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Physical modeling and numerical studies of three-dimensional non-equilibrium multi-temperature flows

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For increasingly non-equilibrium flowfields, the Navier-Stokes equations lose accuracy partially due to the single temperature approximation. To overcome this barrier, a continuum multi-temperature model based on the Bhatnagar-Gross-Krook equation coupled with the Landau-Teller-Jeans relaxation model has been proposed for two-dimensional hypersonic non-equilibrium multi-temperature flow computation. In a recent study, a two-stage fourth-order gas-kinetic scheme (GKS) has been developed for equilibrium flows, which achieves a fourth-order accuracy in space and time as well as high efficiency and robustness. In this paper, targeting for accurate and efficient simulation of multi-temperature non-equilibrium flows, a high-order three-dimensional multi-temperature GKS is constructed under the two-stage fourth-order framework, with the fourth-order Simpson interpolation rule for the newly emerged source term. Simulations on decaying homogeneous isotropic turbulence, low-density nozzle flow, rarefied hypersonic flow over a flat plate, and type IV shock-shock interaction are used to validate the multi-temperature model through the comparison with experimental measurements. The unified gas kinetic scheme (UGKS) results and the Direct Simulation Monte Carlo (DSMC) solutions will be used as well in some cases for validation. Computational results not only confirm the high-order accuracy and quite robustness of this scheme but also show the significant improvement on computational efficiency compared with UGKS and DSMC, especially for the flow in the near continuum regime. Published by AIP Publishing. https://doi.org/10.1063/1.5065455

I. INTRODUCTION

The classification of flow regimes is based on the Knudsen number $Kn$, which is defined as the ratio of the molecular mean free path over a characteristic length scale of the system. The whole flow regime is roughly divided into the continuum flow regime ($Kn \leq 0.001$), continuum-transition regime ($0.001 < Kn \leq 10$), and free molecular regime ($Kn > 10$). The Navier-Stokes (NS) equations with linear relations between stress and strain and Fourier’s laws are adequate to model the equilibrium flow in the continuum flow regime. For the non-equilibrium flow in the continuum-transition regime, the Navier-Stokes equations are well known to be inadequate. However, this continuum-transition regime is important for many scientific and practical engineering applications such as the simulation of micro-scale flows and space exploration vehicles.1 Therefore, accurate models with reliable solutions and lower computational costs for non-equilibrium flow are useful for solving the non-equilibrium flow problem in the near continuum regime.

Available numerical schemes for simulating non-equilibrium flow can be classified into the particle method and deterministic method. Direct simulation Monte Carlo (DSMC)2 uses probabilistic simulation to solve the Boltzmann equation, which is a representative of the particle method and is widely used for rarefied flow simulations. However, in the continuum-transition regime, DSMC requires a great amount of particles and the cell size and time step are limited by the particle mean free path and mean collision time, and it becomes very expensive both in the memory cost and computational time. The deterministic methods, such as Discrete Velocity Methods (DVMs) or Discrete Ordinate Methods (DOMs)3–5 which adopt splitting treatment of free transport and collision, solve the Boltzmann or model equations directly with the discretization of particle velocity space. In the continuum-transition regime, the cell size and time step are also constrained by the particle mean free path and mean collision time, which make these methods prohibitively expensive. Recently, an improved DVM6 is proposed to use a large time step and cell size by coupling the transport and collision in a hybrid flux, where the collisionless flux is computed by the discrete velocity distribution function and the collisional hydrodynamic flux is computed by the NS solver. The multi-scale unified gas kinetic scheme (UGKS)7–10 has been developed successfully for monatomic and diatomic gases for the entire Knudsen number flow. Different from the splitting process used in DSMC and DVM/DOM methods, the distinguishable feature of UGKS is the coupling of the particle transport and collision, which makes the grid size and time step used in UGKS not limited by the particle mean free path.
and collision time. Even though UGKS is currently the most efficient DVM-type multiscale method for flow simulation in the whole flow regime, in view of a considerable number of discrete velocity points to be updated, it is still expensive in the near continuum flow regime than those based on the macroscopic equations. At the same time, for smooth flow, such as those in the boundary layer, a high-order scheme is preferred to get accurate solutions. However, most schemes for the rarefied flow, such as DSMC, DVM/DOM, and UGKS, have only at most second-order accuracy.

To study non-equilibrium flow efficiently, an extended Bhatnagar-Gross-Krook (BGK) model coupled with the Landau-Teller-Jeans relaxation model has been proposed for one-dimensional and two-dimensional non-equilibrium multi-temperature flow computation.\cite{11,12} In the continuum flow regime, the corresponding kinetic scheme goes back automatically to the BGK-NS method. On the other hand, this kinetic scheme solves the non-equilibrium translational and rotational flow quite efficiently in the near continuum regime. In recent studies, an accurate and robust two-stage fourth-order gas-kinetic scheme (GKS) \cite{13,14} has been developed for equilibrium flows, which achieves a fourth-order accuracy in space and time, and shows high efficiency and robustness from the smooth flow to shock problem. In order to capture the delicate flow structure, a high-order non-equilibrium GKS based on the extended BGK method is preferred for simulating the multi-temperature flow efficiently and accurately. In the current study, this high-order non-equilibrium GKS is implemented under the previous two-stage fourth-order framework for three-dimensional multi-temperature flows, and the source term is dealt with by the fourth-order Simpson interpolation rule. Numerical tests from smooth decaying homogeneous isotropic turbulence to challenging hypersonic type IV shock-shock interaction validate the current high-order non-equilibrium GKS. This high-order non-equilibrium GKS not only preserves high accuracy and quite robustness through numerical cases but also shows the significant improvement on computational efficiency in the near continuum flow region.

