Oral presentation | Higher order methods

Higher order methods-I

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[3-C-01] Stable and non-dissipative flux reconstruction schemes using Gauss-Legendre points with kinetic energy and entropy preservation (KEEP) property

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Stable and non-dissipative flux reconstruction schemes using Gauss-Legendre points with kinetic energy and entropy preservation (KEEP) property

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Abstract: Kinetic energy and entropy preserving (KEEP) high-order flux-reconstruction (FR) schemes using Gauss-Legendre points are constructed for the compressible Euler equations. To improve conservation of primary and secondary conserved quantities (i.e., kinetic energy and entropy), the proposed KEEP-FR schemes adopt the new form of flux polynomials, derived for split form of derivatives. The robustness of the proposed schemes is examined through the inviscid Taylor-Green vortex test is conducted. The proposed schemes significantly improve the stability compared to the existing FR schemes using Gauss-Lobatto points which satisfy the kinetic energy preservation property.

Keywords: High-order method, Flux reconstruction method, Non-dissipative scheme, Kinetic-energy and entropy preservation.

1 Introduction

To achieve high-fidelity computations for turbulent flows, non-dissipative schemes and high-order accuracy are demanded. Recently, high-order methods such as discontinuous Galerkin (DG) [1] and flux-reconstruction (FR) [2] methods are getting attention for solving compressible Navior-Stokes equations becuase of their ability to achieve high-order accuracy while remaining its compactness of data structures, which is appropriate for the massive parallel computing using accelerators such as graphic processing unit (GPU). However, it is known that these high-order schemes have a crucial stability problem, and the upwind type Rieman solver is employed to evaluate flux at the boundary, which may introduce substantial numerical dissipation, therefore, non-dissipative high-order schemes are demanded.

In order to improve the stability of non-dissipative high-order schemes, recently, Gassner [3] has introduced a kinetic energy preserving (KEP) DG method with the Gauss–Lobatto points, and more recently, Abe et al. [4] extended the KEP DG scheme to the FR method in split forms based on the Gauss-Lobatto points (KEP-FR-Lobatto). It is known that satisfying kinetic energy preservation properties is important to conduct stable simulations with non-dissipative nature [5, 6, 7, 8, 9, 10, 11]. However, the high-order schemes that satisfy the KEP property using the Gauss-Lobatto nodes tend to be unstable especially for the compressible flows. To further improve the numerical stability of KEP schemes, Kuya et al. [12] has attempted to enhance the preservation of entropy while retaining KEP property (i.e., kinetic energy and entropy preservation (KEEP) property) in finite difference method [13, 14, 15]. In this study, we first extend the KEP-FR-Lobatto proposed by Abe et al. [4] to the FR schemes with KEEP property based on Gauss-Lobatto points (KEEP-FR-Lobatto). However, the schemes are still unstable for the compressible flow simulations. The cause of this numerical instability is that the integration by Gauss-Lobatto quadrature does not guarantee the exact integration when the KEP is considered. This problem of the quadrature rule can be solved by using the Gauss-Legendre points instead of the Gauss-Lobatto points because they can exactly integrate higher degree polynomials. Unlike the Gauss-Lobatto points, the Gauss-Legendre points do not include the grid boundary, therefore, to satisfy the conservation of primary conserved quantities as well as secondary ones such as kinetic energy and entropy on the Gauss-Legendre points, a new form of the flux polynomial is proposed in this study. For the detail derivation of formulations for the proposed schemes and the proof of conservation of the primary and the secondary conserved physical quantities, the reader is referred to [16].

