserving numerical fluxes, the original central method is nonlinearly stable for very short time integration without added numerical dissipation. Due to a page limitation, readers are referred to the original papers for the development of the considered methods. Note that a similar formulation carries over for high order dispersion relation preserving (DRP) central finite difference methods. See Sjögreen & Yee [19] for a study. The methods that will be compared in this paper are the following.

- **ECLOG** - The Tadmor-type entropy conservative method (EC) with logarithmic entropy but without the kinetic energy preserving modification (ECLOG) [18].
- **ECLOGKP** - Tadmor-type method with Ranocha’s kinetic energy preserving modification (ECLOGKP) [6].
- **ECBKPKP** - The Tadmor type entropy conservative (EC) method for Harten’s entropy [7] with $\beta = 2$ (ECBKPKP). It turned out that this method in its base form also satisfies Ranocha’s kinetic energy preservation condition; so there is only one variant for this method [18, 6].
- **ES** - The standard entropy conservative split method (ES) with $\beta = 2$. It is an entropy splitting of the convection flux derivatives— a skew-symmetric form as well [26, 20, 21]. See below for the definition of $\beta$. Note that the computed solutions are highly depend on $\beta$. Here we only set $\beta = 2$ based on the study in [21]
- **ESDS** - The entropy conservative split method with Ducros split (DS) used on the conservative portion of the entropy split flux derivatives (ESDS). This is a heuristically split method as it is a partial Ducros et al. split. Both ESDS and ES use $\beta = 2$ [26, 20, 21, 3].
- **DS** - The Ducros et al. splitting of the convection flux derivatives (DS), without kinetic energy preservation [3].
- **DSKP** - The Ducros et al. splitting of the convection flux derivatives with kinetic energy preservation (DSKP) [3, 6].
- **KGS** - The Kennedy-Gruber-Pirozzoli splitting of the convection flux derivative. This is the form that is kinetic energy preserving and that can be written in conservative form using numerical fluxes [9, 11, 2].

For reference purposes the form of the less known entropy conservative split method of Yee et al. and Sjögreen & Yee is briefly describe here. Entropy splitting for the classical central or DRP (dispersion relation-preserving) central schemes in conjunction with summation-by-parts boundary operators are entropy stable in the sense of possessing an energy estimate [10, 5, 26]. See the recent result by [20, 21] for a followon study of the subject. For the Euler equations the inviscid flux derivative $F(u)_x$ for a perfect gas is split into the following via the entropy variables $W$ discussed in Harten [7].
\[ F_x = \frac{\beta}{\beta + 1} F_x + \frac{1}{\beta + 1} F_W W_x, \quad \beta \neq -1 \]  
\[ W = [w_1, w_2, w_3, w_4, w_5]^T = \frac{p^*}{p} [e + \frac{\alpha - 1}{\gamma - 1} p, -\rho u, -\rho v, -\rho w, \rho]^T, \]  
where \[ p^* = -(p^\rho)^{\frac{1}{\alpha + \gamma}} \] and \[ \beta = \frac{\alpha + \gamma}{1 - \gamma}, \quad \alpha > 0 \text{ or } \alpha < -\gamma. \]  
The conserved entropy is \[ E_H = -\frac{\gamma + \alpha}{\gamma - 1} p^s \frac{1}{\alpha + \gamma}, \] with \[ s = p^\rho. \] See Yee et al. [25, 26] for the formulation, the choice for \( \alpha \) and numerical examples.

The entropy (5) is conserved by ES and ECBKP. The methods ECLOG and ECLOGKP instead conserve the entropy \[ E_L = -\frac{1}{\gamma - 1} \rho \log s. \]  

2. Numerical Results

The nonlinear stability and accuracy of the aforementioned eight methods on a 2D isentropic vortex convection and a 3D Taylor-Green vortex test cases by solving the Euler equations of compressible gas dynamics. Both problems are integrated very long in time. The objective is to evaluate how entropy conservation and kinetic energy preservation affect errors from long time integration.

In order to investigate conservation properties numerically, it is therefore desirable that time discretization errors are kept small. The third-order Runge Kutta (RK3) and the classical fourth-order Runge-Kutta (RK4) with small time step to minimize the time discretization error were considered. Of these two methods, RK4 has a larger region of stability than RK3. Preliminary results showed that the superior accuracy of RK4 made it easier to verify conservation properties, hence the comparison here will only show results by RK4. By design all considered high order methods, except the entropy conservative split methods of Yee et al. [26] and Sjögreen & Yee, are conservative methods, and hence, conserve mass, momentum, and total energy. See the original papers for details.

The pure eighth-order standard central method is not stable after a short time integration for both test problems. Results are not shown here.

