High-Order Gas-Kinetic Scheme in Curvilinear Coordinates for the Euler and Navier-Stokes Solutions

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\textbf{Abstract.} The high-order gas-kinetic scheme (HGKS) has achieved success in simulating compressible flows with Cartesian meshes. To study the flow problems in general geometries, such as the flow over a wing-body, the development of HGKS in general curvilinear coordinates becomes necessary. In this paper, a two-stage fourth-order gas-kinetic scheme is developed for the Euler and Navier-Stokes solutions in the curvilinear coordinates from one-dimensional to three-dimensional computations. Based on the coordinate transformation, the kinetic equation is transformed first to the computational space, and the flux function in the gas-kinetic scheme is obtained there and is transformed back to the physical domain for the update of flow variables inside each control volume. To achieve the expected order of accuracy, the dimension-by-dimension reconstruction based on the WENO scheme is adopted in the computational domain, where the reconstructed variables are the cell averaged Jacobian and the Jacobian-weighted conservative variables. In the two-stage fourth-order gas-kinetic scheme, the point values as well as the spatial derivatives of conservative variables at Gaussian quadrature points have to be used in the evaluation of the time dependent flux function. The point-wise conservative variables are obtained by ratio of the above reconstructed data, and the spatial derivatives are reconstructed through orthogonalization in physical space and chain rule. A variety of numerical examples from the accuracy tests to the solutions with strong discontinuities are presented to validate the accuracy and robustness of the current scheme for both inviscid and viscous flows. The precise satisfaction of the geometrical conservation law in non-orthogonal mesh is also demonstrated through the numerical example.

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1 Introduction

In recent decades, there have been continuous interests and efforts on the development of high-order schemes. With the development of computational aero-acoustics (CAA), large eddy simulations (LES), and direct numerical simulations (DNS), the construction of high-order numerical scheme becomes extremely demanding, and many high-order finite volume schemes on unstructured meshes have been proposed for the complicated geometries [1, 17, 20]. However, the direct implementation in the physical space brings big challenges. The complexity of algorithms and codes increases dramatically because of the difficulty in choosing stencils, especially in the multi-dimensional reconstruction. To overcome the drawback, an efficient way is to apply the finite volume method in the curvilinear coordinate system, where the structured meshes are used. The technique of curvilinear or mapped coordinates is widely used in engineering [15, 44]. In principle, given a suitable mapping function, any problem defined on a general physical domain can be transformed into a computational domain which is equidistant and Cartesian. Although the flexibility may be reduced in comparison with unstructured meshes, the good numerical characteristics are preserved. The first one is the exact global conservation property, which is only approximately satisfied in the high-order finite difference method [27], and the second one is the strict adherence to the integral form for numerical simulations [14]. Furthermore, the standard numerical schemes on the Cartesian and equidistant grids can be used [40].

In the past decades, the gas-kinetic scheme (GKS) based on the Bhatnagar-Gross-Krook (BGK) model [4, 9] has been developed systematically for the computations from low speed flows to supersonic flows [48, 49]. Different from the traditional finite volume and finite difference schemes [41, 43], GKS presents a gas evolution process from kinetic scale to hydrodynamic scale, where both inviscid and viscous fluxes are recovered from a multidimensional time-dependent gas distribution function. Based on the unified coordinate transformation [21], the second-order gas-kinetic scheme was developed under the moving-mesh framework as well [24, 25]. The flux evaluation in the GKS is based on the time evolution of flow variables from an initial piece-wise discontinuous polynomials around each cell interface. Thus, the high-order spatial and temporal evolutions of a gas distribution function are coupled nonlinearly. With the spatial and temporal coupled gas distribution function, the one-stage third-order GKS was developed [30, 33]. In comparison with other high-order schemes with Riemann flux [41], it integrates the flux function over a time step analytically without employing the multi-stage Runge-Kutta techniques [18]. However, with the one-stage gas evolution model, the formulation of GKS can become very complicated for the further improvement, such as the one-stage fourth-
order scheme for three-dimensional computations [31]. Recently, based on the time-dependent flux function of generalized Riemann problem (GRP) [2, 3] and gas-kinetic scheme [48, 49], a two-stage fourth-order method was developed for Lax-Wendroff type flow solvers [26], particularly applied for the hyperbolic conservation laws [29, 35]. With the temporal discretization, a reliable framework was provided for developing GKS into fourth-order and even higher-order accuracy, in which the traditional second-order and third-order flux functions are used [36–38]. More importantly, this scheme is as robust as the second-order scheme and works perfectly from subsonic to hypersonic flows. The robustness is due to the dynamical evolution model of the time dependent flux function. For the construction of high-order scheme, a reliable physical evolution model becomes important, and the delicate flow structures captured in higher-order schemes depend on the quality of the solvers greatly. With the dimensional-by-dimensional WENO reconstruction, the high-order gas-kinetic scheme has been extended to three-dimensional computation with the Cartesian meshes, especially for the direct numerical simulation of compressible isotropic turbulence [7]. The numerical results shows the potentials of HGKS for the numerical simulation of compressible turbulence at very high Mach numbers.

To treat practical problems with general geometries, such as the turbulent boundary layer with non-equidistant grids and the flow over a wing-body with non-Cartesian grids, the development of three-dimensional HGKS in general curvilinear coordinates becomes demanding. In this paper, based on the coordinate transformation, the discretization procedure of finite volume method in curvilinear coordinates is presented. To achieve the spatial accuracy, the WENO-based dimension-by-dimension reconstruction is adopted [40], where the reconstructed variables are the cell averaged Jacobian and the Jacobian-weighted conservative variables. For most high-order schemes based on Riemann solvers [41], only the point-wise values are needed at Gaussian quadrature points, which can be obtained by taking ratio of the reconstructed variables. However, the spatial derivatives of conservative variables in the physical domain is also needed in gas-kinetic scheme, and it plays an equally important role in the two-stage fourth-order temporal discretization. But, the derivatives cannot be provided by the direct spatial reconstruction. According to the chain rule, the spatial derivatives of conservative variables in the computational space can be obtained first. With the procedure of orthogonalization, the spatial derivatives in the local orthogonal coordinates in the physical space are obtained the second-order gas-kinetic solver. Numerical tests with analytical coordinate transformations from one-dimensional to three-dimensional cases, including the accuracy test to the flows with strong discontinuities, are presented to validate the accuracy and robustness of current scheme. The precise satisfaction of geometrical conservation law has been demonstrated numerically as well. In the practical application, the meshes are mostly generated by discrete methods like software. The geometrical metrics need to be interpolated from available discrete points numerically. Currently, we are working on the general geometries, and more examples will be tested in the future. The current scheme provides a solid tool for further studies of complex compressible turbulent flows,
which is our long-term goal.

This paper is organized as follows. In Section 2, the BGK equation and coordinate transformation are introduced. The two-stage fourth-order gas-kinetic scheme is constructed in the curvilinear coordinate in Section 3. Section 4 includes numerical examples to validate the current algorithm. The last section is the conclusion.

2 BGK equation and coordinate transformation

The three-dimensional BGK equation [4, 9] can be written as

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

(2.1)

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

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

(2.2)

where \( \psi = (\psi_1, \cdots, \psi_5)^T = (1, u, v, w, \frac{1}{2}(u^2 + v^2 + w^2 + \varpi^2)) \), the internal variables \( \varpi^2 = \varpi^2_1 + \cdots + \varpi^2_K \), \( d\Xi = du dv dw d\varpi_1 \cdots d\varpi_K \), \( \gamma \) is the specific heat ratio and \( K = (5 - 3\gamma)/(\gamma - 1) \) is the internal degrees of freedom for three-dimensional flows. Taking moments of the BGK equation (2.1), the three-dimensional conservative system can be written as

\[ \frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = 0, \]

where \( Q = (\rho, \rho u, \rho v, \rho w, \rho E)^T \) is the conservative variable, and \( F, G, H \) are fluxes in \( x, y, z \) directions given by

\[
\begin{pmatrix}
F \\
G \\
H
\end{pmatrix} = \int \begin{pmatrix} u \\ v \\ w \end{pmatrix} \psi f d\Xi.
\]

According to the Chapman-Enskog expansion for BGK equation, the macroscopic governing equations can be derived [48, 49]. In the continuum region, the BGK equation can be rearranged and the gas distribution function can be expanded as

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

where \( D_u = \frac{\partial}{\partial t} + u \cdot \nabla \). With the zeroth-order truncation \( f = g \), the Euler equations can be obtained. For the first-order truncation

\[ f = g - \tau (ug_x + vg_y + wg_z + g_t), \]
the Navier-Stokes equations can be obtained. Based on the higher-order truncations, the Burnett and super-Burnett equations can be obtained as well.