In this paper, details on the current extended kinetic model and corresponding macroscopic equations are presented in Sec. II. Section III gives the construction of this high-order non-equilibrium numerical scheme under a two-stage fourth-order framework for solving this extended kinetic model. This is followed by the results and discussion of the non-equilibrium multi-temperature flow computations in Sec. IV. Discussion and conclusion are shown in Sec. V.

II. GAS-KINETIC MODELS AND MACROSCOPIC GOVERNING EQUATIONS FOR DIATOMIC GAS

In this section, the extended kinetic model and its derived macroscopic equations in three dimensions for diatomic gases are presented.

A. Equilibrium translational and rotational temperature model

By modeling the time evolution of a gas distribution function resulting from the free transport and binary elastic collision, the Boltzmann equation has been constructed for monotonic dilute gas. The simplification of the Boltzmann equation given by the BGK model has the following form:\cite{15}

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} + w \frac{\partial f}{\partial z} = g - f = \frac{g - f}{\tau},
\]

where \( f \) is the number density of molecules at the position \((x, y, z)\) and particle velocity \((u, v, w)\) at time \( t \). The left-hand side of Eq. (1) denotes the free transport, and the right-hand side represents the collision term. The relation between the distribution function \( f \) and macroscopic variables, such as mass, momentum, energy, and stress, can be obtained by taking moments of the distribution function. The collision operator in the BGK model shows a simple relaxation process from \( f \) to a local equilibrium state \( g \), with a characteristic time scale \( \tau \) related to the viscosity and heat conduction coefficients. The local equilibrium state is a Maxwellian distribution,

\[
g = \rho \left( \frac{\lambda}{\pi \mu} \frac{n_{s}^{2}}{2} \right) \exp \left[ -\lambda \left( (u - U)^{2} + (v - V)^{2} + (w - W)^{2} + \epsilon^{2} \right) \right],
\]

where \( \rho \) is the density, \((U, V, W)\) are the macroscopic fluid velocities in the \( x-, y-, \) and \( z- \) directions. Here \( \lambda = m/2kT \), where \( m \) is the molecular mass, \( k \) is the Boltzmann constant, and \( T \) is the temperature. For three-dimensional equilibrium diatomic gas, the total number of degrees of freedom \( K = 2 \), the internal variable \( \xi \) accounts for the rotational modes as \( \xi^{2} = \xi_{1}^{2} + \xi_{2}^{2} \), and the specific heat ratio \( \gamma = (K + 5)/(K + 3) \) is determined.

Based on the above BGK model as Eq. (1), the Euler equations can be obtained for a local equilibrium state with \( f = g \). On the other hand, for the Navier-Stokes equations, the stress and Fourier heat conduction terms can be derived with the Chapman-Enskog expansion\cite{16} truncated to the 1st-order,

\[
f = g + Knf_{1} = g - \tau \left( \frac{\partial g}{\partial t} + u \frac{\partial g}{\partial x} + v \frac{\partial g}{\partial y} + w \frac{\partial g}{\partial z} \right).
\]

For the Burnett and super-Burnett equations, the above expansion can be naturally extended,\cite{17} such as \( f = g + Knf_{1} + Kn^{2}f_{2} + Kn^{3}f_{3} + \cdots \). For the above Navier-Stokes solutions, the GKS based on the kinetic BGK model has been well developed.\cite{18} In order to simulate the flow with any realistic Prandtl number, a modification of the heat flux in the energy transport is used in GKS, which is also implemented in the present study.

B. Non-equilibrium translational and rotational temperature model

A single temperature is assumed for translational and rotational modes in the Navier-Stokes equations. However, it loses accuracy in the simulation of the non-equilibrium flow because of the different temperatures for the translational and rotational energy modes. In this subsection, an extended BGK model for non-equilibrium rotational energy is constructed and for the first time, and the corresponding three-dimensional macroscopic governing equations are derived.

For the non-equilibrium multi-temperature diatomic gas flow, the above-mentioned BGK model can be extended in the following form:

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} + w \frac{\partial f}{\partial z} = f^{eq} - f = \frac{f^{eq} - f}{\tau} + \frac{g - f^{eq}}{Zr\tau} = \frac{f^{eq} - f}{\tau} + Q,
\]
where an intermediate equilibrium state \( f^{eq} \) is introduced with two temperatures, one for translational temperature and the other for rotational temperature,

\[
f^{eq} = \rho \left( \frac{\lambda_r}{\pi} \right)^{3/2} \left( \frac{\lambda_r}{\pi} \right) e^{-\lambda_r (u^2 + v^2 + w^2 - \lambda_r \xi_r^2)},
\]

