Two-Stage Fourth-order Gas-kinetic Scheme for Three-dimensional Euler and Navier-Stokes Solutions

Liang Pan\textsuperscript{a} and Kun Xu\textsuperscript{b}

\textsuperscript{a}School of Mathematical Sciences, Beijing Normal University, Beijing 100875, China; \textsuperscript{b}Department of Mathematics and Department of Mechanical and Aerospace Engineering, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

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\textbf{ABSTRACT}
For the one-stage third-order gas-kinetic scheme (GKS), successful applications have been achieved for the three-dimensional compressible flows (Pan 2016). The high-order accuracy of the scheme is obtained by integrating a multidimensional time-accurate gas distribution function over the cell interface within a time step without Gaussian quadrature points and Runge-Kutta time-stepping technique. However, to further increase the order of the scheme, such as the fourth-order one, the formulation becomes very complicated for the multidimensional flow. Recently, a two-stage fourth-order GKS with high efficiency has been constructed for two-dimensional inviscid and viscous flow computations (Li 2016; Pan 2016), and the scheme uses the time accurate flux function and its time derivatives. In this paper, a fourth-order GKS is developed for the three-dimensional flows under the two-stage framework. Based on the three-dimensional WENO reconstruction and flux evaluation at Gaussian quadrature points on a cell interface, the high-order accuracy in space is achieved first. Then, the two-stage time stepping method provides the high accuracy in time. In comparison with the formal third-order GKS (Pan 2015), the current fourth-order method not only improves the accuracy of the scheme, but also reduces the complexity of the gas-kinetic solver greatly. More importantly, the fourth-order GKS has the same robustness as the second-order shock capturing scheme (Xu 2001). Numerical results validate the outstanding reliability and applicability of the scheme for three-dimensional flows, such as turbulent one.

\textbf{KEYWORDS}
two-stage Lax-Wendroff-type time stepping method, fourth-order gas-kinetic scheme, Navier-Stokes equations.

1. Introduction

Over the past half century, the computational fluid dynamics has been developed into a powerful tool for solving the fluid flow problems in industrial applications. Currently, there are a gigantic amount of numerical methods in literature. In comparison with the well-developed second-order schemes, the higher-order methods can provide more accurate solutions, but they are less robust and more complicated. For the high-order schemes, there are generally three parts, i.e. spatial discretization, temporal discretization and flux solvers. For the spatial discretization, many high-order methods have

CONTACT: Liang Pan Email: panliangjlu@sina.com, Kun Xu Email: makxu@ust.hk
been developed, including the discontinuous Galerkin (DG) (Reed 1973; Cockburn 1989, 1998), essential non-oscillatory (ENO) (Harten 1987; Shu 1988), weighted essential non-oscillatory (WENO) (Liu 1994; Jiang 1996; Borges 2008), etc. For most of those methods, the exact and approximate Riemann solvers (Toro 1997) are used for flux evaluation. Due to the first-order evolution of Riemann solvers, the Runge-Kutta method is implemented to achieve higher order temporal accuracy (Gottlieb 1998), in which n-stage is needed for n-th order accuracy. Instead of Riemann solvers, many schemes have been developed based on the time-dependent flux function with high-order evolution, such as the generalized Riemann problem solver (Ben-Artzi 1984, 2006, 2007; Li 2016, 2018), gas-kinetic scheme (Xu 2015, 2001), and AEDR methods (Toro 1997; Titarev 2002). High-order temporal accuracy can be achieved in a one-stage framework with the time integration of the time-dependent flux function. Recently, in order to increase the accuracy and efficiency of these schemes a two-stage fourth-order method has been developed for the time-dependent flux solvers (Li 2016; Pan 2016), where both the flux and temporal derivative of flux function are used in the construction of higher-order schemes. By combining the multi-stage multi-derivative technique, a family of higher-order schemes has been constructed as well (Ji 2018).

In the past decades, the gas-kinetic scheme (GKS) based on the Bhatnagar-Gross-Krook (BGK) model (Bhatnagar 1954; Chapman 1990) has been developed systematically for the compressible flow computations (Xu 2015, 2001, 1998). Different from the traditional CFD methods based on the macroscopic governing equations, the main advantages of the gas-kinetic scheme are the followings. (i) The inviscid and viscous coupling in the flux evolution (Xu 2015, 2001); (ii) Multi-dimensionality with the inclusion of both normal and tangential gradients of flow variables in the flux function across a cell interface (Pan 2016); (iii) Compact stencils can be constructed with the use of the time accurate cell interface flow variables at the next time level (Pan 2016); (iv) Extension to the whole flow regime from the rarefied to the continuum one (Xu 2010, 2012). Recently, with the high-order initial reconstruction, the third-order gas-kinetic schemes have been constructed (Li 2010; Luo 2013; Pan 2016), in which the flux evaluation is based on the moments of spatial-temporal dependent gas distribution function. High-order accuracy can be achieved in a one-stage scheme without Gaussian point integration for spatial accuracy and Runge-Kutta technique for temporal accuracy. However, with the one-stage gas evolution model, the formulation of gas-kinetic scheme can become very complicated for the further development, such as the fourth-order method (Liu 2014), especially for multidimensional computations. The two-stage fourth-order temporal discretization for time-accurate flux solvers in (7) provides a reliable framework to further develop the GKS into fourth-order and even higher accuracy with the implementation of the traditional second-order or third-order flux functions (Pan 2016, 2017; Ji 2018). Most importantly, this scheme is robust, and works perfectly from the subsonic to the hypersonic viscous heat conducting flows. The robustness of the GKS in comparison with Riemann solver based CFD methods is solely due to the differences in the dynamical evolution model of the flux function. The GKS flux follows the dynamics from the particle free transport, to including collisional effect, and to the NS distribution function with the count of intensive particle collisions as the ratio of the time step $\Delta t$ over the particle collision time $\tau$ becoming large. The real physics used in the flux depends on the local $\Delta t/\tau$ (Xu 2017). In real NS computations for the compressible high Mach number flow, the ratio of $\Delta t/\tau$ is not too large as people think of for the validation of the NS modeling (Liu 2018). However, for the Riemann solver based CFD methods, at the beginning of the step it is already assumed that there are infinity number of particle collision to generate distinguishable
waves in the Riemann solution, and the collision needs to be reduced for the NS solutions. Theoretically, there is no such a physical process for the Riemann solver-based Godunov-type schemes for the NS equations. For the second-order schemes, it is hard to distinguish the dynamical differences from the GKS and Riemann solver. However, for the higher-order schemes it seems that a reliable physical evolution model becomes more important due to the absence of large numerical dissipation in the second-order schemes, and the delicate flow structures captured in higher-order schemes depend on the quality of the solvers greatly (Ji 2018).