2 Numerical method

2.1 Flux reconstruction method

Consider the one-dimensional conservation law:

$$\frac{\partial Q}{\partial t} + \frac{\partial U}{\partial x} = 0, \tag{1}$$

where Q represents the conservative variable and U represents the flux. Let the computational domain be divided by M cells or elements E_m, $m = 1, 2, 3, ..., M$. Instead of dealing with elements in global coordinates, E_m, it is convenient to use elements in local coordinates, $\Omega = [-1, 1]$. With ξ varing on Ω,

$$\xi(x) = 2(x - x_m)/\Delta x_m, \tag{2}$$

where x_m represents the center of E_m, and Δx_m represents the width of E_m. The solution Q is approximated by element-wise Lagrange interpolated polynomials of degree K, $Q_m(\xi)$, with no continuity requirement. The main task of FR method is to construct a flux polynomial $U_m(\xi)$ to define the spatial derivatives of the flux at solution points. Eq. (1) is transformed from the global coordinate to the local coordinate by using the derivative of Eq. (2) $\frac{d\xi}{dx}$, as

$$\frac{\Delta x_m}{2}\frac{\partial Q_m(\xi)}{\partial t} + \frac{\partial U_m(\xi)}{\partial \xi} = 0 \tag{3}$$

In order to derive the flux polynomial $U_m(\xi)$, the FR method introduces the solution point ξ_p and the Lagrange interpolated polynomials are constructed from discrete physical quantities at $(K + 1)$ solution points, $U_{m,p}$. Let the Lagrange basis function in Ω be l_p,

$$l_p(\xi) = \prod_{s=0,s\neq p}^{K} \frac{\xi - \xi_s}{\xi_p - \xi_s}, \tag{4}$$

then Kth order Lagrange interpolated polynomials based on physical quantity, ϕ, at the solution points can be written as

$$[\phi]_m(\xi) = \sum_{p=0}^{K} \phi_{m,p} l_p(\xi), \tag{5}$$

where $\phi_{m,p}$ is arbitrary physical quantity at solution point ξ_p in the mth cell. Note that in this paper, the notation of $[\,\cdot\,]_m(\xi)$ means the cell-wise Lagrange interpolation in the mth cell. For simplicity, $[\,\cdot\,]_m(\xi)$ abbreviate to $[\,\cdot\,]_m$ in the rest of this paper. According to Eq. (5), the discontinuous flux polynomials and the solution polynomials are defined:

$$[U]_m = \sum_{p=0}^{K} U_{m,p} l_p(\xi), \qquad [Q]_m = \sum_{p=0}^{K} Q_{m,p} l_p(\xi). \tag{6}$$

Due to the lack of information from the adjacent cell, the flux polynomials constructed by the cell-wise Lagrange interpolation (discontinuous flux polynomials) become discontinuous at the grid boundaries, however, to ensure the conservation of physical quantities, the flux polynomial $U_m(\xi)$ at the boundary must be common. To this end, the upwind-type Riemann flux, found in a finite volume method, is introduced at each interface as a common flux in the general FR framework. Then the discontinuous flux polynomial is modified by using the gap between the common flux and the value at the boundaries with correction polynomials. Therefore, the continuous flux polynomial is,

$$U_m(\xi) = U_m^{\text{modified}}(\xi) = [U]_m + \left\{\widetilde{U}_{m-\frac{1}{2}} - [U]_m(-1)\right\} g_L(\xi) + \left\{\widetilde{U}_{m+\frac{1}{2}} - [U]_m(1)\right\} g_R(\xi), \tag{7}$$

where $[U]_m(\xi)$ is the Lagrange interpolated (discontinuous flux) polynomial, $\widetilde{U}_{m\pm 1/2}$ are the common fluxes at right and left interfaces, $[U](-1)$ is the left boundary value of the discontinuous flux polynomials, $[U](1)$ is the right boundary value of the discontinuous flux polynomials, g_L is the left correction polynomial, and g_R is the right correction polynomial. Here, the left and right correction polynomials,

g_L and g_R, are degree $K+1$ and must satisfy,

$$g_L(-1) = 1, \quad g_L(1) = 0, \tag{8}$$

and

$$g_R(\xi) = g_L(-\xi). \tag{9}$$

For the boundary values, the following notation is used in this paper:

$$[U]_m(-1) = [U]^R_{m-1/2}, \qquad [U]_m(1) = [U]^L_{m+1/2}. \tag{10}$$

Now the continuous flux polynomial is constructed, thus, the discrete spacial derivative equation at each solution point is defined by taking analytical differentiation of Eq. (7):

$$\begin{aligned} \left.\frac{\partial U_m(\xi)}{\partial \xi}\right|_{\xi_p} &= \left.\frac{\partial U_m^{\text{modified}}(\xi)}{\partial \xi}\right|_{\xi_p} \\ &= \underbrace{\left.\frac{[U]_m}{\partial \xi}\right|_{\xi_p}}_{\text{Discontinuous flux term}} \underbrace{+ \left\{\widetilde{U}_{m-\frac{1}{2}} - [U]^R_{m-1/2}\right\} \left.\frac{dg_L(\xi)}{d\xi}\right|_{\xi_p} + \left\{\widetilde{U}_{m+\frac{1}{2}} - [U]^L_{m+1/2}\right\} \left.\frac{dg_R(\xi)}{d\xi}\right|_{\xi_p}}_{\text{Correction term}}, \end{aligned} \tag{11}$$

where $[\ \cdot\ ]|_{\xi_p}$ represents values at the solution points. The derivative of the discontinuous flux polynomial and the correction polynomial are called the discontinuous flux term and the correction term, respectively. Finally, the physical quantity in the next time step at the solution points can be solved explicitly by time discretization schemes.

2.2 Proposed KEEP-FR scheme

In order to numerically improve the conservation of secondary conserved physical quantities, the split forms are introduced in some studies of the finite volume and finite difference methods. In the proposed scheme, the idea of the split form is extended to the FR framework. The spatial derivative for arbitrary functions of $a(x)$ and $b(x)$ can be written in the divergence and two-part split forms by using the product rule,

$$(\text{Divergence}) \quad \frac{\partial ab}{\partial x}, \tag{12}$$

$$(\text{Two}-\text{part split}) \quad a\frac{\partial b}{\partial x} + b\frac{\partial a}{\partial x}. \tag{13}$$

Among various split forms introduced in the finite volume and finite difference method, many of which achieves the preservation of the primary and secondary conserved physical quantity are constructed by the combination of the two-pair split forms. To use the idea of split form, instead of using the general FR framework shown in Eq. (7), which is only able to reflect the divergence form, we propose a new form of flux polynomial:

$$\begin{aligned} ab_m(\xi) &= [a]_m[b]_m + [a]_m[b]^*_m + [a]^*_m[b]_m \\ [a]^*_m &= \left[\widetilde{a}_{m-\frac{1}{2}} - [a]^R_{m-\frac{1}{2}}\right] g_L + \left[\widetilde{a}_{m+\frac{1}{2}} - [a]^L_{m+\frac{1}{2}}\right] g_R. \end{aligned} \tag{14}$$

Since the Gauss-Legendre points do not locate at grid boundaries, when the split form is adapted in the discontinuous flux polynomials $[a]_m[b]_m$, a new form of the correction terms is required to construct continuous flux polynomials as in Eq. (14). The general FR scheme employs constant common fluxes and correction polynomials for the modification of the discontinuous flux polynomial as in Eq. (7). Unlike the general flux polynomial, the proposed flux polynomials adopt the $2K$th order polynomials $[a]_m[b]_m$ (the multiplication of two Kth order Lagrange interpolated polynomials) for discontinuous flux terms, and the $2K+1$th order polynomials such as $[a]_m g_L(\xi)$ (the multiplication of Kth order Lagrange interpolated polynomials and $K+1$th order correction polynomials) for correction terms as in Eq. (14). For the fluxes at the boundaries, $\widetilde{\phi}$, we use arithmetic mean of adjacent boundary values,

$$\widetilde{\phi}_{m\pm\frac{1}{2}} = \frac{[\phi]^R_{m\pm\frac{1}{2}} + [\phi]^L_{m\pm\frac{1}{2}}}{2}, \tag{15}$$