(5)

where \( \lambda_r = m/2kT_r \) is related to the translational temperature \( T_r \) and \( \lambda_r = m/2kT_r \) accounts for the rotational temperature \( T_r \). Therefore, the right-hand side collision operator contains two terms corresponding to the elastic and inelastic collisions, respectively, where the relaxation process becomes \( f \rightarrow f^{eq} \rightarrow g \) and the inelastic collision process from \( f^{eq} \) to \( g \) takes a much longer time \( T_\tau \tau \) than that of elastic collision process by \( T \). The additional term \( Q_\tau \) in the collision part accounts for the energy exchange between the translational and rotational energy, which contributes to the source term for the corresponding three-dimensional macroscopic flow evolution. The above three-dimensional extended BGK model is a natural extension for the two-dimensional extended BGK model.\(^{12}\)

The relation between mass \( \rho \), momentum \( \rho U, \rho V, \rho W \), total energy \( \rho E \), and rotational energy \( \rho E_r \) with the distribution function \( f \) is given by

\[
W = \left( \begin{array}{c}
\rho \\
\rho U \\
\rho V \\
\rho W \\
\rho E \\
\rho E_r \\
\end{array} \right) = \int \psi_\alpha d\Xi, \quad \alpha = 1, 2, 3, 4, 5, 6,
\]

(6)

where \( d\Xi = du dv dw \xi_r d\xi_r \) and \( \psi_\alpha \) is the component of the vector for moments

\[
\psi = (\psi_1, \psi_2, \psi_3, \psi_4, \psi_5, \psi_6)^T
\]

\[
= (1, u, v, w, \frac{1}{2}(u^2 + v^2 + w^2 + \xi_r^2), \frac{1}{2} \xi_r^2)^T.
\]

As a new temperature \( \lambda_r \) is introduced, the constraint of rotational energy relaxation has to be imposed on the above extended kinetic model to self-consistently determine all unknowns. Since only mass, momentum, and total energy are conserved during particle collisions, the compatibility condition for the collision term turns into

\[
\int \left( \frac{f^{eq} - f}{\tau} + Q_\tau \right) \psi_\alpha d\Xi = S = (0, 0, 0, 0, 0, s)^T, \quad \alpha = 1, 2, 3, 4, 5, 6.
\]

(7)

The source term for the rotational energy is from the energy exchange between translational and rotational ones during inelastic collision. The source term for the rotational energy is modeled through the Landau-Teller-Jeans-type relaxation model,

\[
s = \frac{(\rho E_r)^{eq} - \rho E_r}{Z_r \tau}.
\]

(8)

The equilibrium energy \( (\rho E_r)^{eq} \) is determined by the assumption \( T_r = T_s = T \) such that

\[
(\rho E_r)^{eq} = \frac{\rho}{2\lambda_r^{eq}} \lambda_r^{eq} = \frac{K + 3}{4} \rho E - \frac{1}{2} \rho(U^2 + V^2 + W^2).
\]

(9)

Here, the collision number \( Z_r \) is related to the ratio of the elastic collision frequency to the inelastic frequency. The particle collision time multiplied by a rotational collision number \( Z_r \) models the relaxation process for the rotational energy to equilibrate with the translational one. The value \( Z_r \) used in the current study is as in the work of Parker,\(^{19}\)

\[
Z_r = \frac{Z^{eq}_r}{1 + (\pi^{3/2}/2)\sqrt{T/T_r} + (\pi + \pi^2/4)(T_r/T)},
\]

(10)

where the quantity \( T^* \) is the characteristic temperature of intermolecular potential and \( Z^{eq}_r \) is the limiting value. Over a temperature range from 30 K to 3000 K for nitrogen, the values \( Z^{eq}_r = 23.0 \) and \( T^* = 91.5 \) K are used. The local temperature \( T \) in the above equation is the translational temperature. More advanced models for the energy relaxation are discussed in referred work.\(^{20}\)

Using the intermediate state given by Eq. (5), with the frozen of rotational energy exchange, the first-order Chapman-Enskog expansion gives

\[
f = f^{eq} + Knf_1 = f^{eq} - \tau \left( \frac{\partial f^{eq}}{\partial t} + u \frac{\partial f^{eq}}{\partial x} + v \frac{\partial f^{eq}}{\partial y} + w \frac{\partial f^{eq}}{\partial z} \right).
\]

(10)

The corresponding macroscopic non-equilibrium multi-temperature continuum equations in three-dimensions can be derived, as shown in the Appendix,

\[
\partial W = \left( \begin{array}{c}
\rho \\
\rho U \\
\rho V \\
\rho W \\
\rho E \\
\rho E_r \\
\end{array} \right) F = \left( \begin{array}{c}
\rho U \\
\rho U^2 + p \\
\rho UV \\
\rho UW \\
(\rho E + p)U \\
(\rho E + p)V \\
\end{array} \right) G = \left( \begin{array}{c}
\rho V \\
\rho UV \\
\rho VW \\
\rho WV \\
(\rho E + p)V \\
(\rho E + p)W \\
\end{array} \right),
\]

\[
H = \left( \begin{array}{c}
\rho W \\
\rho UW \\
\rho WV \\
\rho WV + p \\
(\rho E + p)W \\
\rho E_r W \\
\end{array} \right),
\]

with

\[
F_v = \left( \begin{array}{c}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
U \tau_{xx} + V \tau_{xy} + W \tau_{xz} + q_x \\
U \tau_{xx} + q_x \\
\end{array} \right) \quad G_v = \left( \begin{array}{c}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
U \tau_{xx} + V \tau_{xy} + W \tau_{xz} + q_y \\
V \tau_{xx} + q_y \\
\end{array} \right) \quad H_v = \left( \begin{array}{c}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
U \tau_{xx} + V \tau_{xy} + W \tau_{xz} + q_z \\
W \tau_{xx} + q_z \\
\end{array} \right).
\]
where \( \rho E = \frac{1}{2} \rho (U^2 + 3RT) + KRT \) is the total energy and \( \rho E_r = \rho RT \), with \( K = 2 \) being the rotational energy. The pressure \( p \) is related to the translational temperature as \( p = \rho RT \).