In this paper, with the two-stage fourth-order discretization, a multidimensional fourth-order gas-kinetic scheme is constructed for simulating three-dimensional flows. High-order accuracy in space is achieved by the three-dimensional WENO method (Liu 1994; Jiang 1996; Borges 2008) and Gaussian quadrature points for the numerical fluxes. In comparison with the formal three-dimensional scheme (Pan 2015), the current fourth-order scheme reduces the complexity of the gas-kinetic flux solver greatly, and improves the robustness of scheme. Many numerical tests, including both inviscid and viscous, and low and high speed flow computations, will be used to validate the current fourth-order method. Numerical results show that the current scheme has the same reliability and applicability as the well-developed second-order scheme, but is much more accurate and effective to capture the complicated flow structures. With the count of the degrees of freedom for the description of a flow field, the current scheme provides state-of-art solutions from a higher-order scheme from the incompressible to the hypersonic flow simulations.

This paper is organized as follows. In Section 2, BGK equation and finite volume scheme are briefly reviewed. The general formulation for the two-stage temporal discretization is introduced in Section 3, and the procedure of spatial reconstruction is given in Section 4. Section 5 includes numerical examples to validate the current algorithm. The last section is the conclusion.

2. BGK equation and finite volume scheme

The three-dimensional BGK equation (Bhatnagar 1954; Chapman 1990) can be written as

\[ f_t + u f_x + v f_y + w f_z = \frac{g - f}{\tau}, \]  

where \( u = (u, v, w) \) is the particle velocity, \( f \) is the gas distribution function, \( g \) is the three-dimensional Maxwellian distribution, and \( \tau \) is the collision time. The collision term satisfies the compatibility condition

\[ \int \frac{g - f}{\tau} \psi d\Xi = 0, \]  

where \( \psi = (\psi_1, ..., \psi_5)^T = (1, u, v, w, \frac{1}{2}(u^2 + v^2 + w^2 + \xi^2))^T \), the internal variables \( \xi^2 \) equals to \( \xi^2 = \xi_1^2 + ... + \xi_K^2 \), \( d\Xi = dudvdwd\xi_1...d\xi_K \), \( K \) is the degrees of freedom, and the specific heat ratio \( \gamma = (K + 5)/(K + 3) \) for three-dimensional flows. In the
continuum region, the gas distribution function can be expanded as

\[ f = g - \tau D_u g + \tau D_u (\tau D_u) g - \tau D_u [\tau D_u (\tau D_u) g] + \ldots, \]

where \( D_u = \frac{\partial}{\partial t} + u \cdot \nabla \). Based on the Chapman-Enskog expansion, the macroscopic equations can be derived (Xu 2015, 2001). With the zeroth-order truncation \( f = g \), the Euler equations can be obtained. With the first-order truncation

\[ f = g - \tau (ug_x + vg_y + wg_z + g_t), \]

the Navier-Stokes equations can be obtained. With the higher order truncations, the Burnett and super-Burnett equations can be derived. Thus, in the gas-kinetic scheme, the Euler and Navier-Stokes solutions can be obtained according to the Chapman-Enskog expansion without solving the macroscopic equations.

Taking moments of Eq.(1) and integrating over the control volume \( V_{ijk} = x_i \times y_j \times z_k \) with \( x_i = [x_i - \Delta x/2, x_i + \Delta x/2], y_j = [y_j - \Delta y/2, y_j + \Delta y/2], z_k = [z_k - \Delta z/2, z_k + \Delta z/2] \), the semi-discretized finite volume scheme can be written as

\[
\frac{dQ_{ijk}}{dt} = \mathcal{L}(Q_{ijk}) = \frac{1}{|V_{ijk}|} \left[ \int_{y_j \times z_k} (F_{i+1/2,j,k} - F_{i-1/2,j,k})dydz \\
+ \int_{x_i \times z_k} (G_{i,j+1/2,k} - G_{i,j-1/2,k})dxdz \\
+ \int_{x_i \times y_j} (H_{i,j,k+1/2} - H_{i,j,k-1/2})dxdy \right],
\]

where \( Q = (\rho, \rho U, \rho V, \rho W, \rho E)^T \) are the conservative flow variables, \( Q_{ijk} \) is the cell averaged value over control volume \( V_{ijk} \) and \( |V_{ijk}| = \Delta x \Delta y \Delta z \). For the three-dimensional computation, the Gaussian quadrature for the numerical fluxes is used to achieve the accuracy in space, and the numerical fluxes in x-direction is given as an example

\[
\int_{y_j \times z_k} F_{i+1/2,j,k}dydz = \Delta y \Delta z \sum_{m,n=1}^{M} \omega_{mn} F(x_{i+1/2,m,n}, t),
\]

where \( x_{i+1/2,m,n} = (x_{i+1/2}, y_{jm}, z_{kn}), (y_{jm}, z_{kn}), m, n = 1, \ldots, M \) are the Gaussian quadrature points for \( y_j \times z_k \) and \( \omega_{mn} \) are quadrature weights, and \( M = 2 \) is used in this paper. Based on the spatial reconstruction, which will be presented in the following section, the reconstructed point value and the spatial derivatives at each Gaussian quadrature points can be obtained and the numerical fluxes \( F(x_{i+1/2,m,n}, t) \) can be provided by the flow solvers. Similarly, the numerical fluxes in the y and z-directions can be obtained as well