In order to construct the numerical scheme in curvilinear coordinates, the coordinate transformation from the physical domain \((x, y, z)\) to the computational domain \((\xi, \eta, \zeta)\) is considered

\[
\left( \frac{\partial (x, y, z)}{\partial (\xi, \eta, \zeta)} \right) = \begin{pmatrix}
x_\xi & x_\eta & x_\zeta 
\end{pmatrix}.
\]

With the transformation above, the BGK equation (2.1) can be transformed as

\[
\frac{\partial}{\partial t} \left( J f \right) + \frac{\partial}{\partial \xi} \left( [u\hat{\xi}x + v\hat{\xi}y + w\hat{\xi}z] f \right) + \frac{\partial}{\partial \eta} \left( [u\hat{\eta}x + v\hat{\eta}y + w\hat{\eta}z] f \right) + \frac{\partial}{\partial \zeta} \left( [u\hat{\zeta}x + v\hat{\zeta}y + w\hat{\zeta}z] f \right) = \frac{g - f}{\tau} J, \tag{2.3}
\]

where \(J\) is the Jacobian of transformation, and the metrics above are given as follows

\[
\begin{pmatrix}
\hat{\xi}_x & \hat{\xi}_y & \hat{\xi}_z \\
\hat{\eta}_x & \hat{\eta}_y & \hat{\eta}_z \\
\hat{\zeta}_x & \hat{\zeta}_y & \hat{\zeta}_z
\end{pmatrix} = \begin{pmatrix}
y_\eta \hat{\zeta}_z - z_\eta \hat{\zeta}_y & z_\eta \hat{x}_z - x_\eta \hat{x}_y & x_\eta \hat{y}_z - y_\eta \hat{y}_x \\
y_\zeta \hat{x}_z - z_\zeta \hat{x}_y & z_\zeta \hat{y}_z - x_\zeta \hat{y}_x & x_\zeta \hat{x}_y - y_\zeta \hat{x}_z \\
y_\zeta \hat{y}_z - z_\zeta \hat{y}_x & z_\zeta \hat{x}_y - x_\zeta \hat{x}_z & x_\zeta \hat{x}_z - y_\zeta \hat{x}_y \\
\end{pmatrix}.
\]

Taking moments of Eq. (2.3), we can obtain the conservative system in curvilinear coordinate

\[
\frac{\partial \hat{Q}}{\partial t} + \frac{\partial \hat{F}}{\partial \xi} + \frac{\partial \hat{G}}{\partial \eta} + \frac{\partial \hat{H}}{\partial \zeta} = 0, \tag{2.4}
\]

where \(\hat{Q} = J Q\) and \(\hat{F}, \hat{G}, \hat{H}\) are fluxes in \(\xi, \eta, \zeta\) directions given by

\[
\hat{F} = \int [u\hat{\xi}x + v\hat{\xi}y + w\hat{\xi}z] \psi f d\Xi, \\
\hat{G} = \int [u\hat{\eta}x + v\hat{\eta}y + w\hat{\eta}z] \psi f d\Xi, \\
\hat{H} = \int [u\hat{\zeta}x + v\hat{\zeta}y + w\hat{\zeta}z] \psi f d\Xi.
\]

Eq. (2.4) can be also obtained by taking coordinate transformation for macroscopic Euler equation, and numerical scheme can be constructed in finite volume framework with Riemann solvers \([41]\). In order to construct the high-order scheme with Lax-Wendroff type flow solvers \([28]\), i.e. the spatial and temporal coupled flux solvers, the geometric metrics and the corresponding numerical fluxes need to be further considered.
Integrating Eq. (2.4) over the control volume $V_{ijk}$, the semi-discretized finite volume scheme can be written as

$$\frac{d\hat{Q}_{ijk}}{dt} = \mathcal{L} (\hat{Q}_{ijk}) = \frac{1}{|V_{ijk}|} \left[ \int_{\eta_j-\Delta\eta/2}^{\eta_j+\Delta\eta/2} \int_{\zeta_k-\Delta\zeta/2}^{\zeta_k+\Delta\zeta/2} (\hat{F}_{i+1/2,j,k}^{\eta,j} - \hat{F}_{i-1/2,j,k}^{\eta,j}) d\eta d\zeta \\
+ \int_{\xi_i-\Delta\xi/2}^{\xi_i+\Delta\xi/2} \int_{\zeta_k-\Delta\zeta/2}^{\zeta_k+\Delta\zeta/2} (\hat{G}_{i,j+1/2,k}^{\eta,j} - \hat{G}_{i,j-1/2,k}^{\eta,j}) d\eta d\zeta \\
+ \int_{\zeta_k-\Delta\zeta/2}^{\zeta_k+\Delta\zeta/2} \int_{\eta_j-\Delta\eta/2}^{\eta_j+\Delta\eta/2} (\hat{H}_{i,j,k+1/2}^{\eta,j} - \hat{H}_{i,j,k-1/2}^{\eta,j}) d\eta d\zeta \right], \quad (2.5)$$

where $|V_{ijk}| = \Delta\xi\Delta\eta\Delta\zeta$. The numerical fluxes in $\xi$-direction are given as example. To achieve the spatial accuracy, the Gaussian quadrature is used over the cell interface and we have

$$\hat{F}_{i+1/2,j,k}(t) = \int_{\eta_j-\Delta\eta/2}^{\eta_j+\Delta\eta/2} \int_{\zeta_k-\Delta\zeta/2}^{\zeta_k+\Delta\zeta/2} \hat{F}_{i+1/2,j,k}^{\eta,j} d\eta d\zeta \\
= \Delta\eta\Delta\zeta \sum_{m,n=1}^{2} \omega_{mn} \hat{F}(\xi_{i+1/2,j,m,k,n},t), \quad (2.6)$$

where $\xi_{i+1/2,j,m,k,n}$ is the Gauss quadrature point of cell interface $[\eta_j-\Delta\eta/2,\eta_j+\Delta\eta/2] \times [\zeta_k-\Delta\zeta/2,\zeta_k+\Delta\zeta/2]$ with $\zeta = \xi_{i+1/2}$, and $\omega_{mn},m,n = 1,2$ are quadrature weights. The numerical fluxes $\hat{G}_{i,j+1/2,k}(t)$ and $\hat{H}_{i,j,k+1/2}(t)$ in $\eta,\zeta$ directions can be defined as well. According to the definition of $\hat{F}$, the numerical fluxes in Eq. (2.6) at quadrature point can
each Gaussian quadrature point, which can be determined sequentially

\[ \tilde{F}(\xi_{i+1/2,jn,k_n},t) = \begin{pmatrix} \tilde{F}_p \\ \tilde{F}_{pu} \\ \tilde{F}_{pv} \\ \tilde{F}_{pE} \end{pmatrix} = S_\xi \int \tilde{u} \tilde{\psi} f(x_{i+1/2,jn,k_n},t,\tilde{u},\xi) d\tilde{\Xi}, \]

where \( S_\xi = \sqrt{\frac{\xi_x^2}{\xi_x^2 + \xi_y^2 + \xi_z^2}}, \) \( d\tilde{\Xi} = d\tilde{u} d\tilde{v} d\tilde{w} d\xi^1 \cdots d\xi^K. \) The local particle velocity is given by

\[ (\tilde{u},\tilde{v},\tilde{w}) = (u,v,w) \cdot (n_x,n_y,n_z), \]

where \( n_x \) is the normal direction, and \( n_y,n_z \) are two orthogonal tangential directions at each Gaussian quadrature point, which can be determined sequentially

\[ n_x = \left( \frac{\xi_y \xi_z}{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}}, \xi_z \xi_x, \xi_x \xi_y \right)/\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}, \]
\[ n_z = \left( \frac{\xi_y \xi_z}{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}}, \right)/\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}, \]
\[ n_y = n_z \times n_x. \]