Meanwhile, the viscous normal stress terms are
\[
\tau_{xx} = \tau_p [\frac{2}{3} \rho \frac{\partial U}{\partial x} + \frac{1}{3} \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z}] - \rho K \frac{1}{1 + \frac{1}{\lambda_f}} \frac{1}{1 + \frac{1}{\lambda_r}} Z_r \frac{1}{2(K + 3)} Z_f \frac{1}{2(K + 3)} Z_f,
\]
\[
\tau_{yy} = \tau_p [\frac{2}{3} \rho \frac{\partial V}{\partial y} + \frac{1}{3} \frac{\partial U}{\partial x} + \frac{\partial W}{\partial z}] - \rho K \frac{1}{1 + \frac{1}{\lambda_f}} \frac{1}{1 + \frac{1}{\lambda_r}} Z_r \frac{1}{2(K + 3)} Z_f \frac{1}{2(K + 3)} Z_f,
\]
\[
\tau_{zz} = \tau_p [\frac{2}{3} \rho \frac{\partial W}{\partial z} + \frac{1}{3} \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y}] - \rho K \frac{1}{1 + \frac{1}{\lambda_f}} \frac{1}{1 + \frac{1}{\lambda_r}} Z_r \frac{1}{2(K + 3)} Z_f \frac{1}{2(K + 3)} Z_f,
\]
with viscous shear stress term given by
\[
\tau_{xy} = \tau_{yx} = \tau_p \left[ \frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right],
\]
\[
\tau_{xz} = \tau_{zx} = \tau_p \left[ \frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right],
\]
\[
\tau_{yz} = \tau_{zy} = \tau_p \left[ \frac{\partial V}{\partial z} + \frac{\partial W}{\partial y} \right],
\]
and heat conduction terms are
\[
q_x = \tau_p \frac{1}{4} \frac{\partial}{\partial x} \left( \frac{1}{\lambda_f} + \frac{1}{\lambda_r} \right),
\]
\[
q_y = \tau_p \frac{1}{4} \frac{\partial}{\partial y} \left( \frac{1}{\lambda_f} + \frac{1}{\lambda_r} \right),
\]
\[
q_z = \tau_p \frac{1}{4} \frac{\partial}{\partial z} \left( \frac{1}{\lambda_f} + \frac{1}{\lambda_r} \right).
\]
The following terms are related to the governing equation of rotational energy \( \rho E_r \) as
\[
\tau_r = \frac{3}{2} \rho K \frac{1}{1 + \frac{1}{\lambda_f}} \frac{1}{1 + \frac{1}{\lambda_r}} Z_r \frac{1}{2(K + 3)} Z_f \frac{1}{2(K + 3)} Z_f,
\]
\[
q_{rx} = \tau_p \frac{1}{4} \frac{\partial}{\partial x} \frac{1}{\lambda_r},
\]
\[
q_{ry} = \tau_p \frac{1}{4} \frac{\partial}{\partial y} \frac{1}{\lambda_r},
\]
\[
q_{rz} = \tau_p \frac{1}{4} \frac{\partial}{\partial z} \frac{1}{\lambda_r}.
\]
The source term in Eq. (10) is given by
\[
S = (0, 0, 0, 0, 0, (\rho E_r c)_f - \rho E_r). \frac{Z_r}{Z_f}.
\]

In the limiting case of small departure from equilibrium, the rotational energy equation becomes
\[
(\rho E_r)_t + (\rho E_r U)_x + (\rho E_r V)_y + (\rho E_r W)_z = \rho R \frac{3}{Z_r} \frac{3}{K} (T_r - T_i).
\]

Based on the leading Euler system for approximating the time-derivative term, the above equation becomes
\[
T_r - T_i = -\frac{2}{3} Z_r \tau T (U_x + V_y + W_z).
\]

Therefore, the normal bulk viscosity term can be exactly recovered from
\[
\frac{2}{3} \frac{K}{K + 3} \tau_p (U_x + V_y + W_z) = \rho R \frac{K}{Z_r} \frac{3}{K + 3} (T_r - T_i).
\]

With the above macroscopic modeling equations for a multi-temperature system, the non-equilibrium flow in the near continuum regime is modeled beyond the NS assumption. The bulk viscosity is replaced by a relaxation term between translational and rotational energy, which seems more physically meaningful than the bulk viscosity assumption \(^{11,12}\) for the flows with temperature non-equilibrium. In this paper, the nonlinear system [Eq. (10)] is solved with the flux function provided through the time-dependent integral solution from Eq. (4). This flux function couples the inviscid and all dissipative terms and has advantages in comparison with the traditional NS solver, where the Riemann solver and central difference are used for the inviscid and viscous terms.