\[
\int_{x_i \times z_k} G_{i,j+1/2,k}dxdz = \Delta x \Delta z \sum_{m,n=1}^{M} \omega_{mn} G(x_{im,j+1/2,kn}, t),
\]

\[
\int_{x_i \times y_j} H_{i,j,k+1/2}dxdy = \Delta x \Delta y \sum_{m,n=1}^{M} \omega_{mn} H(x_{im,jn,k+1/2}, t).
\]
In the gas-kinetic scheme, the numerical fluxes at the Gaussian quadrature point can be obtained by taking moments of the gas distribution function

\[
F(x_{i+1/2}, j_m, k_n, t) = \int \psi u f(x_{i+1/2}, j_m, k_n, t, u, \xi) du dv dw d\xi,
\]

where \( f(x_{i+1/2}, j_m, k_n, t, u, \xi) \) is provided by the integral solution of BGK equation Eq.(1) at the cell interface

\[
f(x_{i+1/2}, j_m, k_n, t, u, \xi) = \frac{1}{\tau} \int_0^t g(x', t', u, \xi) e^{-\frac{(t-t')}{\tau}} dt' + e^{-\frac{t}{\tau}} f_0(-u, \xi),
\]

where \( x_{i+1/2}, j_m, k_n \) is the location of cell interface, \( x_{i+1/2} = x' + u(t-t'), y_{j_m} = y' + v(t-t'), z_{k_n} = z' + w(t-t') \) is the trajectory of particles, \( f_0 \) is the initial gas distribution and \( g \) is the corresponding equilibrium state. For the second-order scheme, the second-order gas-kinetic solver for the three-dimensional flows can be expressed as

\[
f(x_{i+1/2}, j_m, k_n, t, u, \xi) = (1 - e^{-\frac{t}{\tau}}) g_0 + ((t + \tau) e^{-\frac{t}{\tau}} - \tau)(a_1 u + a_2 v + a_3 w) g_0 \\
+ (t - \tau + \tau e^{-\frac{t}{\tau}}) \bar{g}_0 \\
+ e^{-\frac{t}{\tau}} g_r [1 - (\tau + t)(a_{1r} u + a_{2r} v + a_{3r} w) - \tau A_r] |H(u)| \\
+ e^{-\frac{t}{\tau}} g_l [1 - (\tau + t)(a_{1l} u + a_{2l} v + a_{3l} w) - \tau A_l] |1 - H(u)|,
\]

where more details about gas distribution function is found in (Xu 2001, 2015; Pan 2015). With the second-order gas-kinetic solver Eq.(7), the second-order accuracy in time can be achieved by one step integration. In the one-stage gas evolution model, the third-order and fourth-order gas-kinetic solver has been developed as well. The formulation of one-stage gas-kinetic solvers, which can be found in (Li 2010; Luo 2013; Liu 2014), become very complicated, especially for the multidimensional computations (Liu 2014). It is the complicated formulation that has become a barrier of developing high-order gas-kinetic schemes.

3. Fourth-order temporal discretization

Recently, a two-stage fourth-order time-accurate discretization was developed for Lax-Wendroff flow solvers, particularly applied for hyperbolic equations with the generalized Riemann problem (GRP) solver (Li 2016) and gas-kinetic scheme (Pan 2016). Such method provides a reliable framework to develop a three-dimensional fourth-order gas-kinetic scheme with a second-order flux function Eq.(7). Consider the following time-dependent equation

\[
\frac{\partial \mathbf{q}}{\partial t} = \mathcal{L}(\mathbf{q}),
\]

with the initial condition at \( t_n \), i.e.,

\[
\mathbf{q}(t = t_n) = \mathbf{q}^n,
\]
where \( \mathcal{L} \) is an operator for spatial derivative of flux. The time derivatives are obtained using the Cauchy-Kovalevskaya method,

\[
\frac{\partial \mathbf{w}^n}{\partial t} = \mathcal{L}(\mathbf{q}^n), \quad \frac{\partial}{\partial t} \mathcal{L}(\mathbf{q}^n) = \frac{\partial}{\partial \mathbf{q}} \mathcal{L}(\mathbf{q}^n) \mathcal{L}(\mathbf{q}^n).
\]

Introducing an intermediate state at \( t^* = t_n + \Delta t/2 \),

\[
\mathbf{q}^* = \mathbf{q}^n + \frac{1}{2} \Delta t \mathcal{L}(\mathbf{q}^n) + \frac{1}{8} \Delta t^2 \frac{\partial}{\partial t} \mathcal{L}(\mathbf{q}^n),
\]

the corresponding time derivatives are obtained as well for the intermediate stage state,

\[
\frac{\partial \mathbf{q}^*}{\partial t} = \mathcal{L}(\mathbf{w}^*), \quad \frac{\partial}{\partial t} \mathcal{L}(\mathbf{q}^*) = \frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{q}^*) \mathcal{L}(\mathbf{q}^*).
\]

Then, the state \( \mathbf{q} \) can be updated with the following formula

\[
\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \mathcal{L}(\mathbf{q}^n) + \frac{1}{6} \Delta t^2 (\frac{\partial}{\partial t} \mathcal{L}(\mathbf{q}^n) + 2 \frac{\partial}{\partial t} \mathcal{L}(\mathbf{q}^*)).
\]

(10)

It can be proved that for hyperbolic equations the above time stepping method Eq.(9) and Eq.(10) provides a fourth-order time accurate solution for \( \mathbf{q}(t) \) at \( t = t_n + \Delta t \). For the conservation laws with source terms

\[
\frac{\partial \mathbf{q}}{\partial t} = \mathcal{L}(\mathbf{q}) + \mathbf{S}(\mathbf{q}),
\]

the two-stage fourth-order temporal discretization Eq.(9) and Eq.(10) can be directly used with the inclusion of \( \partial_t \mathbf{S}(\mathbf{q}) \). More details of the analysis can be found in (Li 2016).