Denote \( (a_{ij}) \) is the inverse of \( (n_x,n_y,n_z), \) each component of \( \tilde{F}(\xi_{i+1/2,jn,k_n},t) \) can be given by the combination of fluxes in the local orthogonal coordinate

\[
\begin{align*}
\left\{ \begin{array}{l}
\tilde{F}_p = S_\xi F_{\tilde{p}}, \\
\tilde{F}_{pu} = S_\xi (a_{11} F_\tilde{p}\tilde{u} + a_{12} F_\tilde{p}\tilde{v} + a_{13} F_\tilde{p}\tilde{w}), \\
\tilde{F}_{pv} = S_\xi (a_{21} F_\tilde{p}\tilde{u} + a_{22} F_\tilde{p}\tilde{v} + a_{23} F_\tilde{p}\tilde{w}), \\
\tilde{F}_{pE} = S_\xi F_{\tilde{p}E}, \\
\end{array} \right.
\end{align*}
\]

where the fluxes in the local coordinate can be obtained as follows

\[ (F_{\tilde{p}},F_{\tilde{p}u},F_{\tilde{p}v},F_{\tilde{p}E})^T = \int \tilde{u} \tilde{\psi} f(x_{i+1/2,jn,k_n},t,\tilde{u},\xi) d\tilde{\Xi}, \]

and \( \tilde{\psi} = (1,\tilde{u},\tilde{v},\tilde{w},(\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2 + \xi^2)/2)^T. \) The procedure above shows that the spatial reconstruction, including the conservative variables and their spatial derivatives, needs to be conducted in the orthogonal local coordinate \( (n_x,n_y,n_z) \) in the physical domain.

With the integral solution of BGK equation, the gas distribution function can be constructed as follows

\[ f(x_{i+1/2,jn,k_n},t,u,\xi) = \frac{1}{\tau} \int_0^t g(x',t',u,\xi) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_0(-ut,\xi), \]
where \( \tilde{u} = (\tilde{u}, \tilde{v}, \tilde{w}) \) is denoted as \( u = (u, v, w) \) for simplicity in this section, \( x_{i+1/2,jm,k_l} = (x_{i+1/2}, y_{jm}, z_{k_l}) \) is the location of Gaussian quadrature point, \( x' = x_{i+1/2} - u(t-t') \), \( y' = y_{jm} - v(t-t') \), \( z' = z_{k_l} - w(t-t') \) are the trajectory of particles, \( f_0 \) is the initial gas distribution function, and \( g \) is the corresponding equilibrium state. With the reconstruction of macroscopic variables, the gas distribution function at cell interface can be expressed as

\[
f(x_{i+1/2,jm,k_l}, t, u, \zeta) = (1-e^{-t/\tau})g_0 + ((t+\tau)e^{-t/\tau} - \tau)(\bar{\varphi}_1 u + \bar{\varphi}_2 v + \bar{\varphi}_3 w)g_0 \\
+ (t-\tau + \tau e^{-t/\tau})\tilde{A}g_0 \\
+ e^{-t/\tau}g_v[1-(\tau+t)(a_1^l u + a_2^l v + a_3^l w-\tau A^l)]H(u) \\
+ e^{-t/\tau}g_l[1-(\tau+t)(a_1^l u + a_2^l v + a_3^l w-\tau A^l)](1-H(u)),
\]

where the equilibrium state \( g_0 \) and corresponding conservative variables \( Q_0 \) at the quadrature point can be determined by the compatibility condition (2.2)

\[
\int \psi g_0 d\Xi = Q_0 = \int_{u>0} \psi g_l d\Xi + \int_{u<0} \psi g_r d\Xi,
\]

and the coefficients in Eq. (2.8) can be determined by the reconstructed directional derivatives and compatibility condition

\[
\langle a_1^k \rangle = \frac{\partial Q_k}{\partial n_x}, \quad \langle a_2^k \rangle = \frac{\partial Q_k}{\partial n_y}, \quad \langle a_3^k \rangle = \frac{\partial Q_k}{\partial n_z}, \quad \langle a_1^l u + a_2^l v + a_3^l w + A^l \rangle = 0,
\]

\[
\langle \varphi_1 \rangle = \frac{\partial Q_0}{\partial n_x}, \quad \langle \varphi_2 \rangle = \frac{\partial Q_0}{\partial n_y}, \quad \langle \varphi_3 \rangle = \frac{\partial Q_0}{\partial n_z}, \quad \langle \varphi_1 u + \varphi_2 v + \varphi_3 w + \bar{A} \rangle = 0,
\]

where \( k = l, r, \) and \( \langle \cdots \rangle \) are moments of the equilibrium \( g \) and defined by

\[
\langle \cdots \rangle = \int g(\cdots) \psi d\Xi.
\]

More details of the gas-kinetic scheme can be found in [48].

### 3 High-order scheme in curvilinear coordinate

#### 3.1 Spatial reconstruction

To achieve the high-order spatial accuracy, the fifth-order WENO reconstruction [8, 23, 32] is adopted. In the curvilinear coordinates, the reconstruction is conducted for the cell averaged variables \( \mathcal{J} Q \) and \( \mathcal{J} \). However, the reconstructed variables \( Q \) and spatial derivatives \( \frac{\partial Q}{\partial n_x}, \frac{\partial Q}{\partial n_y}, \frac{\partial Q}{\partial n_z} \) are needed for the gas-kinetic solver, and the special treatment is needed for reconstruction. The procedure is given as follows:
1. For each Gaussian quadrature point $\xi = \xi_{i+1/2}$, the local coordinate $(n_x, n_y, n_z)$ is determined according to Eq. (2.7). For a general coordinate transformation, the local coordinate is different for each quadrature point. More computational cost will be introduced for the reconstruction because the variables need to be projected into different local coordinate.

2. According to one-dimensional WENO-Z reconstruction [8], the cell averaged reconstructed values at $\xi = \xi_{i+1/2}$ can be constructed

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

where $\ell_1, \ell_2 = -2, \ldots, 2$. With the WENO reconstruction in the horizontal direction over the interval $[\xi_{k-\ell_2} - \Delta \xi / 2, \xi_{k-\ell_2} + \Delta \xi / 2]$, the line-averaged values with $\eta = \eta_{ju}$ can be given

$$( J Q_l )_{ju, k-\ell_2, r} ( J Q_r )_{ju, k-\ell_2, r} ( J Q_0 )_{ju, k-\ell_2, r}.$$

With the WENO reconstruction in the vertical direction, the point values at Gaussian quadrature point $\xi = \xi_{i+1/2}$, $\eta = \eta_{ju}$ can be given

$$( J Q_l )_{ju, k-\ell_2, r} ( J Q_r )_{ju, k-\ell_2, r} ( J Q_0 )_{ju, k-\ell_2, r}.$$

With the identical procedure, the reconstructed Jacobian can be also obtained at the Gaussian quadrature point $\xi = \xi_{i+1/2}$, $\eta = \eta_{ju}$ as well

$$( J )_{ju, k-\ell_2, r} ( J )_{ju, k-\ell_2, r} ( J )_{ju, k-\ell_2, r}.$$

For simplicity, the subscripts corresponding to the Gaussian quadrature points and the variables at the left, right and across the cell interface are omitted. With the reconstruction of $( J Q )$ and $J$, the point value $Q$ can be calculated by

$$Q = \frac{( J Q )}{J}.$$

The procedure above is standard for the classical scheme with Riemann solvers [41], and the numerical methods can be extended to the curvilinear coordinates directly. With the spatial and temporal decoupled fluxes, the Runge-Kutta method is need for temporal accuracy. To implement the spatial-temporal coupled flow solvers, the spatial derivatives at Gaussian quadrature points need to be calculated accurately, which is key for achieving high-order accuracy.