giving central-type (non-dissipative) fluxes. Since the new form of continuous flux polynomials is constructed, the spacial derivative can be defined by the analytical differentiation of the continuous flux polynomials. By using the product rule, the spacial derivative of Eq. (14) yields extra terms, that do not appear in the conventional FR framework, as

$$\begin{aligned}\frac{\partial ab_m(\xi)}{\partial \xi} d\xi &= \frac{\partial\left([a]_m[b]_m + [a]_m[b]^*_m + [a]^*_m[b]_m\right)}{\partial \xi} \\ &= [a]_m\frac{\partial [b]_m}{\partial \xi} + \frac{\partial [a]_m}{\partial \xi}[b]_m + [a]_m\frac{\partial [b]^*_m}{\partial \xi} + \frac{\partial [a]^*_m}{\partial \xi}[b]_m + \underbrace{\frac{\partial [a]_m}{\partial \xi}[b]^*_m + [a]^*_m\frac{\partial [b]_m}{\partial \xi}}_{\text{Extra terms}}.\end{aligned} \tag{16}$$

In terms of the conservation, the extra terms does not have any effect if and only if the Gauss-Legendre points and the right Radau polynomial are adopted as the solution points and the left correction polynomial. Hereby, in this study, the discrete spatial derivatives at each solution point are defined:

$$\left.\frac{\partial ab_m(\xi)}{\partial \xi}\right|_{\xi_p} = [a]_m|_{\xi_p}\left.\frac{\partial [b]_m}{\partial \xi}\right|_{\xi_p} + \left.\frac{\partial [a]_m}{\partial \xi}\right|_{\xi_p}[b]_m|_{\xi_p} + [a]_m|_{\xi_p}\left.\frac{\partial [b]^*_m}{\partial \xi}\right|_{\xi_p} + \left.\frac{\partial [a]^*_m}{\partial \xi}\right|_{\xi_p}[b]_m|_{\xi_p}. \tag{17}$$

Since $[a]^{\text{modified}}_m = [a]_m + [a]^*_m$, where $[a]^{\text{modified}}_m$ is defined by the conventional FR framework as Eq. (11), Eq. (17) can be simplified as

$$\left.\frac{\partial ab_m(\xi)}{\partial \xi}\right|_{\xi_p} = [a]_m|_{\xi_p}\left.\frac{\partial [b]^{\text{modified}}}{\partial \xi}\right|_{\xi_p} + [b]_m|_{\xi_p}\left.\frac{\partial [a]^{\text{modified}}}{\partial \xi}\right|_{\xi_p}. \tag{18}$$

Eq. (18) becomes a similar form as the two-pair split as shown in Eq. (13). Therefore, the split forms constructed by the combination of the two-pair split forms can be represented in the FR framework. A specific split form, which improves the KEEP property given by Kuya [12], is investigated in this study.

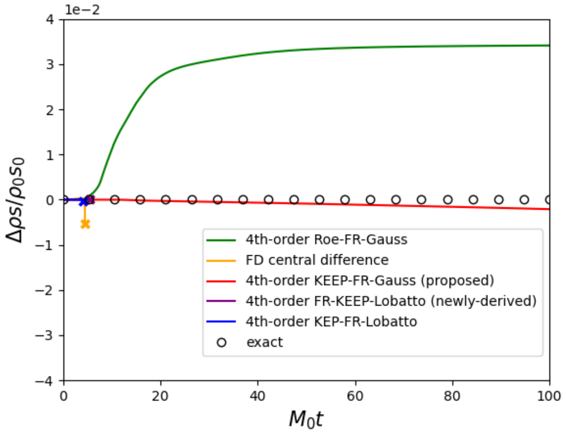
3 Numerical test

The numerical stability and conservation property of the proposed KEEP-FR schemes are evaluated by the inviscid Taylor-Green vortex test. In this test, vortices get smaller and smaller in time and thus eventually become unresolved. Therefore, this test reveals the numerical stability of schemes in practical turbulent simulations where grid size resolution is not always sufficient. The initial flow conditions of the inviscid Taylor-Green vortex are given by