### III. HIGH-ORDER FINITE VOLUME NON-EQUILIBRIUM GAS-KINETIC SCHEME

The extended model proposed in Sec. II B is solved based on the conservative finite volume method GKS.\(^{18}\) The numerical fluxes at cell interfaces are evaluated based on the general time-dependent gas distribution solution. In this paper, a high-order non-equilibrium finite volume GKS will be constructed, where the additional source term is dealt with by the fourth-order Simpson interpolation rule.

#### A. Three-dimensional finite volume scheme

Taking moments of Eq. (4) and integrating over the control volume \( V_{ijk} = \Delta_i \Delta_j \Delta_k \), with \( \Delta_i = [x_i - \Delta_i^2, x_i + \Delta_i^2] \), \( \Delta_j = [y_j - \Delta_j^2, y_j + \Delta_j^2] \), and \( \Delta_k = [z_k - \Delta_k^2, z_k + \Delta_k^2] \), the three-dimensional non-equilibrium finite volume scheme can be written as
\[
\frac{dW_{ijk}}{dt} = L(W_{ijk}) = \frac{1}{|V_{ijk}|} \left[ \int_{V_{ijk}} (F_{1-2,j,k} - F_{1+1,j,k}) dy dz + \int_{V_{ijk}} (G_{1-1,j,k} - G_{1+1,j,k}) dx dz + \int_{V_{ijk}} (H_{1-1,j,k} - G_{1+1,j,k}) dx dy + S_{ijk} \right],
\]
where \( f(x_{i+1/2,j,k}, t, \mathbf{u}, \xi) \) is based on the integral solution of BGK equation [Eq. (4)] at the cell interface,
\[
\begin{align*}
 f(x_{i+1/2,j,k}, t, \mathbf{u}, \xi_r) &= \frac{1}{\tau} \int_{t_0}^{t} f^{eq}(x', t', \mathbf{u}, \xi_r)e^{-(t-t')/\tau} dt' \\
 &+ e^{-t/\tau} f_0(-\mathbf{u}, \xi_r),
\end{align*}
\]
where \( x_{i+1/2,j,k} = \mathbf{0} \) is the location of the cell interface, \( \mathbf{u} = (u, v, w) \) is the particle velocity, and \( x_{i+1/2,j,k} = \mathbf{x}' + \mathbf{u}(t - t') \) is the trajectory of particles. \( f_0 \) is the initial gas distribution, and \( f^{eq} \) is the corresponding intermediate equilibrium state as Eq. (5). \( f^{eq} \) and \( f_0 \) can be constructed as
\[
 f^{eq} = f_0^eq(1 + \bar{a}x + \bar{b}y + \bar{c}z + \bar{A}t),
\]
and
\[
\int \psi_{\alpha} f_0^{eq} d\Xi = \int_{a=0} \psi_{\alpha} f_{l}^{eq} d\Xi + \int_{a=0} \psi_{\alpha} f_{r}^{eq} d\Xi,
\]
where \( f_{l}^{eq} \) and \( f_{r}^{eq} \) are the initial gas distribution functions on both sides of a cell interface. \( f_0^{eq} \) is the initial equilibrium state located at the cell interface, which can be determined through the compatibility condition

For a second-order flux, the time-dependent gas distribution function at the cell interfaces is evaluated as
\[
\begin{align*}
 f(x_{i+1/2,j,k}, t, \mathbf{u}, \xi_r) &= (1 - e^{-t/\tau}) f_0^{eq} + ((t + \tau)e^{-\tau t} - \tau(\bar{a}u + \bar{b}v + \bar{c}w)f_0^{eq} + (t + \tau e^{t/\tau})A f_0^{eq} \\
 &+ e^{-t/\tau} f_{l}^{eq} [1 - (t + \tau)(a_l u + b_l v + c_l w) - \tau A_l](1 - H(\bar{u})) \\
 &+ e^{-t/\tau} f_{r}^{eq} [1 - (t + \tau)(a_r u + b_r v + c_r w) - \tau A_r]H(\bar{u}),
\end{align*}
\]
where the coefficients in Eq. (15) can be determined by the spatial derivatives of macroscopic flow variables and the compatibility condition. For three-dimensional diatomic gas, the expansion of spatial variation \( \partial f^{eq}/\partial x \) is given by
\[
\begin{align*}
 \frac{\partial f^{eq}}{\partial x} &= \frac{1}{\rho} (a_1 + a_2 u + a_3 v + a_4 w + a_5(u^2 + v^2 + w^2) + a_6 \xi_r^2) f^{eq} \\
 &= -\rho f^{eq},
\end{align*}
\]
where all coefficients in Eq. (16) can be explicitly determined by the relations between the microscopic and macroscopic variables at the cell interface, i.e., \( W = \int \psi_{\alpha} f^{eq} d\mathbf{u} d\xi \) and \( \partial W/\partial x = (1/\rho)\int \psi_{\alpha} f^{eq} d\mathbf{u} d\xi \), where \( W = (\rho, \rho U, \rho V, \rho W, \rho E, \rho E_r) \) are the flow variables. The components of coefficients \( a \) in Eq. (16) can be expressed as
\[
\begin{align*}
 a_6 &= 2 \lambda_2^2 K (2 \frac{\partial (\rho E_r)}{\partial x} - \frac{1}{2} \frac{K}{\lambda_r} \frac{\partial \rho}{\partial x}), \\
 a_5 &= 2 \lambda_2^2 (B - 2U A_1 - 2V A_2 - 2W A_3), \\
 a_4 &= 2 \lambda_r A_3 - 2W a_s, \\
 a_3 &= 2 \lambda_r A_2 - 2V a_s, \\
 a_2 &= 2 \lambda_r A_1 - 2U a_s, \\
 a_1 &= \frac{\partial \rho}{\partial x} - a_2 U - a_3 V - a_4 W \\
 &- a_5 (U^2 + V^2 + W^2 + \frac{3}{\lambda_r}) - a_6 \frac{K}{2 \lambda_r},
\end{align*}
\]
with the defined variables
\[
B = 2\frac{\partial (pE - pE)}{\partial x} - (U^2 + V^2 + W^2 + 3\frac{1}{\lambda_i}) \frac{\partial \rho}{\partial x},
\]
\[
A_1 = \frac{\partial (pU)}{\partial x} - U \frac{\partial \rho}{\partial x},
\]
\[
A_2 = \frac{\partial (pV)}{\partial y} - V \frac{\partial \rho}{\partial y},
\]
\[
A_3 = \frac{\partial (pW)}{\partial z} - W \frac{\partial \rho}{\partial z}.
\]