3. According to WENO-Z reconstruction above, the spatial derivatives of the reconstructed variables at Gaussian quadrature points $\xi = \xi_{i+1/2}$, $\eta = \eta_{ju}$ can be given

$$( \partial_\xi ( J Q_l ) )_{ju, k-\ell_2, r} ( \partial_\xi ( J Q_r ) )_{ju, k-\ell_2, r} ( \partial_\xi ( J Q_0 ) )_{ju, k-\ell_2, r},$$

$$( \partial_\eta ( J Q_l ) )_{ju, k-\ell_2, r} ( \partial_\eta ( J Q_r ) )_{ju, k-\ell_2, r} ( \partial_\eta ( J Q_0 ) )_{ju, k-\ell_2, r},$$

$$( \partial_\xi ( J Q_l ) )_{ju, k-\ell_2, r} ( \partial_\xi ( J Q_r ) )_{ju, k-\ell_2, r} ( \partial_\xi ( J Q_0 ) )_{ju, k-\ell_2, r}. $$
and

\[
(\partial_\xi J_l)_{j_m,k_n}, (\partial_\eta J_l)_{j_m,k_n}, (\partial_\zeta J_l)_{j_m,k_n}, \quad (\partial_\xi J_r)_{j_m,k_n}, (\partial_\eta J_r)_{j_m,k_n}, (\partial_\zeta J_r)_{j_m,k_n},
\]

\[
(\partial_\xi J_0)_{j_m,k_n}, (\partial_\eta J_0)_{j_m,k_n}, (\partial_\zeta J_0)_{j_m,k_n}.
\]

4. The spatial derivatives \(Q_\xi, Q_\eta, Q_\zeta\) in the computational domain can be obtained by the above reconstructed \((JQ)_{\xi}, (JQ)_{\eta}, (JQ)_{\zeta}\) and chain rule as well

\[
Q_\xi = \frac{(JQ)_{\xi} - Q_{J_\xi}}{J},
\]

\[
Q_\eta = \frac{(JQ)_{\eta} - Q_{J_\eta}}{J},
\]

\[
Q_\zeta = \frac{(JQ)_{\eta} - Q_{J_\zeta}}{J}.
\]

However, what we need is the directional derivatives \(\frac{\partial Q}{\partial n_x}, \frac{\partial Q}{\partial n_y}, \frac{\partial Q}{\partial n_z}\). According to the chain rule, the spatial derivatives can be rewritten as

\[
Q_\xi = Q_\xi x_\xi + Q_\eta y_\xi + Q_\zeta z_\xi,
\]

\[
Q_\eta = Q_\xi x_\eta + Q_\eta y_\eta + Q_\zeta z_\eta,
\]

\[
Q_\zeta = Q_\xi x_\zeta + Q_\eta y_\zeta + Q_\zeta z_\zeta.
\]

The normalized spatial derivatives can be considered as the directional derivatives along the following direction

\[
Q_\xi' = \frac{Q_\xi}{|x_\xi|}, \quad \tau_1 = \frac{(x_\xi, y_\xi, z_\xi)}{|x_\xi|},
\]

\[
Q_\eta' = \frac{Q_\eta}{|x_\eta|}, \quad \tau_2 = \frac{(x_\eta, y_\eta, z_\eta)}{|x_\eta|},
\]

\[
Q_\zeta' = \frac{Q_\zeta}{|x_\zeta|}, \quad \tau_3 = \frac{(x_\zeta, y_\zeta, z_\zeta)}{|x_\zeta|},
\]

where \(\tau_1, \tau_2, \tau_3\) can be obtained from the coordinate transformation. For the Cartesian mesh, they coincide with \(n_x, n_y, n_z\). However, for the general meshes, they are not orthogonal. The procedure of orthogonalization is used to generate the spatial derivatives in the local orthogonal coordinate for the calculation of numerical fluxes

\[
\frac{\partial Q}{\partial n_x} = Q_{\xi}',
\]

\[
\frac{\partial Q}{\partial n_y} = \frac{1}{(\tau_2, n_y)} Q_{\eta}' - \frac{(\tau_2, n_z)}{(\tau_2, n_y)} \frac{\partial Q}{\partial n_z},
\]

\[
\frac{\partial Q}{\partial n_z} = \frac{1}{(\tau_1, n_z)} Q_{\zeta}' - \frac{(\tau_1, n_y)}{(\tau_1, n_z)} \frac{\partial Q}{\partial n_y} - \frac{(\tau_1, n_z)}{(\tau_1, n_z)} \frac{\partial Q}{\partial n_z}.
\]
Thus, the spatial derivatives in the local orthogonal coordinate are fully determined. The fourth step is analytical and no error is introduced. So long as the spatial accuracy is achieved in the second and third step, the order of accuracy can be maintained by the procedures above.

### 3.2 Temporal discretization

A two-stage fourth-order time-accurate discretization was developed for Lax-Wendroff flow solvers with the generalized Riemann problem (GRP) solver [29] and the gas-kinetic scheme (GKS) [35]. Consider the following time-dependent equation

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

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

\[
q(t = t_n) = q^n,
\]

where \( \mathcal{L} \) is an operator for spatial derivative of flux. The state \( q^{n+1} \) at \( t_{n+1} = t_n + \Delta t \) can be updated with the following formula

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

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

It can be proved that for hyperbolic equations the above temporal discretization provides a fourth-order time accurate solution for \( q^{n+1} \).

In order to develop the high-order scheme in the curvilinear coordinate, the semi-discretized finite volume scheme

\[
\frac{d\hat{Q}_{ijk}}{dt} = \mathcal{L}(\hat{Q}_{ijk}),
\]

can be discretized according to the two-stage temporal method. To implement two-stage method, the following notation is introduced by Eq. (2.6)

\[
\hat{F}_{i+1/2,j,k}(\delta) = \int_{t_n}^{t_{n+\delta}} \hat{F}_{i+1/2,j,k}(t) \, dt = \int_{t_n}^{t_{n+\delta}} \sum_{m,n=1}^{2} S_{mn} \int \tilde{u} \psi f(x_{i+1/2,j,m}, \tilde{u}, \varsigma) d\tilde{\xi} dt,
\]

and it can be expanded as the following linear form in the time interval \([t_n, t_n + \Delta t] \)

\[
\hat{F}_{i+1/2,j,k}(t) = \hat{F}_{i+1/2,j,k}^{n} + \partial_t \hat{F}_{i+1/2,j,k}^{n}(t - t_n).
\]
Integrate over $[t_n, t_n + \Delta t / 2]$ and $[t_n, t_n + \Delta t]$, we have the following two equations

\[
\hat{F}^n_{i+1/2,j,k} \Delta t + \frac{1}{2} \partial_t \hat{F}^n_{i+1/2,j,k} \Delta t^2 = \hat{F}^n_{i+1/2,j,k}(\Delta t),
\]

\[
\frac{1}{2} \hat{F}^n_{i+1/2,j,k} \Delta t + \frac{1}{8} \partial_t \hat{F}^n_{i+1/2,j,k} \Delta t^2 = \hat{F}^n_{i+1/2,j,k}(\Delta t / 2).
\]

By solving the linear system, the coefficients $\hat{F}^n_{i+1/2,j,k}$ and $\partial_t \hat{F}^n_{i+1/2,j,k}$ can be determined. Similarly, the fluxes and temporal derivatives in $\eta$ and $\zeta$ directions can be also obtained. Thus, the operator and its temporal derivative at $t^n$ can be given by

\[
\mathcal{L}(\hat{Q}^n_{ijk}) = -\frac{1}{|V_{ijk}|} \left[ (\hat{F}^n_{i+1/2,j,k} - \hat{F}^n_{i-1/2,j,k}) + (\hat{G}^n_{i,j+1/2,k} - \hat{G}^n_{i,j-1/2,k}) + (\hat{H}^n_{i,j,k+1/2} - \hat{H}^n_{i,j,k-1/2}) \right],
\]

\[
\mathcal{L}_t(\hat{Q}^n_{ijk}) = -\frac{1}{|V_{ijk}|} \left[ (\partial_t \hat{F}^n_{i+1/2,j,k} - \partial_t \hat{F}^n_{i-1/2,j,k}) + (\partial_t \hat{G}^n_{i,j+1/2,k} - \partial_t \hat{G}^n_{i,j-1/2,k}) + (\partial_t \hat{H}^n_{i,j,k+1/2} - \partial_t \hat{H}^n_{i,j,k-1/2}) \right].
\]

With the reconstruction at the intermediate state, $\mathcal{L}_t(\hat{Q}^n_{ijk})$ can be constructed. More details of the two-stage fourth-order scheme can be found in [29, 35].