In this paper the above two-stage fourth-order method will be extended to the three-dimensional flows. For the semi-discretized finite volume scheme

\[
\frac{dQ_{ijk}}{dt} = \mathcal{L}(Q_{ijk}),
\]

three-dimensional semi-discretized finite volume scheme becomes a particular case of the general ODE system. The two-stage method Eq.(9) and Eq.(10) can be extended directly for Eq.(3). For the gas-kinetic scheme, the gas evolution is a relaxation process from kinetic to hydrodynamic scale through the exponential function, and the corresponding flux is a complicated function of time. In order to obtain the time derivatives of the flux function at \( t_n \) and \( t^* = t_n + \Delta t/2 \) with the correct physics, the flux function should be approximated as a linear function of time within a time interval. According to the numerical fluxes at the Gauss quadrature points Eq.(5), the following notation
is introduced

\[
F_{i+1/2,j,k}(Q^n, t) = \sum_{m,n=1}^{M} \omega_{mn} F(x_{i+1/2,j,m,k}, t),
\]

\[
F_{i+1/2,j,k}(Q^n, \delta) = \int_{t_n}^{t_{n+\delta}} F_{i+1/2,j,k}(Q^n, t) dt,
\]

where \(F(x_{i+1/2,j,m,k}, t)\) is obtained according to Eq.(5) and the subscript of \(Q\) is omitted. In the time interval \([t_n, t_n + \Delta t]\), the flux is expanded as follows

\[
F_{i+1/2,j,k}(Q^n, t) = F^n_{i+1/2,j,k} + \partial_t F^n_{i+1/2,j,k}(t - t_n).
\]

The coefficients \(F_{i+1/2,j,k}(Q^n, t)\) and \(\partial_t F_{i+1/2,j,k}(Q^n, t_n)\) can be determined as follows,

\[
F_{i+1/2,j,k}(Q^n, t_n) \Delta t + \frac{1}{2} \partial_t F_{i+1/2,j,k}(Q^n, t_n) \Delta t^2 = F_{i+1/2,j,k}(Q^n, \Delta t),
\]

\[
\frac{1}{2} F_{i+1/2,j,k}(Q^n, t_n) \Delta t + \frac{1}{8} \partial_t F_{i+1/2,j,k}(Q^n, t_n) \Delta t^2 = F_{i+1/2,j,k}(Q^n, \Delta t/2).
\]

By solving the linear system, we have

\[
F_{i+1/2,j,k}(Q^n, t_n) = (4F_{i+1/2,j,k}(Q^n, \Delta t/2) - F_{i+1/2,j,k}(Q^n, \Delta t))/\Delta t,
\]

\[
\partial_t F_{i+1/2,j,k}(Q^n, t_n) = 4(F_{i+1/2,j,k}(Q^n, \Delta t) - 2F_{i+1/2,j,k}(Q^n, \Delta t/2))/\Delta t^2.
\]

Similarly, the numerical fluxes \(G^n_{i,j+1/2,k}\) in the y-direction and \(H_{i,j,k+1/2}\) in z-direction can be obtained as well. With the numerical fluxes and temporal derivatives, \(\mathcal{L}(Q^n_{ijk})\) and \(\mathcal{L}_t(Q^n_{ijk})\) can be given as follows

\[
\mathcal{L}(Q^n_{ijk}) = \frac{1}{\Delta x} (F_{i+1/2,j,k}(Q^n, t_n) - F_{i-1/2,j,k}(Q^n, t_n))
+ \frac{1}{\Delta y} (G_{i,j+1/2,k}(Q^n, t_n) - G_{i,j-1/2,k}(Q^n, t_n))
+ \frac{1}{\Delta z} (H_{i,j,k+1/2}(Q^n, t_n) - H_{i,j,k-1/2}(Q^n, t_n)),
\]

(11)

\[
\mathcal{L}_t(Q^n_{ijk}) = \frac{1}{\Delta x} (\partial_t F_{i+1/2,j,k}(Q^n, t_n) - \partial_t F_{i-1/2,j,k}(Q^n, t_n))
+ \frac{1}{\Delta y} (\partial_t G_{i,j+1/2,k}(Q^n, t_n) - \partial_t G_{i,j-1/2,k}(Q^n, t_n))
+ \frac{1}{\Delta z} (\partial_t H_{i,j,k+1/2}(Q^n, t_n) - \partial_t H_{i,j,k-1/2}(Q^n, t_n)).
\]

(12)

According to Eq.(9), \(Q^n_{ijk}\) at \(t_n\) can be updated. With the similar procedure, the numerical fluxes and temporal derivatives at the intermediate stage can be constructed and \(\mathcal{L}_t(Q^n_{ijk})\) can be given as well. According to Eq.(9) and Eq.(10), \(Q^{n+1}_{ijk}\) at \(t_{n+1}\) can be updated.
4. Spatial reconstruction

The above time evolution solution is based on the high-order initial reconstruction for macroscopic flow variables and WENO reconstruction (Liu 1994; Jiang 1996; Borges 2008) is adopted for the spatial reconstruction. For the three dimensional computation, the reconstruction procedure for the cell interface $x_{i+1/2,j,k}$ is given as an example, and the stencil for reconstruction is given in Fig.1. The point value $Q_l$, $Q_r$ and $Q_0$ and first-order derivatives at the Gauss quadrature points $(x_{i+1/2}, y_{jm}, z_{kn})$, $m, n = 1, ..., 2$ need to be constructed. The detailed procedure is given as follows

**Figure 1.** Schematics of spatial reconstruction at the cell interface $(i + 1/2, j, k)$.

1. According to one dimensional reconstruction, the cell averaged reconstructed values and cell averaged spatial derivatives

$$
(Q_l)_{j-\ell_1,k-\ell_2}, (Q_r)_{j-\ell_1,k-\ell_2}, (Q_0)_{j-\ell_1,k-\ell_2}, \quad (\partial_x Q_l)_{j-\ell_1,k-\ell_2}, (\partial_x Q_r)_{j-\ell_1,k-\ell_2}, (\partial_x Q_0)_{j-\ell_1,k-\ell_2},
$$

can be constructed for the stencil shown in Fig.1, where $\ell_1, \ell_2 = -2, ..., 2$.