In a similar way, the temporal variation of \( \frac{\partial \rho}{\partial t} \) can be expanded and the corresponding coefficients can be obtained from the compatibility condition for the Chapman-Enskog expansion,
\[
\int \psi_o \left( \frac{\partial f_{eq}}{\partial t} + u \frac{\partial f_{eq}}{\partial x} + v \frac{\partial f_{eq}}{\partial y} + w \frac{\partial f_{eq}}{\partial z} \right) d\Xi = 0,
\]
where the above six equations uniquely determine six unknowns in \( A \), i.e., \( A = A_1 + A_2 + A_3 + A_4 + A_5 + A_6 \).

Here, the second-order accuracy in time can be achieved by one step integration, with the time-dependent gas-kinetic flux solver Eq. (15). Based on a higher-order expansion of the equilibrium state around a cell interface, the one-stage third-order GKS has been developed successfully.22 However, the one-stage gas-kinetic solver becomes very complicated for even higher-order schemes, especially for three-dimensional computations. In order to reduce the complexity of high-order scheme, the technique of a two-stage fourth-order method will be used here for the development of a fourth-order scheme for the non-equilibrium flow.

**B. Two-stage high-order temporal discretization**

In recent studies, 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 and the GKS.14 Such methods provide a reliable framework to develop a high-order three-dimensional non-equilibrium GKS with a second-order flux function Eq. (15) only, where the source terms will be treated by high-order interpolation. A key point for this two-stage high-order method is to use the time derivative of a flux function. In order to obtain the time derivative of a flux function at \( t_n \) and \( t_n + \Delta t/2 \), the flux function should be approximated as a linear function of time within a time interval.

According to the numerical fluxes at cell interface Eq. (13), the following notation is introduced:
\[
F_{i+1/2,j,k}(W^n, t_n) = \int_{t_n}^{t_n + \frac{\Delta t}{2}} F_{i+1/2,j,k}(W^n, t) dt
\]
\[
= \int_{t_n}^{t_n + \frac{\Delta t}{2}} F_{i+1/2,j,k}(W^n, t_n) dt.
\]

In the time interval \([t_n, t_n + \Delta t/2]\), the flux is expanded as the following linear form:
\[
F_{i+1/2,j,k}(W^n, t) = F_{i+1/2,j,k}(W^n, t_n) + \frac{\partial F_{i+1/2,j,k}(W^n, t_n)}{\partial t}(t - t_n).
\]

Based on Eq. (17) and linear expansion of flux as Eq. (18), the coefficients \( F_{i+1/2,j,k}(W^n, t_n) \) and \( \frac{\partial F_{i+1/2,j,k}(W^n, t_n)}{\partial t} \) can be determined by integrating Eq. (17) with \( \Delta t/2 \) and \( \Delta t \),
\[
F_{i+1/2,j,k}(W^n, t_n + \Delta t) + \frac{\partial F_{i+1/2,j,k}(W^n, t_n)}{\partial t} \Delta t^2 = F_{i+1/2,j,k}(W^n, \Delta t),
\]
\[
\frac{1}{2} F_{i+1/2,j,k}(W^n, t_n) \Delta t + \frac{1}{8} \frac{\partial F_{i+1/2,j,k}(W^n, t_n)}{\partial t} \Delta t^2 = F_{i+1/2,j,k}(W^n, \Delta t/2).
\]

By solving the linear system, we have
\[
F_{i+1/2,j,k}(W^n, t_n) = (4F_{i+1/2,j,k}(W^n, \Delta t/2) - F_{i+1/2,j,k}(W^n, \Delta t))/\Delta t,
\]
\[
\frac{\partial F_{i+1/2,j,k}(W^n, t_n)}{\partial t} = (4F_{i+1/2,j,k}(W^n, \Delta t/2) - F_{i+1/2,j,k}(W^n, \Delta t/2))/\Delta t^2.
\]

and
\[
F_{i+1/2,j,k}(W^n, t), \quad \frac{\partial F_{i+1/2,j,k}(W^n, t)}{\partial t} \text{ for the intermediate state } t \text{ can be constructed similarly.}
\]