### 3.3 One-dimensional scheme in non-equidistant grids

As a particular case, the method for one-dimensional flow degenerates to the scheme in non-equidistant grids. For one-dimensional flows, the finite volume scheme (2.5) can be simplified as

\[
\frac{d(JQ)_i}{dt} = -\frac{1}{\Delta \xi} (\hat{F}^n_{i+1/2} - \hat{F}^n_{i-1/2}),
\]

where $F_{i+1/2}$ is the numerical flux in the physical domain. To implement the high-order gas-kinetic scheme, the point value $Q_{i+1/2}$ and spatial derivative $(Q_x)_{i+1/2}$ are needed. With the reconstructed for cell averaged variable $(JQ)$ and cell averaged Jacobian $J$, the point value is given by

\[
Q_{i+1/2} = \frac{(JQ)_{i+1/2}}{J_{i+1/2}}.
\]

With the coordinate transformation, the relation of spatial derivative can be expressed as

\[
Q_{\xi} = Q_x \xi_x.
\]
The spatial derivative can be calculated by

\[(Q_x)_{i+1/2} = \frac{(Q_x)_{i+1/2}}{(x_{i+1/2})},\]

where \((Q_x)_{i+1/2}\) is given by the chain rule

\[(Q_x)_{i+1/2} = \left(\frac{(J Q)_{i+1/2} - Q_{i+1/2}(J_x)_{i+1/2}}{J_{i+1/2}}\right).

With the above procedure, the one-dimensional gas-kinetic scheme is obtained.

4 Numerical tests

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

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

where \(\epsilon = 0.01\) and \(C = 1\). For the viscous flow, we have

\[\tau = \frac{v}{p} + C \left| \frac{p_l - p_r}{p_l + p_r} \right| \Delta t,\]

where \(p_l\) and \(p_r\) denote the pressure on the left and right sides of the cell interface, \(v\) is the dynamic viscous coefficient, and \(p\) is the pressure at the cell interface. The ratio of specific heats takes \(\gamma = 1.4\). 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.

Remark 4.1. In this paper, all examples are tested with analytical coordinate transformations. In practice, the meshes are mostly generated by discrete methods like software. The geometrical metrics need to be interpolated from available discrete points at Gaussian points. The interpolation is critical for the high order accuracy and geometrical conservation law [47]. More examples with general geometries will be tested in the future for the practical application.

4.1 Accuracy tests

The advection of density perturbation for the one-dimensional to three-dimensional flows are presented to test the order of accuracy. For the one-dimensional case, the physical domain is \([0,2]\) and the initial conditions are set as follows

\[\rho_0(x) = 1 + 0.2\sin(\pi x), \quad p_0(x) = 1, \quad U_0(x) = 1.\]
Table 1: Accuracy test: 1D advection of density perturbation with nonuniform meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>order</th>
<th>$L^2$ error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>2.5450E-03</td>
<td></td>
<td>2.0040E-03</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>8.0378E-05</td>
<td>4.9847</td>
<td>6.3372E-05</td>
<td>4.9829</td>
</tr>
<tr>
<td>40</td>
<td>2.5856E-06</td>
<td>4.9582</td>
<td>2.0277E-06</td>
<td>4.9659</td>
</tr>
<tr>
<td>80</td>
<td>8.1489E-08</td>
<td>4.9877</td>
<td>6.3762E-08</td>
<td>4.9910</td>
</tr>
<tr>
<td>160</td>
<td>2.5499E-09</td>
<td>4.9980</td>
<td>1.9959E-09</td>
<td>4.9975</td>
</tr>
<tr>
<td>320</td>
<td>7.9780E-11</td>
<td>4.9983</td>
<td>6.2447E-11</td>
<td>4.9982</td>
</tr>
<tr>
<td>640</td>
<td>2.5150E-12</td>
<td>4.9973</td>
<td>1.9801E-12</td>
<td>4.9789</td>
</tr>
</tbody>
</table>

Table 2: Accuracy test: 1D advection of density perturbation with uniform meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>order</th>
<th>$L^2$ error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.7066E-03</td>
<td></td>
<td>1.3691E-03</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>5.7014E-05</td>
<td>4.9036</td>
<td>4.4846E-05</td>
<td>4.9321</td>
</tr>
<tr>
<td>40</td>
<td>1.8059E-06</td>
<td>4.9804</td>
<td>1.4147E-06</td>
<td>4.9863</td>
</tr>
<tr>
<td>80</td>
<td>5.6518E-08</td>
<td>4.9979</td>
<td>4.4293E-08</td>
<td>4.9972</td>
</tr>
<tr>
<td>160</td>
<td>1.7678E-09</td>
<td>4.9986</td>
<td>1.3852E-09</td>
<td>4.9989</td>
</tr>
<tr>
<td>320</td>
<td>5.5340E-11</td>
<td>4.9975</td>
<td>4.3366E-11</td>
<td>4.9973</td>
</tr>
<tr>
<td>640</td>
<td>1.7396E-12</td>
<td>4.9973</td>
<td>1.3633E-12</td>
<td>4.9913</td>
</tr>
</tbody>
</table>

The periodic boundary conditions are imposed at both ends of the physical domain and the exact solutions are

$$\rho(x,t) = 1 + 0.2\sin(\pi(x-t)), \quad p(x,t) = 1, \quad U(x,t) = 1.$$ 

The computational domain is $[0,2]$ as well, and a nonuniform mesh is provided by the following coordinate transformation

$$x = \xi + 0.05\sin(\pi\xi),$$

where $N$ uniform cells are used in computational domain. In order to get the cell integrated flow variables, three-point Gaussian quadrature is used inside each cell to evaluate the values without losing accuracy. As reference, the mesh with $N$ uniform cells in physical domain is tested as well. The $L^1$ and $L^2$ errors and orders of accuracy at $t=2$ are presented in Table 1 and Table 2 for both nonuniform and uniform meshes, respectively. The expected order of accuracy are achieved with the mesh refinement.