2. With the one-dimensional WENO reconstruction in the horizontal direction, the averaged value and the averaged spatial derivatives

$$
(Q_l)_{jm,k-\ell_2}, (Q_r)_{jm,k-\ell_2}, (Q_0)_{jm,k-\ell_2}, \quad (\partial_x Q_l)_{jm,k-\ell_2}, (\partial_x Q_r)_{jm,k-\ell_2}, (\partial_x Q_0)_{jm,k-\ell_2},
$$

over the interval $[z_{k-\ell_2} - \Delta z/2, z_{k-\ell_2} + \Delta z/2]$ with $y = y_{jm}$, can be given.

3. With one-dimensional WENO reconstruction in the vertical direction, the point value and spatial derivatives

$$
(Q_l)_{jm,kn}, (Q_r)_{jm,kn}, (Q_0)_{jm,kn}, \quad (\partial_x Q_l)_{jm,kn}, (\partial_x Q_r)_{jm,kn}, (\partial_x Q_0)_{jm,kn}, \quad (\partial_y Q_l)_{jm,kn}, (\partial_y Q_r)_{jm,kn}, (\partial_y Q_0)_{jm,kn}, \quad (\partial_z Q_l)_{jm,kn}, (\partial_z Q_r)_{jm,kn}, (\partial_z Q_0)_{jm,kn},
$$

can be fully given at the Gaussian quadrature points $(x_{i+1/2}, y_{jm}, z_{kn})$. 

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With the reconstructed point value and spatial derivatives at each Gaussian quadrature point \((x_{i+1/2}, y_j, z_k)\), the numerical fluxes can be obtained by Eq.(4), Eq.(5) and Eq.(7).

In the computation, without special statement, the fifth-order WENO-JS reconstruction (Jiang 1996) is adopted for the flow with discontinuities and the linear scheme is used for the smooth flows to reduce the dissipation.

5. Numerical experiments

In this section, numerical tests for both inviscid and viscous flows will be presented to validate our numerical scheme. For the inviscid flow, the collision time \(\tau\) takes

\[
\tau = \epsilon \Delta t + C \frac{p_l - p_r}{p_l + p_r} \Delta t,
\]

where \(p_l\) and \(p_r\) denote the pressures on the left and right sides of the cell interface. In the computation, \(\epsilon = 0.01\) and \(C = 1\). For the viscous flow, we have

\[
\tau = \frac{\mu}{p} + \frac{p_l - p_r}{p_l + p_r} \Delta t,
\]

where \(\mu\) is the viscous coefficient and \(p\) is the pressure at the cell interface, and it will reduce to \(\tau = \mu/p\) in the smooth flow regions. \(\Delta t\) is the time step which is determined according to the CFL number, which takes 0.4 in the computation. The reason for including artificial dissipation through the additional term in the particle collision time is to enlarge the kinetic scale physics in the discontinuous region for the construction of a numerical shock structure through the particle free transport and inadequate particle collision in order to keep the non-equilibrium property.

For the smooth flow, the WENO reconstruction can be used directly on the conservative flow variables. For the flow with strong discontinuity, the characteristic variables can be used in the reconstruction. Based on \(A_{i+1/2,j} = (\partial F/\partial Q)_{Q=Q^*}\), where \(Q\) are the conservative variables, \(F(Q)\) are the corresponding fluxes, and \(Q^* = (Q_{i,j,k} + Q_{i+1,j,k})/2\), the cell averaged and point conservative values can be projected into the characteristic field by \(\omega = RQ\), where \(R\) is the matrix corresponding to right eigenvectors of \(A\). The reconstruction scheme is applied on the characteristic variables \(\omega\). With the reconstructed polynomials for characteristic variables, the conservative flow variables can be recovered by the inverse projection.

5.1. Accuracy tests

The first case is the advection of density perturbation for the inviscid flow, and the initial condition is given as follows

\[
\rho(x, y, z) = 1 + 0.2 \sin(\pi(x + y + z)), \quad p(x, y, z) = 1, \quad u(x, y, z) = 1, \quad v(x, y, z) = 1, \quad w(x, y, z) = 1.
\]

The computational domain is \([0, 2] \times [0, 2] \times [0, 2]\), and the periodic boundary conditions are applied in both directions. The exact solution is the perturbation which propagates
with the velocity $(1,1,1)$. The $L^1$ and $L^2$ errors and orders at $t = 2$ with $N \times N \times N$ uniform mesh cells are presented in Tab.1, which shows that the expected accuracy can be also achieved for the three-dimensional inviscid computation.

<table>
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<th>$L^1$ error</th>
<th>Order</th>
<th>$L^2$ error</th>
<th>Order</th>
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<td></td>
<td>3.9071E-02</td>
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<td>2.5039E-04</td>
<td>7.2857</td>
</tr>
<tr>
<td>$40 \times 40 \times 40$</td>
<td>2.0710E-05</td>
<td>4.9485</td>
<td>8.1338E-06</td>
<td>4.9441</td>
</tr>
<tr>
<td>$80 \times 80 \times 80$</td>
<td>7.3189E-07</td>
<td>4.8225</td>
<td>2.8983E-07</td>
<td>4.8106</td>
</tr>
</tbody>
</table>

Table 1. Accuracy tests: density perturbation advection by the high-order GKS.