2.1. Gas Dynamics Test Case for Smooth Flow: 2D Isentropic Vortex Convection

The two-dimensional isentropic vortex convection problem of compressible gas dynamics is a test case to examine the stability and accuracy of numerical methods under long time integration. The challenge with this problem is to maintain stability without losing accuracy. The problem has initial data

\[ \rho(x, y) = ((1 - \frac{(\gamma - 1)b^2}{8\gamma\pi^2})e^{1-r^2})^{\frac{1}{\gamma-1}} \]  
\[ u(x, y) = u_\infty - \frac{b(y - y_0)}{2\pi} e^{(1-r^2)/2} \]  
\[ v(x, y) = v_\infty + \frac{b(x - x_0)}{2\pi} e^{(1-r^2)/2} \]  
\[ p(x, y) = \rho(x, y)^\gamma, \]
where \( r^2 = x^2 + y^2 \), \( b = 5 \), \( \gamma = 1.4 \), \( u_\infty = 1 \), and \( v_\infty = 0 \). The exact solution is the initial data translated, \( u(x,t) = u_0(x - u_\infty t, y - v_\infty t) \). The computational domain is of size \( 0 \leq x \leq 18, 0 \leq y \leq 18 \) with periodic boundary conditions. The center of the vortex is chosen to be \( (x_0, y_0) = (9, 9) \). The computations use a grid with \( 100 \times 100 \) uniformly distributed grid points.

This test case is solved to a final time \( T = 1440 \). This is twice as long as most of our previous studies where end time 720 has been regularly used. The CFL number is set to 0.4, leads to a fairly small time step. The entire integration uses about 80,000 time steps.

Figure 1 shows the kinetic energy and the two entropies as function of time for the eight methods. Also included is the maximum norm of the error to obtain a better idea of the properties of the solutions. Methods KGS, DS, and ESDS blow up before time 300, while the four methods that conserve entropy all run to the final time. However, the methods that do not blow up have very large errors after time 300. Figure 2 shows a close up of the result of Fig. 1.

The results might at first glance appear to be counterintuitive, especially considering that our previous investigation on the same isotropic vortex test case was stable for longer times. One possible explanation is that the current smaller CFL number is now requiring many more time steps with a slightly different time integration path than another larger CFL time step to reach a given time (the previous investigations used CFL=0.8 or 1). We conjecture that the instabilities make the solution grow with the number of time steps, which makes the blow up occur at earlier times as the CFL-number decreases.

The entropies are not perfectly conserved for longer times. The likely explanation is that the poor accuracy for long times makes time discretization error significant. This in turn, destroys the conservation, when entropy conservation holds only for the semi-discrete problem. However, as seen from the zoomed-in plots, the entropy and kinetic energy are very close to being constant, up to the time when the errors become large. This is an improvement that we expected to see with the more accurate time integration.

Note that results by ES and ESDS are highly depend on \( \beta \). Here we set \( \beta = 2 \) based on the study in [21].

2.2. Gas Dynamics Shock-Free Turbulence Test Case – 3D Taylor-Green Vortex

The 3D Taylor-Green vortex problem [24] has been used to evaluate nonlinear stability and accuracy of numerical methods as a shock-free low speed compressible turbulence since it was first proposed in 1937. The problem has smooth and well-resolved initial data. The size of the spatial scales in the flow field decreases as time evolves. This test case gives a good way to assess how well a numerical scheme handles the small scales that appear in the solution. The influence of numerical dissipation is very visible in some quantities, such as the total enstrophy, as the flow evolves in time. For previous studies on coarse grid computations of some of the considered methods comparing with a fine grid DNS solutions, see Sjögren and Yee [18, 21].

The present discussion of numerical results is confined to a coarse grid DNS comparison among methods. It is noted that for this Taylor-Green inviscid problem, small scales are generated that eventually cause large errors in the solution due to inadequate resolution. This probably occurring around \( T = 5 \). Another issue is that for very low dissipative or non-dissipative numerical methods for the simulation of turbulent flows, even with extreme grid refinement, grid convergence cannot be obtained as the original inviscid Euler equations are chaotic in nature. With sufficient but not excess numerical dissipations, than one is solving the equivalent of a Navier-Stokes equations. See Yee & Sjögren [27] for a study.