For the two-dimensional case, the physical domain is $[0,2] \times [0,2]$ and the initial conditions are given as follows

$$\rho_0(x,y) = 1 + 0.2\sin(\pi(x+y)), \quad p_0(x,y) = 1, \quad U_0(x,y) = 1, \quad V_0(x,y) = 1.$$
The periodic boundary conditions are imposed at boundaries and the exact solutions are

\[ \rho(x,y,t) = 1 + 0.2\sin(\pi(x+y-t)), \quad p(x,y,t) = 1, \]
\[ U(x,y,t) = 1, \quad V(x,y,t) = 1. \]

The computational domain is \([0,2] \times [0,2]\), and \(N \times N\) uniform cells are used. The nonuniform orthogonal mesh and nonuniform nonorthogonal mesh are tested respectively, where the orthogonal is given by

\[ \begin{align*}
x &= \xi + 0.05\sin(\pi\xi), \\
y &= \eta + 0.05\sin(\pi\eta),
\end{align*} \]

the nonorthogonal mesh is given by

\[ \begin{align*}
x &= \xi + 0.05\sin(\pi\xi)\sin(\pi\eta), \\
y &= \eta + 0.05\sin(\pi\xi)\sin(\pi\eta),
\end{align*} \]

and the orthogonal and nonorthogonal meshes with \(40 \times 40\) cells are presented in Fig. 2 as example. As reference, the uniform mesh with \(N^2\) cells in the physical domain is also tested. Two-dimensional Gauss quadratures are used to provide the initial conditions. The \(L^1\) and \(L^2\) errors and orders of accuracy at \(t = 2\) with \(N^2\) cells are presented in Table 3, Table 4 and Table 5 for nonuniform orthogonal meshes, nonorthogonal meshes and uniform meshes. The expected accuracy can be also achieved for the current scheme.
Table 3: Accuracy test: 2D advection of density perturbation with nonuniform orthogonal meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>order</th>
<th>$L^2$ error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^2$</td>
<td>9.3427E-03</td>
<td>5.3475E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$20^2$</td>
<td>3.0710E-04</td>
<td>4.9270</td>
<td>1.7197E-04</td>
<td>4.9585</td>
</tr>
<tr>
<td>$40^2$</td>
<td>9.7453E-06</td>
<td>4.9778</td>
<td>5.4578E-06</td>
<td>4.9777</td>
</tr>
<tr>
<td>$80^2$</td>
<td>3.0561E-07</td>
<td>4.9949</td>
<td>1.7120E-07</td>
<td>4.9945</td>
</tr>
<tr>
<td>$160^2$</td>
<td>2.9939E-10</td>
<td>4.9972</td>
<td>1.7120E-10</td>
<td>4.9971</td>
</tr>
</tbody>
</table>

Table 4: Accuracy test: 2D advection of density perturbation with nonuniform nonorthogonal meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>order</th>
<th>$L^2$ error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^2$</td>
<td>2.0481E-02</td>
<td>1.2061E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$20^2$</td>
<td>9.4574E-04</td>
<td>4.4367</td>
<td>5.3232E-04</td>
<td>4.5019</td>
</tr>
<tr>
<td>$40^2$</td>
<td>3.1638E-05</td>
<td>4.9017</td>
<td>1.7690E-05</td>
<td>4.9112</td>
</tr>
<tr>
<td>$80^2$</td>
<td>9.9865E-07</td>
<td>4.9856</td>
<td>5.6017E-07</td>
<td>4.9809</td>
</tr>
<tr>
<td>$160^2$</td>
<td>3.1326E-08</td>
<td>4.9945</td>
<td>1.7701E-08</td>
<td>4.9839</td>
</tr>
<tr>
<td>$320^2$</td>
<td>9.8696E-10</td>
<td>4.9882</td>
<td>5.7052E-10</td>
<td>4.9554</td>
</tr>
</tbody>
</table>

Table 5: Accuracy test: 2D advection of density perturbation with uniform meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>order</th>
<th>$L^2$ error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^2$</td>
<td>6.7911E-03</td>
<td>3.7248E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$20^2$</td>
<td>2.2028E-04</td>
<td>4.9462</td>
<td>1.2245E-04</td>
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</tr>
<tr>
<td>$40^2$</td>
<td>7.0197E-06</td>
<td>4.9718</td>
<td>3.8911E-06</td>
<td>4.9758</td>
</tr>
<tr>
<td>$80^2$</td>
<td>2.2575E-07</td>
<td>4.9585</td>
<td>1.2518E-07</td>
<td>4.9580</td>
</tr>
<tr>
<td>$160^2$</td>
<td>7.7220E-09</td>
<td>4.8696</td>
<td>4.2895E-09</td>
<td>4.8670</td>
</tr>
<tr>
<td>$320^2$</td>
<td>3.0956E-10</td>
<td>4.6406</td>
<td>1.7222E-10</td>
<td>4.6384</td>
</tr>
</tbody>
</table>

The three-dimensional accuracy test is presented as well, which is the start point of the simulation of complex flows with complicated geometry. The physical domain is $[0,2] \times [0,2] \times [0,2]$ and the initial condition is set as follows

$$
\rho_0(x,y,z) = 1 + 0.2\sin(\pi(x+y+z)), \quad p_0(x,y,z) = 1,
U_0(x,y,z) = 1, \quad V_0(x,y,z) = 1, \quad W_0(x,y,z) = 1.
$$

The periodic boundary conditions are applied at boundaries, and the exact solutions are

$$
\rho(x,y,z,t) = 1 + 0.2\sin(\pi(x+y+z-t)), \quad p(x,y,z,t) = 1,
U(x,y,z,t) = 1, \quad V(x,y,z,t) = 1, \quad W(x,y,z,t) = 1.
$$

The computational domain is $[0,2] \times [0,2] \times [0,2]$. The nonuniform orthogonal mesh and nonuniform nonorthogonal mesh are tested respectively, where the orthogonal mesh is
Table 6: Accuracy test: 3D advection of density perturbation with nonuniform orthogonal meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>Order</th>
<th>$L^2$ error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>2.6560E-02</td>
<td></td>
<td>1.0639E-02</td>
<td></td>
</tr>
<tr>
<td>$20^3$</td>
<td>9.0703E-04</td>
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<td>3.5650E-04</td>
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<td>2.9298E-05</td>
<td>4.9522</td>
<td>1.1508E-05</td>
<td>4.9531</td>
</tr>
<tr>
<td>$80^3$</td>
<td>3.5179E-07</td>
<td>4.9440</td>
<td>3.7407E-07</td>
<td>4.9432</td>
</tr>
<tr>
<td>$160^3$</td>
<td>5.3343E-08</td>
<td>4.8351</td>
<td>1.3126E-08</td>
<td>4.8328</td>
</tr>
</tbody>
</table>

Table 7: Accuracy test: 3D advection of density perturbation with nonuniform nonorthogonal meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>Order</th>
<th>$L^2$ error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>3.5692E-02</td>
<td></td>
<td>1.4482E-02</td>
<td></td>
</tr>
<tr>
<td>$20^3$</td>
<td>4.2433E-03</td>
<td>4.6482</td>
<td>6.1955E-04</td>
<td>4.5469</td>
</tr>
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<td>4.8458</td>
<td>2.1579E-05</td>
<td>4.8435</td>
</tr>
<tr>
<td>$80^3$</td>
<td>1.6323E-06</td>
<td>4.9223</td>
<td>7.0200E-07</td>
<td>4.9420</td>
</tr>
<tr>
<td>$160^3$</td>
<td>5.6847E-08</td>
<td>4.8437</td>
<td>2.3694E-08</td>
<td>4.8888</td>
</tr>
</tbody>
</table>

Table 8: Accuracy test: 3D advection of density perturbation with uniform meshes.