5.2. **Three-dimensional Sod problem**

This problem is a fully three-dimensional extension of Sod problem. The computational domain is $(x,y,z) \in [0,1] \times [0,1] \times [0,1]$, and the initial condition is given as follows

$$(\rho,U,V,p) = \begin{cases} (1,0,0,1), & 0 \leq \sqrt{x^2+y^2+z^2} < 0.5, \\ (0.125,0,0,0.1), & 0.5 < \sqrt{x^2+y^2+z^2} \leq 1. \end{cases}$$

The exact solution of this problem can be given by the following one-dimensional system with geometric source terms

$$\frac{\partial Q}{\partial t} + \frac{\partial F(Q)}{\partial r} = S(Q),$$

where

$$Q = \begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix}, F(Q) = \begin{pmatrix} \rho U \\ \rho U^2 + p \\ U(\rho E + p) \end{pmatrix}, S(Q) = -\frac{d-1}{r} \begin{pmatrix} \rho U \\ \rho U^2 \\ U(\rho E + p) \end{pmatrix}.$$

The radial direction is denoted by $r$, $U$ is the radial velocity, $d$ is the number of space dimensions and $\gamma = 1.4$. The two-stage fourth-order gas-kinetic scheme is used to solve this equation and the numerical results with 10000 cells are given as the reference solutions. In the computation, the uniform mesh with $\Delta x = \Delta y = \Delta z = 1/100$ is used. The symmetric boundary condition is imposed on the plane with $x = 0$, $y = 0$ and $z = 0$, and the non-reflection boundary condition is imposed on the plane with $x = 1$, $y = 1$ and $z = 1$. The three-dimensional density and pressure distributions are given in Fig.2, and the density and pressure distribution along the line $y = z = 0$ are given in Fig.3. The numerical results agree well with the reference solutions.

<table>
<thead>
<tr>
<th>mesh</th>
<th>Two-stage GKS</th>
<th>RK4 HLLC</th>
<th>RK4 exact-RS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10 \times 10 \times 10$</td>
<td>0.9526</td>
<td>0.7488</td>
<td>1.1856</td>
</tr>
<tr>
<td>$20 \times 20 \times 20$</td>
<td>6.9264</td>
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<td>$40 \times 40 \times 40$</td>
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<td>61.8699</td>
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<tr>
<td>$80 \times 80 \times 80$</td>
<td>418.5974</td>
<td>284.2182</td>
<td>474.1962</td>
</tr>
</tbody>
</table>

Table 2. Three-dimensional Sod problem: computational time (in seconds) for different scheme.
Figure 2. Three-dimensional Sod problem: the three-dimensional density and pressure distributions with $\Delta x = \Delta y = \Delta z = 1/100$.

Figure 3. Three-dimensional Sod problem: the density and pressure distributions with $\Delta x = \Delta y = \Delta z = 1/100$ along the line $y = z = 0$.

Based on the above three-dimensional Riemann problem, the computational efficiency of the current scheme is presented together with the traditional fourth-order Runge-Kutta scheme with the exact and approximate HLLC Riemann solvers (Toro 1997). The CPU times are recorded after running 5 time steps for each scheme with a single processor of Intel Core i7 4790 CPU @3.60GHz, and the CPU times with different mesh sizes for each scheme are presented in Table.2. Due to the simple HLLC flux function, the Runge-Kutta method with HLLC Riemann solver is more efficient than the current scheme. Due the iterative procedure, the Runge-Kutta method with exact Riemann solver costs more time. However, even for the inviscid flow cases, the current scheme solves the Navier-Stokes equations. If the Godunov type scheme is extended to the Navier-Stokes equations, the computational cost will at least be doubled. Thus, for the high-order schemes and for the viscous flow computations, the design of high-order time accurate gas-kinetic solver is worthwhile.

5.3. Flow impinging on sphere

In this case, the inviscid hypersonic flows impinging on a unit sphere are tested to validate robustness of the current scheme with different Mach numbers with $\gamma = 1.4$. In the computation, a $40 \times 40 \times 40$ mesh shown in Fig.4 is used, which representing the domain $[-1.75, -1] \times [-0.4\pi, 0.4\pi] \times [0.1\pi, 0.9\pi]$ in the spherical coordinate $(r, \phi, \theta)$. 
Figure 4. Flow impinging on sphere: the computational mesh (a), density distribution with Mach number $Ma = 5$ (b) and 8 (c).

Figure 5. Flow impinging on sphere: the Mach number (a), pressure (b) distributions for $Ma = 5$, and the Mach number (c), pressure (d) distributions for $Ma = 8$ at the plane with $\phi = 0$.

The density distributions in the whole domain, Mach number and pressure distributions at the plane with $\phi = 0$ for the Mach number $Ma = 5$ and 8 are shown in Fig.4 and Fig.5, where the shock is well captured by the current scheme and the carbuncle phenomenon does not appear (Pandolfi 2001).

5.4. Rayleigh-Taylor instability

The Rayleigh-Taylor instability occurs when an interface between two different fluids with different densities experiences a pressure gradient opposing the density gradient (Chen 1999). This interface is unstable and any disturbance tends to grow, leading to the penetration of both fluids into each other. If the initial interface displacement is random, the Rayleigh-Taylor instability usually evolves into complicated turbulent mixing. In this case, the three-dimensional Rayleigh-Taylor instability is tested in a rectangular box with domain $[0, 0.25] \times [0, 0.25] \times [0, 1]$ with a gravity pointed downward $g = (0, 0, g)$, $g = -0.1$. The source terms and temporal derivative are

$$S(Q) = (0, 0, 0, \rho g, \rho W g),$$
$$\partial_t S(Q) = (0, 0, 0, \rho g, (\rho W)tg).$$
Figure 6. Rayleigh-Taylor instability: the fluid interface from a single-mode perturbation at $t = 3, 4, 5, 6, 7, 8$.

Figure 7. Rayleigh-Taylor instability: the density distribution at $x = 0$, $x = W/2$ and $x = y$ with $t = 3, 4, 5, 6, 7, 8$.