The same RK4 time discretization and CFL number 0.4 are used here. The end time is 20 instead of the standard end time 10 to observe the solution behavior a twice as long. The 3D Euler equations of compressible gas dynamics are solved with \( \gamma = 5/3 \). The computational domain is a cube with side
Figure 1. Inviscid 2D compressible vortex convection with $100^2$ grid points: Comparison of kinetic energy, entropy $E_H$, maximum-norm of error, and entropy $E_L$ vs. time for the 8 methods.

length $2\pi$. The computation is made on a uniform grid with $64^3$ grid points and initial data

$$
\rho = 1, \quad p = 100 + \{(\cos(2z) + 2)(\cos(2x) + \cos(2y)) - 2\}/16
$$

(11)

$$
u = \sin x \cos y \cos z, \quad v = -\cos x \sin y \cos z, \quad w = 0,
$$

(12)

with periodic boundary conditions in all three directions.

Note that for such a coarse grid DNS computations

Figure 3 shows the enstrophy vs. time to end time 20. It is interesting to see the behavior of doubling the time integration duration. Figure 4 shows the comparison of kinetic energy, entropy $E_H$, maximum-norm of error, and entropy $E_L$ vs. time for the eight methods. Figure 5 shows the zoomed in result of Fig. 4.

Method ESDS becomes unstable at around time 6, and method DSKP becomes unstable around time 7. All other schemes ran to completion. The kinetic energy and entropy results show the quantity with its value at time zero subtracted, e.g. e.g. the kinetic energy ($E_{kin}(t)$) shown is $E_{kin}(t) - E_{kin}(0)$. The ES method starts to lose some energy at a later time. Otherwise the stable results are similar. ECLOGKP and KGS are indistinguishable, and fall on top of each other in the zoomed in figure. One surprising result is that method ECBKP is expected to preserve kinetic energy in the same manner does not. The
Figure 2. Inviscid 2D compressible vortex convection with $100^2$ grid points: Comparison of kinetic energy, entropy $E_H$, maximum-norm of error, and entropy $E_L$ vs. time for the 8 methods. Zoom of Fig. 1.

other stable methods are a little off, but it is only visible in the closeup. Methods ES and ECBKP fall on top of each other, as we would expect, since these two schemes conserve the entropy in a discretized sense. Method ECLOGKP is also on top of ES and ECBKP, making it hard to visualize the differences in the results.

In the logarithmic entropy function comparison method ES deviates a little bit more at later time. This is not expected as it conserves Harten’s entropy almost perfectly. Methods ECLOGKP and ECLOG conserve entropy as illustrated in the figure where their solutions are on top of each other. Overall, ECLOGKP, ECLOG, ECBKP, KGS, and DS are very similar, one has to zoom in very much on the plots to see any differences for this test case. However, differences might be larger for other flow problems. As can be seen, for this test case, method ES behaves somewhat different. DSKP and ESDS are not performing well. It is noted again that results by ES and ESDS are highly depend on $\beta$. Here we set $\beta = 2$ based on the study in [21]
3. Summary

For the two considered 2D smooth flow and 3D shock free turbulent test cases, all four methods that conserve an spatial entropy (ECLOG, ECLOGKP, ECBKP, and ES), ran to completion without blowing up using RK4 and CFL=0.4. The heuristically split methods (DS, DSKP, KGS, and ESDC with $\beta = 2$), showed more varied behavior, with ESDS and DSKP being stable for one problem but not the other. These experiments indicate that entropy conservation provides stability improvement, but the kinetic energy preservation property is not directly correlated with stability. It should be stressed, that the results were obtained using a fairly small time step.

Although all four methods ESDS, KGS, DS, and DSKP fail on the isentropic vortex problem, DS and DSKP are both competitive with the entropy conserving methods. This is due to the fact that at the time at which these methods fail, the entropy conserving schemes are already losing their accuracy. It is of questionable value to be able to run the computation to very long times, if all accuracy is lost at an earlier time. It is noted that method KGS performed very well for the Taylor-Green vortex, but blew up on the isentropic vortex problem. The results confirm that nonlinear stability is very problem dependent when dealing with coupled nonlinear systems of equations. One idea to fully investigate the nonlinear stability would be to run with completely random initial data. This way all modes would be present initially. This would cause any unstable mode to show up directly.

Moreover, the aforementioned solution behavior of the eight different spatial discretizations are based on the RK4 time discretization with CFL=0.4. The solution behavior by ES and ESDS are only for $\beta = 2$. Performance of these spatial methods would be different using a different CFL for RK4 or a different time discretization.

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Figure 4. Inviscid 3D Taylor-Green Vortex with $64^3$ grid points: Comparison of kinetic energy, entropy $E_H$, maximum-norm of error, and entropy $E_L$ vs. time for the 8 methods.
Figure 5. Inviscid 3D Taylor-Green Vortex with $64^3$ grid points: Comparison of kinetic energy, entropy $E_H$, maximum-norm of error, and entropy $E_L$ vs. time for the 8 methods. Zoom of Fig. 4.
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