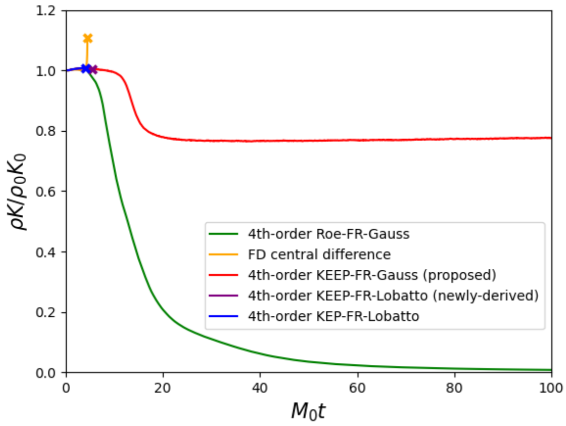
$$\begin{cases} \rho = \rho_0, \\ u = M_0 \sin(x)\cos(y)\cos(z), \\ v = -M_0\cos(x)\sin(y)\cos(z), \\ w = 0, \\ p = \dfrac{1}{\gamma} + \dfrac{\rho_0 M_0^2}{16}\left[\cos(2x) + \cos(2y)\right]\left[\cos(2z) + 2\right], \end{cases} \tag{19}$$

where the initial density and Mach number are set to $\rho_0 = 1.0$ and $M_0 = 0.4$. For the time marching, the four-stage fourth-order Runge-Kutta scheme is used. As a reference, the results obtained by the existing 4th-order KEP-FR-Lobatto scheme, finite difference 2nd-order central difference scheme, 4th-order general FR scheme in Eq. (11) with Roe common flux based on the Gauss-Legendre points (Roe-FR-Gauss), and newly-derived 4th-order KEEP-FR-Lobatto are compared. The computational domain is a $[0, 2\pi]^3$ periodic box with 64 degree of freedom (16 cells $\times$ 4 solution points for the FR scheme, and 64 cells for the finite difference scheme).

Figure 1 shows the time evolution of the total kinetic energy and total entropy conservation error. The total kinetic energy decreases in any cases due to the compressibility effect. The proposed KEEP-FR scheme using the Gauss-Legendre points achieves the stable computation by preserving the entropy



(a) Total entropy error



(b) Total kinetic energy

Figure 1: Time evolution of (a) total entropy error and (b) total kinetic energy.

well. In contrast, the existing 4th-order KEP-FR-Lobatto has become unstable at the early stage of the computation, and the stability of this scheme is about the same as the finite difference 2nd-order central difference scheme, which is known as an unstable scheme. The newly-derived 4th-order KEEP-FR-Lobatto scheme slightly improved the stability compared to 4th-order KEP-FR-Lobatto, however, it is not sufficient to conduct the compressible flow simulations stably. The 4th-order Roe-FR-Gauss scheme shows the stable computation, however the kinetic energy drops and the entropy increases non-physically due to the numerical dissipation.

4 Conclusion and Future Work

To satisfy the primary conservation as well as kinetic energy and entropy preserving (KEEP) property, the new form of flux polynomials based on Gauss-Legendre points that can reflect the idea of split form is proposed. The proposed flux polynomial can be extended to many forms of split forms constructed by the combination of the two-pair split forms developed in the finite difference and finite volume methods. In this study, the split form which satisfies KEEP property is investigated. We discuss more detail about the derivation of formulation for proposed schemes, and the proof of conservation of primary and secondary conserved physical quantity in [16]. The proposed scheme achieves superior numerical stability in the inviscid Taylor-Green vortex test, which has never been achieved in central-type FR schemes. The extension of the proposed scheme to the Navior-Stokes equation to achieve high-fidelity compressible turbulent flow simulations is in progress.

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