For each step, $\rho_t$ and $(\rho W)_t$ can be extracted from

$$\frac{\partial Q_{ijk}}{\partial t} = \mathcal{L}(Q_{ijk}) + \mathcal{S}(Q_{ijk}),$$

and Eq.(9) and Eq.(10) can be implemented directly. Periodic boundary conditions are applied at the four sides, while symmetric boundary conditions are applied at the top and bottom walls. The instability develops from the imposed single mode initial perturbation

$$\frac{h(x, y)}{D} = 0.05\left[ \cos\left(\frac{2\pi x}{D}\right) + \cos\left(\frac{2\pi y}{D}\right) \right],$$

13
where $h$ is the height of the interface and $D$ is the box width. The dimensionless parameters is the Atwood number

$$A = \frac{\rho_h - \rho_l}{\rho_h + \rho_l},$$

where $\rho_h, \rho_l$ are densities of heavy and light fluids, respectively. In the computation, the Atwood number $A = 1/3$ is used. The fluid interface from a single-mode perturbation at $t = 3, 4, 5, 6, 7, 8$ are given in Fig.6, and the density distribution at $x = 0, x = W/2$ and $x = y$ with $t = 3, 4, 5, 6, 7, 8$ are given in Fig.7. As expected, the heavy and light fluids penetrate into each other as time increases. The light fluid rises to form a bubble and the heavy fluid falls to generate a spike.

Figure 8. Lid-driven cavity flow: the velocity profiles $U$ and $V$ in the symmetry $x - y$-plane along the vertical and horizontal centerlines with $Re = 1000, 400$ and 100.

Figure 9. Lid-driven cavity flow: The mean velocity profiles $U$ and $V$ in the symmetry $x - y$-plane along the vertical and horizontal centerlines with $Re = 3200$. 

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5.5. **Lid-driven cavity flow**

The lid-driven cavity problem is one of the most important benchmarks for numerical Navier-Stokes solvers. The fluid is bounded by a unit cubic $[0, 1] \times [0, 1] \times [0, 1]$ and driven by a uniform translation of the top boundary with $y = 1$. The monatomic gas with $\gamma = 5/3$ is used, such that there is no bulk viscosity involved. Early three-dimensional cavity-flow calculations were carried out by De Vahl Davis and Mallinson (Debonis 1976) and Goda (Goda 1979). In this case, the flow is simulated with Mach number $Ma = 0.15$ and all the boundaries are isothermal and nonslip. Numerical simulations are conducted with three Reynolds numbers of $Re = 1000$, $400$ and $100$ using $65 \times 65 \times 65$ meshes. The convergent solution is obtained, and the $u$-velocity profiles along the vertical centerline line, $v$-velocity profiles along the horizontal centerline in the symmetry $x-y$ plane and the benchmark data (Albensoeder 2005; Shu 2003) are shown in Fig.8. The simulation results match well with the benchmark data. The flow at $Re = 3200$ corresponds to unsteady state solutions, which have been studied extensively (Prasad 1989). The mean velocity profiles in the symmetry plane along the vertical and the horizontal centerlines of the numerical solutions and experimental measurements (Prasad 1989) are presented Fig.9. The agreement between them shows that the three-dimensional high-order gas-kinetic scheme is capable of simulating complex three-dimensional unsteady flows.

5.6. **Compressible homogeneous turbulence**

The high-order gas-kinetic scheme is applied for the direct numerical simulations (DNS) of the compressible decaying homogeneous isotropic turbulence. The flow is computed within a square box defined as $-\pi \leq x, y, z \leq \pi$, and the periodic boundary conditions are used in all directions for all the flow variables (Luo 2009; Samtaney 2001; Li 2014). In the computation, the domain is discretized with a uniform Cartesian mesh cells $N^3$. A divergence-free random initial velocity field $u_0$ is generated for a given spectrum with a specified root mean square $u'$ as follows

$$u' = \frac{\langle u \cdot u \rangle}{3}^{1/2},$$

where $\langle ... \rangle$ is a volume average over the whole computational domain. The specified spectrum for velocity is given by

$$E(k) = A_0 k^4 \exp(-2k^2/k_0^2),$$

where $k$ is the wave number, $k_0$ is the wave number at spectrum peaks, $A$ is a constant chosen to get a specified initial kinetic energy. The initial volume averaged turbulent kinetic energy $K_0$ and the initial large-eddy-turnover time $\tau$ is given by

$$K_0 = \frac{3A_0}{64} \sqrt{2\pi} k_0^5, \quad \tau = \sqrt{\frac{32}{A_0} (2\pi)^{1/4} k_0^{-7/2}}.$$
Figure 10. Compressible homogeneous turbulence. Left: the iso-surfaces of $Q$ criterion colored by velocity magnitude at time $t/\tau = 2$ with $128^3$ cells; right: the pressure distribution with $z = -\pi$ at time $t/\tau = 1$.

Figure 11. Compressible homogeneous turbulence: the time history of $K(t)/K_0$ (a), $\rho_{rms}(t)/Ma_t^2$ (b) and $S_u(t)$ and time history of $K(t)/K_0$ (c) with $Ma_\lambda = 0.2, 0.5$ and 0.6 with respect to $t/\tau$ (d).

Taylor microscale Reynolds number $Re_\lambda$ and turbulence Mach number $Ma_t$ are given as

$$Re_\lambda = \frac{\langle \rho \rangle u' \lambda}{\langle \mu \rangle} = \frac{(2\pi)^{1/4}}{4} \frac{\rho_0}{\mu_0} \sqrt{2A_0 k_0^{3/2}} ,$$

$$Ma_t = \frac{\sqrt{3} u'}{c_s} = \frac{\sqrt{3} u'}{\sqrt{\gamma T_0}} ,$$
where $\lambda$ is Taylor microscale

$$
\lambda^2 = \frac{(u')^2}{<(\partial_1 u_1)^2>}
$$

The dynamic viscosity is determined by

$$
\mu = \mu_0\left(\frac{T}{T_0}\right)^{0.76},
$$

where $\mu_0$ and $T_0$ can be determined from $Re_{\lambda}$ and $Ma_t$ with initialized $u'$ and $p_0 = 1$. The time history of the kinetic energy, root-mean-square of density fluctuation and skewness factor for velocity slope are defined as