With these notations, the three-dimensional high-order non-equilibrium algorithm for multi-temperature flow is given by

(i) With the initial reconstruction, update \( W^* \) at \( t_n + \Delta t/2 \) by
\[
W^{n+1}_{ijk} = W^n_{ijk} - \frac{1}{\Delta x} \left[ F_{i+1/2,j,k}(W^n, \Delta t/2) - F_{i-1/2,j,k}(W^n, \Delta t/2) \right] - \frac{1}{\Delta y} \left[ G_{i+1/2,j,k}(W^n, \Delta t/2) - G_{i-1/2,j,k}(W^n, \Delta t/2) \right] - \frac{1}{\Delta z} \left[ H_{i,j+1/2,k}(W^n, \Delta t/2) - H_{i,j-1/2,k}(W^n, \Delta t/2) \right] + S^n_{ijk} \Delta \tau / 2,
\]
and compute the fluxes and their derivatives by Eq. (19) for future use,
\[
F_{i+1/2,j,k}(W^n, t_n), \quad G_{i+1/2,j,k}(W^n, t_n), \quad H_{i,j+1/2,k}(W^n, t_n), \quad \frac{\partial F_{i+1/2,j,k}(W^n, t_n)}{\partial t}, \quad \frac{\partial G_{i+1/2,j,k}(W^n, t_n)}{\partial t}, \quad \frac{\partial H_{i,j+1/2,k}(W^n, t_n)}{\partial t}.
\]

(ii) Reconstruct the intermediate value \( W^{*+1}_{ijk} \) and compute
\[
\frac{\partial F_{i+1/2,j,k}(W^*, t_n)}{\partial t}, \quad \frac{\partial G_{i+1/2,j,k}(W^*, t_n)}{\partial t}, \quad \frac{\partial H_{i,j+1/2,k}(W^*, t_n)}{\partial t}, \quad \frac{\partial F_{i+1/2,j,k}(W^*, t_n)}{\partial t} \text{ at } t_n + \Delta t/2.
\]

(iii) Update \( W_{ijk}^{n+1} \) by
\[
W_{ijk}^{n+1} = W^n_{ijk} - \frac{\Delta t}{\Delta x} \left[ S^n_{i+1/2,j,k} - S^n_{i-1/2,j,k} \right] - \frac{\Delta t}{\Delta y} \left[ S^n_{ij+1/2,k} - S^n_{ij-1/2,k} \right] - \frac{\Delta t}{\Delta z} \left[ S^n_{i,j+k+1/2} - S^n_{i,j,k-1/2} \right] + S^n_{ijk} \Delta \tau.
\]
C. Fourth-order Simpson interpolation for source term

Let \( s^r_{ijk} \) denote the source component for rotational energy \( \rho E_r \), while other components in the source term \( S_{ijk} \) are zero. Here, \( \rho E_r \) can be updated using a semi-implicit scheme based on the fourth-order Simpson interpolation rule.

(i) Update \( (\rho E_r)^s \) at \( t^s = t_n + \Delta t/2 \) by

\[
(\rho E_r)^s_{ijk} = (\rho E_r)^n_{ijk} + (RHS)^s_{ijk} + \Delta t^s/2 \left( s^r_{ijk} + s^{r+1}_{ijk} \right),
\]

\[
s^r_{ijk} = (\rho E_r)^{eq}_{ijk} - (\rho E_r)^n_{ijk},
\]

\[
s^{r+1}_{ijk} = (\rho E_r)^{eq}_{ijk} - (\rho E_r)^{n+1}_{ijk},
\]

thus

\[
(\rho E_r)^s_{ijk} = \frac{2(Z_r \tau)^{n+1}_{ijk}}{2(Z_r \tau)^{n+1}_{ijk} + \Delta t^s} \left[ (\rho E_r)^n_{ijk} + (RHS)^s_{ijk} + \Delta t^s/2 \left( s^n_{ijk} + s^{n+1}_{ijk} \right) \right], \tag{22}
\]

where \( \Delta t^s = \Delta t/2 \) and \( (RHS)^s_{ijk} \) represents the component for rotational energy on the right-hand side of Eq. (20) without the source term. \( (\rho E_r)^s_{ijk} \) can be updated based on the fourth-order Simpson interpolation rule.

(ii) Update \( (\rho E_r)^{n+1} \) at \( t^{n+1} \) by

\[
(\rho E_r)^{n+1}_{ijk} = (\rho E_r)^n_{ijk} + (RHS)^{n+1}_{ijk} + \Delta t/6 \left( s^n_{ijk} + 4s^{n+1}_{ijk} + s^{n+1}_{ijk} \right),
\]

\[
s^{n+1}_{ijk} = (\rho E_r)^{eq}_{ijk} - (\rho E_r)^{n+1}_{ijk},
\]

thus

\[
(\rho E_r)^{n+1}_{ijk} = \frac{6(Z_r \tau)^{n+1}_{ijk}}{6(Z_r \tau)^{n+1}_{ijk} + \Delta t} \left[ (\rho E_r)^n_{ijk} + (RHS)^{n+1}_{ijk} + \Delta t/6 \left( s^n_{ijk} + 4s^{n+1}_{ijk} + (Z_r \tau)^{n+1}_{ijk} \right) \right], \tag{23}
\]

where \( (RHS)^{n+1}_{ijk} \) represents the component for rotational energy on the right-hand side of Eq. (21) without the source term. The right-hand side terms in Eq. (23) are known after updating the flow variables through fluxes at \( t^{n+1} \), so \( (\rho E_r)^{n+1} \) can be updated based on the fourth-order Simpson interpolation rule.