<table>
<thead>
<tr>
<th>mesh</th>
<th>$L^1$ error</th>
<th>Order</th>
<th>$L^2$ error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
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<td></td>
</tr>
<tr>
<td>$20^3$</td>
<td>6.3946E-04</td>
<td>4.8743</td>
<td>2.5037E-04</td>
<td>4.8926</td>
</tr>
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<td>8.1505E-06</td>
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</tr>
<tr>
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<td>4.6240</td>
<td>1.1391E-08</td>
<td>4.6231</td>
</tr>
</tbody>
</table>

given by

\[
\begin{cases}
    x = \xi + 0.05\sin(\pi \xi), \\
    y = \eta + 0.05\sin(\pi \eta), \\
    z = \zeta + 0.05\sin(\pi \zeta),
\end{cases}
\]

the nonorthogonal mesh is given by

\[
\begin{cases}
    x = \xi + 0.05\sin(\pi \xi)\sin(\pi \eta)\sin(\pi \zeta), \\
    y = \eta + 0.05\sin(\pi \xi)\sin(\pi \eta)\sin(\pi \zeta), \\
    z = \zeta + 0.05\sin(\pi \xi)\sin(\pi \eta)\sin(\pi \zeta),
\end{cases}
\]

and $N^3$ uniform cells are used in the computational domain. As reference, $N^3$ uniform cells in the physical domain is also tested. The $L^1$ and $L^2$ errors and orders of accuracy at $t = 2$ with $N^3$ cells are presented in Table 6, Table 7 and Table 8 for nonuniform orthogonal meshes, nonorthogonal meshes, and uniform meshes. The expected accuracy is also achieved for the current scheme for the three-dimensional cases.
4.2 Geometric conservation law

The geometric conservation law (GCL) [12] is also tested by the two-dimensional and three-dimensional nonuniform nonorthogonal meshes given above. The GCL is mainly about the maintenance of a uniform flow passing through a non-uniform non-orthogonal mesh. The initial condition for the two-dimensional case is

\[ \rho_0(x,y) = 1, \quad p_0(x,y) = 1, \quad U_0(x,y) = 1, \quad V_0(x,y) = 1, \]

and the initial condition for the three-dimensional case is

\[ \rho_0(x,y,z) = 1, \quad p_0(x,y,z) = 1, \quad U_0(x,y,z) = 1, \quad V_0(x,y,z) = 1, \quad W_0(x,y,z) = 1. \]

The periodic boundary conditions are adopted as well. The \( L^1 \) and \( L^2 \) errors at \( t = 0.5 \) for the two-dimensional case with \( N^2 \) cells are given in Table 9, and for the three-dimensional case with \( N^3 \) cells are given in Table 10. The results show that the errors reduce to the machine zero. The current scheme is based on the coordinate transformation given by a smooth function, which preserves the geometric conservation law analytically. For a general mesh, the special treatment of the metrics and Jacobian is needed [47].

<table>
<thead>
<tr>
<th>2D mesh</th>
<th>( L^1 ) error</th>
<th>( L^2 ) error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10(^2)</td>
<td>2.9805E-15</td>
<td>2.3133E-15</td>
</tr>
<tr>
<td>20(^2)</td>
<td>5.7204E-15</td>
<td>3.6866E-15</td>
</tr>
<tr>
<td>40(^2)</td>
<td>7.5987E-15</td>
<td>4.7070E-15</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3D mesh</th>
<th>( L^1 ) error</th>
<th>( L^2 ) error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10(^3)</td>
<td>1.0896E-14</td>
<td>4.9111E-15</td>
</tr>
<tr>
<td>20(^3)</td>
<td>1.5292E-14</td>
<td>6.7811E-15</td>
</tr>
<tr>
<td>40(^3)</td>
<td>1.8241E-14</td>
<td>8.1087E-15</td>
</tr>
</tbody>
</table>

4.3 One dimensional Riemann problems

In this case, two examples of one-dimensional Riemann problems are tested. The physical domain for the 1D case are \([0,1]\), and the computational domain is expressed as

\[ x = \xi + 0.1 \sin(2\pi \xi). \]

The first one is the Sod problem, and the initial condition is given as follows

\[ (\rho, U, p) = \begin{cases} 
(1,0,1), & 0 \leq x < 0.5, \\
(0.125,0,0.1), & 0.5 \leq x \leq 1.
\end{cases} \]
The non-reflecting boundary conditions are used at both ends, and 100 uniform cells are used in the computational domain. The density, velocity and pressure distributions at $t = 0.2$ are presented in Fig. 3. The current scheme well captures the exact solutions. The
second one is the Woodward-Colella blast wave problem [45], and the initial conditions are given as follows

\[(ρ, U, p) = \begin{cases} 
(1, 0, 1000), & 0 \leq x < 0.1, \\
(1, 0, 0.01), & 0.1 \leq x < 0.9, \\
(1, 0, 100), & 0.9 \leq x \leq 1. 
\end{cases}\]

The reflected boundary conditions are imposed on both ends, and 400 non-uniform cells are used in the computational domain. The density, velocity and pressure distributions at \(t = 0.038\) are presented in Fig. 3, which validate the robustness and resolution of currents scheme for the 1D strong discontinuity.

### 4.4 Two-dimensional Riemann problem

In this case, two examples of two-dimensional Riemann problems are tested. The meshes with \(40 \times 40\) cells are shown in Fig. 4 as example. The initial conditions for the first problem are

\[(ρ, U, V, p) = \begin{cases} 
(1, 0.75, -0.5, 0.5), & x > 0.5, y > 0.5, \\
(2, 0.75, 0.5, 0.5), & x < 0.5, y > 0.5, \\
(1, -0.75, 0.5, 0.5), & x < 0.5, y < 0.5, \\
(3, -0.75, -0.5, 0.5), & x > 0.5, y < 0.5, 
\end{cases}\]

in which four initial contacts waves interact with each other and result in a more complicated pattern. For these cases, the nonuniform orthogonal meshes

\[
\begin{align*}
x &= \xi + 0.05\sin(2\pi \xi), \\
y &= \eta + 0.05\sin(2\pi \eta),
\end{align*}
\]

![Figure 4: 2D Riemann problem: the nonuniform orthogonal and nonorthogonal mesh 40 × 40 cells.](image)
and nonuniform nonorthogonal meshes
\[
\begin{align*}
x &= \xi + 0.05\sin^2(2\pi \xi)\sin(2\pi \eta), \\
y &= \eta + 0.05\sin(2\pi \xi)\sin^2(2\pi \eta),
\end{align*}
\]
are tested respectively, where both the physical and computational domain are \([0,1] \times [0,1]\). The non-reflecting boundary conditions are used in all boundaries. Meanwhile, the meshes are given by symmetrically corresponding the boundaries. The density distributions for the first case at \(t=0.4\) and for the second case at \(t=0.25\) on the nonuniform orthogonal and nonorthogonal meshes with \(500 \times 500\) cells are presented in Fig. 5, respectively. The complicated flow structures are well captures by the current scheme with different type of meshes.

### 4.5 Double Mach reflection

This problem was extensively studied by Woodward and Colella [45] for the inviscid flow. The computational domain is \([0,4] \times [0,1]\), and a solid wall lies at the bottom of the computational domain starting from \(x = 1/6\). Initially a right-moving Mach 10 shock is positioned at \((x,y) = (1/6,0)\), and makes a 60° angle with the \(x\)-axis. The initial pre-shock and post-shock conditions are

\[
\begin{align*}
(\rho, U, V, p) &= (8, 4.125\sqrt{3}, -4.125, 116.5), \\
(\rho, U, V, p) &= (1.4, 0, 0, 1).
\end{align*}
\]

For this case, the nonuniform orthogonal meshes
\[
\begin{align*}
x &= \xi - 0.05\sin(2\pi \xi), \\
y &= \eta - 0.05\sin(2\pi \eta),
\end{align*}
\]
and nonuniform nonorthogonal meshes

\[
\begin{align*}
x &= \xi - 0.05\sin^2(2\pi \xi)\sin(2\pi \eta), \\
y &= \eta - 0.05\sin(2\pi \xi)\sin^2(2\pi \eta),
\end{align*}
\]

are tested respectively, where both the physical and computational domain are \([0,4] \times [0,1]\). The local meshes for the area \([2,3] \times [0,1]\) with \(160 \times 40\) cells are shown in Fig. 6 as example. The reflective boundary condition is used at the wall, while for the rest of bottom boundary, the exact post-shock condition is imposed. At the top boundary, the flow variables are set to describe the exact motion of the Mach 10 shock. The density distributions with \(800 \times 200\) uniform mesh points at \(t=0.2\) are shown in Fig. 7. The current scheme resolves the flow structure under the triple Mach stem clearly with the distorted meshes.