$$
K(t) = \frac{1}{2} < \rho u \cdot u >,
$$

$$
\rho_{rms}(t) = \sqrt{<(\rho - \bar{\rho})^2>},
$$

$$
S_u(t) = \sum_i <(\partial_i u_i)^3> / <(\partial_i u_i)^2>{3/2}.
$$

In the computation, $A_0 = 1.3 \times 10^{-4}$, $k_0 = 8$, $Re_{\lambda} = 72$ and $Ma_t = 0.5$, and the uniform meshes with $64^3$, $128^3$ and $256^3$ cells are used. The iso-surfaces of $Q$ criterion colored by velocity magnitude and the pressure distribution with $z = -\pi$ at time $t/\tau = 1$ are given in Fig.10. The time history of normalized kinetic energy $K(t)/K_0$, normalized root-mean-square of density fluctuation $\rho_{rms}(t)/Ma_t^2$ and skewness factor $S_u(t)$ with respect to $t/\tau$ are given in Fig.11. The numerical results agree well with the reference data. With fixed initial $Re_{\lambda} = 72$ and $128^3$ cells, the cases with $Ma_t = 0.2, 0.5, 0.6$ are tested, and the time histories of normalized kinetic energy $K(t)/K_0$ are given in Fig.11 as well. With the increase of $Ma_t$, the dynamic viscosity increases, and the kinetic energy gets dissipated more rapidly.

5.7. **Taylor-Green Vortex**

This problem is aimed at testing the performance of high-order methods on the direct numerical simulation of a three-dimensional periodic and transitional flow defined by a simple initial condition, i.e. the Taylor-Green vortex (Bull 2014; Debonis 2013). With a uniform temperature field, the initial flow field is given by

$$
\begin{align*}
 u &= V_0 \sin(\frac{x}{L}) \cos(\frac{y}{L}) \cos(\frac{z}{L}), \\
 v &= -V_0 \cos(\frac{x}{L}) \sin(\frac{y}{L}) \cos(\frac{z}{L}), \\
 w &= 0, \\
 p &= p_0 + \frac{p_0 V_0^2}{16} (\cos(\frac{2x}{L}) + \cos(\frac{2y}{L})) (\cos(\frac{2z}{L}) + 2).
\end{align*}
$$

The fluid is then a perfect gas with $\gamma = 1.4$ and the Prandtl number is $Pr = 0.71$. Numerical simulations are conducted with two Reynolds numbers $Re = 1600$ and 280. The flow is computed within a periodic square box defined as $-\pi L \leq x, y, z \leq \pi L$. The
characteristic convective time $t_c = L/V_0$. In the computation, $L = 1, V_0 = 1, \rho_0 = 1,$ and the Mach number takes $M_0 = V_0/c_0 = 0.1$, where $c_0$ is the sound speed. The volume-averaged kinetic energy can be computed from the flow as it evolves in time, which is expressed as

$$E_k = \frac{1}{\rho_0 \Omega} \int_{\Omega} \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u} \, d\Omega,$$

where $\Omega$ is the volume of the computational domain, and the dissipation rate of the kinetic energy is given by

$$\varepsilon_k = -\frac{dE_k}{dt}.$$

The numerical results of the current scheme with $128 \times 128 \times 128$ mesh points for the normalized volume-averaged kinetic energy and dissipation rate with Reynolds numbers $Re = 1600$ and 280 are presented in Fig.12 and Fig.14, which agree well with the data in (Debonis 2013; Wang 2015). The iso-surfaces of $Q$ criteria colored by velocity magnitude at $t = 5$ and 10 are shown in Fig.13 for $Re = 1600$ and in Fig.15 for $Re = 280$. The evolution of flow structure is evident, starting from large vortices and decaying into more complex structures. Different from many other higher-order methods, the current scheme has no internal degrees of freedom to be updated within
Figure 14. Taylor-Green Vortex problem: the kinetic energy $E_k$ and dissipation rate $-\frac{dE_k}{dt}$ with fourth-order scheme for $Re = 280$.

Figure 15. Taylor-Green Vortex problem: the iso-surfaces of $Q$ criterion colored by velocity magnitude at time $t = 5, 10$ for $Re = 280$.

each cell.

Figure 16. Taylor-Green Vortex problem: the dissipation rate $-\frac{dE_k}{dt}$ without Gaussian quadrature for $Re = 1600$.

In many finite volumes type high-order schemes for three-dimensional flows, the Gaussian quadrature is not used for the flux evaluation, and it make the computation more efficient. For this case, the numerical results of the dissipation rate without Gaussian quadrature with the same mesh points is given in Fig.16, where the peak of the dissipation rate can not be reached.
6. Conclusion

In this paper, based on the two-stage time stepping method, a fourth-order gas-kinetic scheme is proposed for the three-dimensional inviscid and viscous flow computations. With the three-dimensional WENO-JS reconstruction, a gas-kinetic scheme with higher-order spatial and temporal accuracy is developed. In comparison with the classical methods based on the first-order Riemann solver, for the same fourth-order accuracy in time the current scheme only uses two stages instead of four stages with the Runge-Kutta time-stepping technique. As a result, the two-stage GKS can be more efficient than the four-stage methods with the absence of two time consuming reconstructions. For the Navier-Stokes solutions, the current scheme doesn’t separate inviscid and viscous terms and they are treated uniformly from the same initial WENO-type reconstruction. The GKS can present very accurate viscous flow solutions due to its multidimensional flux function at a cell interface, where the gradients in both normal and tangential directions of flow variables participate in the gas evolution. The fourth-order GKS not only has the expected order of accuracy for the smooth flow, but also has favorable shock capturing property for the discontinuous solutions. Most importantly, the numerical tests clearly demonstrate that the current fourth-order scheme has the same robustness as the second-order one. The scheme has been tested from the smooth flows to the flows with discontinuities, and from the low speed to the hypersonic ones. For the three dimensional Navier-Stokes solutions, the current scheme is one of the state-of-art methods in the capturing of complicated flow structures.

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