### 4.6 Flows past a cylinder

In this case, the inviscid hypersonic flows impinging on a cylinder are tested to validate robustness of the current scheme for the inviscid flow. For this case, the computational domain is \([0.5,1.5] \times [-0.5,0.5]\), and the physical domain is expressed as

\[
\begin{align*}
x &= \xi \cos(\pi \eta), \\
y &= \xi \sin(\pi \eta).
\end{align*}
\]

In the computation, \(60 \times 60\) cells are used shown in Fig. 8, which are given uniformly in the computational domain. This problem is initialized by a flow moving towards to a cylinder with different Mach numbers. The reflective boundary condition is imposed on
the surface of cylinder, and the outflow boundary condition is set on the left boundary. The Mach number distributions for the flows with $Ma = 5$, 8, and 10 are presented in Fig. 8, which show that the current scheme can capture strong shocks very well without carbuncle phenomenon [39]. The robustness of the scheme is well validated.

The viscous low speed flows over a cylinder is tested as well. In this case, the free stream velocity is $U_{\infty} = 1$ and $Ma_{\infty} = 0.15$. The physical domain is expressed as

$$\begin{align*}
  x &= 2\xi^2 \cos(\pi\eta), \\
  y &= 2\xi^2 \sin(\pi\eta),
\end{align*}$$

where $(\xi, \eta) \in [0.5, 4.5] \times [0, 2]$. 360 $\times$ 180 uniform cells are used for the computational do-
main, the non-slip boundary condition is used on the walls and the characteristic boundary condition is used for the inflow and outflow boundary. The streamlines and mesh distribution for $Re = 20$ and $40$ are presented in Fig. 9. The length of the recirculation region from the rearmost point of the cylinder to the end of the wake increases with the Reynolds number. The length for the current scheme and the previous results are presented in Table 11.

Table 11: Low speed flows past a cylinder: recirculation length $L$ with $Re = 20$ and $40$.

<table>
<thead>
<tr>
<th>Reference</th>
<th>$Re = 20$</th>
<th>$Re = 40$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dennis &amp; Chang [13]</td>
<td>0.940</td>
<td>2.345</td>
</tr>
<tr>
<td>Fornberg [16]</td>
<td>0.910</td>
<td>2.240</td>
</tr>
<tr>
<td>He &amp; Doolen [19]</td>
<td>0.921</td>
<td>2.245</td>
</tr>
<tr>
<td>Wu &amp; Shu [46]</td>
<td>0.930</td>
<td>2.310</td>
</tr>
<tr>
<td>present</td>
<td>0.911</td>
<td>2.245</td>
</tr>
</tbody>
</table>

4.7 Viscous shock tube

This problem was introduced to test the performances of current scheme for viscous flows [10]. In this case, an ideal gas is at rest in a two-dimensional unit box $[0,1] \times [0,1]$. A
membrane located at $x = 0.5$ separates two different states of the gas and the dimensionless initial states are

$$(\rho, U, p) = \begin{cases} (120, 0, 120/\gamma), & 0 < x < 0.5, \\ (1.2, 0, 1.2/\gamma), & 0.5 < x < 1, \end{cases}$$

where $\gamma = 1.4$, Reynolds number $Re = 200$ and Prandtl number $Pr = 0.73$. In the computation, this case is tested in the physical domain $[0,1] \times [0,0.5]$, a symmetric boundary condition is used on the top boundary $x \in [0,1], y = 0.5$. Non-slip boundary condition for velocity, and adiabatic condition for temperature are imposed at solid wall boundaries. For this case, the identical transformations, which are given for the double Mach reflection problem, are used. The meshes with $50 \times 25$ cells are shown in Fig. 4 as example.

The membrane is removed at time zero and wave interaction occurs. A shock wave, followed by a contact discontinuity, moves to the right with Mach number $Ma = 2.37$ and reflects at the right end wall. After the reflection, it interacts with the contact discontinuity. The contact discontinuity and shock wave interact with the horizontal wall and create a thin boundary layer during their propagation. The solution will develop complex two-dimensional shock/shear/boundary-layer interactions. The density distributions on the orthogonal and nonorthogonal meshes with $500 \times 250$ cells are presented in Fig. 11. The results match well with each other. The density profiles along the lower
wall for $Re = 200$ are also presented in Fig. 12, and numerical results deviate with other slightly due to different mesh size along the lower wall.

This case is also tested by the curved geometries and the meshes are given in Fig. 13. Two mappings from the computational domain to physical domain are written as

\[
\begin{align*}
\begin{cases}
x = \xi, \\
y = \eta(0.95 + 0.05\cos(2\pi \xi))
\end{cases},
\end{align*}
\]

and

\[
\begin{align*}
\begin{cases}
x = \xi, \\
y = \eta(0.95 - 0.05\cos(2\pi \xi))
\end{cases},
\end{align*}
\]

where $(\xi, \eta) \in [-0.5, 0.5] \times [-0.5, 0.5]$. Due to the symmetric condition at $\eta = 0$, the computational domain takes $(\xi, \eta) \in [-0.5, 0.5] \times [-0.5, 0]$, and $2N \times N$ uniform cells are used. The mesh distributions are given in Fig. 13 for two mappings with $50 \times 25$ cells, respectively. The density distributions for two mappings with $500 \times 250$ cells are given in Fig. 14. Due to the curved boundaries, the different flow structures are obtained.
4.8 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 [5, 11]. With a uniform temperature field, the initial flow field is given by

\[ u = V_0 \sin \left( \frac{x}{L} \right) \cos \left( \frac{y}{L} \right) \cos \left( \frac{z}{L} \right), \]
\[ v = -V_0 \cos \left( \frac{x}{L} \right) \sin \left( \frac{y}{L} \right) \cos \left( \frac{z}{L} \right), \]
\[ w = 0, \]
\[ p = p_0 + \rho_0 V_0^2 \left[ \cos \left( \frac{2x}{L} \right) + \cos \left( \frac{2y}{L} \right) \right] \left[ \cos \left( \frac{2z}{L} \right) + 2 \right]. \]

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 \( Re = 280 \). 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

\[ E_k = \frac{1}{\rho_0 \Omega} \int \frac{1}{2} \rho u \cdot ud\Omega, \]

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

\[ \varepsilon_k = -\frac{dE_k}{dt}. \]
Figure 15: Taylor-Green vortex problem: the kinetic energy $E_k$ and dissipation rate $-dE_k/dt$ for $Re = 280$.

In the computation, the nonorthogonal mesh is considered

$$
\begin{align*}
x &= \xi + 0.05\sin \xi \sin \eta \sin \zeta, \\
y &= \eta + 0.05\sin \xi \sin \eta \sin \zeta, \\
z &= \zeta + 0.05\sin \xi \sin \eta \sin \zeta.
\end{align*}
$$

As reference, the uniform Cartesian mesh is used as well. The numerical results with $96 \times 96 \times 96$ mesh points for the normalized volume-averaged kinetic energy and dissipation rate with Reynolds numbers $Re = 280$ are presented in Fig. 15, which agree well with the data in [42].

## 5 Conclusion

In this paper, a two-stage fourth-order gas-kinetic scheme in curvilinear coordinates is developed for the Euler and Navier-Stokes solutions. With the two-stage temporal discretization [29, 35], a reliable framework is provided for constructing a fourth-order scheme under the gas-kinetic framework. To treat practical problems with general geometry, such as the turbulent boundary layer and the flow over a wing-body configuration, the development of a three-dimensional HGKS in general curvilinear coordinates becomes necessary. To achieve the high-order accuracy, the dimension-by-dimension WENO-type reconstruction is adopted in the computational domain, where the reconstructed Jacobian and the product of flow variables and local Jacobian are used to get the point-wise values and spatial derivatives of conservative variables at Gaussian quadrature points in the computational domain. However, for the gas-kinetic flow solver, the spatial derivatives of conservative variables in the physical domain is needed as well, which is obtained through a procedure of orthogonalization and chain rule in the local orthogonal coordinates for the flux evaluation in the normal direction. The one-
dimensional to three-dimensional numerical tests from the accuracy test to the solutions with strong discontinuities are presented to validate the accuracy and robustness of the current scheme. The geometrical conservation law is precisely satisfied by the current scheme as well. The current development of HGKS provides a valuable high-order method for the complicated flow simulation in the complex geometries.

Acknowledgments

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References