IV. NUMERICAL EXAMPLES

In this section, numerical tests from smooth flow to hyper-sonic ones will be presented to validate our numerical scheme. The collision time \( \tau \) takes

\[
\tau = \frac{\mu}{p} + \frac{c[|PL - PR|]}{|pL + pR|} \Delta t,
\]

where \( \mu \) is the viscous coefficient obtained from Sutherland’s law and \( C \) is set to 1.5 in the computation. \( p_L \) and \( p_R \) denote the pressure on the left- and right-hand sides at the cell interface, which reduces to \( \tau = \mu \rho \) in the smooth flow region. \( \Delta t \) is the time step determined according to the Courant-Friedrichs-Lewy (CFL) condition with the CFL number 0.3 in the computations.

A. Decaying homogeneous isotropic turbulence

Decaying homogeneous isotropic turbulence (DHIT) provides a benchmark for testing the dissipative behavior of the numerical scheme. In the current study, the reference experiment is conducted by Comte-Bellot and Corrsin,\(^{23}\) with the Taylor Reynolds number \( Re = 71.6 \) and the turbulent Mach number \( Ma = 0.2 \). Here, the computation domain is a \((2\pi)^3\) box with 128\(^3\) uniform grids. The Vreman-type large eddy simulation (LES) model\(^{24, 25}\) is implemented with the periodic boundary condition in 6 faces. In this GKS, the turbulence model is coupled to get the newly defined collision time as in previous studies.\(^{26, 28}\)

The turbulent fluctuating velocity as \( u' \), the Taylor microscale \( \lambda \), the Taylor Reynolds number \( Re = c/\lambda \), and the turbulent Mach number \( Ma \) are defined as

\[
u' = \frac{(u_1^2 + u_2^2 + u_3^2)^{1/2}}{3},
\]

\[
\lambda^2 = \frac{u'^2}{\langle \partial u_1/\partial x_1 \rangle^2},
\]

\[
Re = \frac{u'\lambda}{\nu},
\]

\[
Ma = \frac{(u_1^2 + u_2^2 + u_3^2)^{1/2}}{c},
\]

where \((\cdots)\) represents the space average in the computation domain. \( c \) represents the local sound speed, and \( \nu \) represents the kinematic viscosity coefficient as \( \mu/\rho \). The initial velocity field is computed from the experiment’s energy spectral, with constant pressure, density, and temperature. For multi-temperature simulation, because the true temperature cannot be recovered in this artificial system, the specific collision number \( Z_r = 5 \) is chosen considering the nitrogen gas for \( Z_r = 5 \) at the room temperature. The rotational temperature is initiated with the same value as the translational temperature.

The following quantities of turbulence have been computed in our simulations:
FIG. 1. Comparison of TKE spectral on high order equilibrium GKS, high order GKS, and second order GKS with the collision number $Z_r = 5$ at dimensionless time $t^* = 0.87$. The experimental data are from the experiment.

$$E(\kappa) = \frac{1}{2} \int_{\kappa_{\text{min}}}^{\kappa_{\text{max}}} \Phi_{ii}(\kappa) \delta(|\kappa| - \kappa) d\kappa,$$

$$M_{\text{loc}} = \left( \frac{u_1^2 + u_2^2 + u_3^2}{c} \right)^{1/2},$$

$$\Delta T = \frac{T_{\text{m}} - R_{\text{ot}}}{T_0},$$

where velocity spectral $\Phi_{ii}$ is the Fourier transform of two-point correlation, with the wave number $\kappa_{\text{min}} = 0$ and $\kappa_{\text{max}} = 64$. $T_0$ is the initial temperature, while $T_{\text{m}}$ and $R_{\text{ot}}$ represent the translational temperature and rotational temperature, respectively.

Figure 1 shows the turbulence kinetic energy (TKE) spectral at dimensionless time $t^* = 0.87$, based on the high order equilibrium GKS, high order GKS, and second order GKS. Without the special statement, high order GKS denotes the current high order non-equilibrium multi-temperature GKS. In the high wavenumber region, TKE spectral from the high order GKS is closer to the experiment result, which outweighs the results from the second order GKS. High order accuracy is achieved in the high order GKS, which has the advantage of simulating the non-equilibrium multi-temperature flow when the smooth equilibrium region appears. Besides, small difference resulting from the different bulk viscosity term between the high order equilibrium GKS and high order GKS is observed in this TKE spectral. This different behavior is also verified by the PDF of the local Mach number $M_{\text{loc}}$ and the contours of $\Delta T$ shown in Fig. 2 as the maximum difference between the translational temperature and rotational temperature on the $z = 0.5$ plane at dimensionless time $t^* = 0.87$ is no more than 1.2%.

**B. Low-density nozzle flow**

A low-thrust rocket engine has been used for the control of altitude and trajectory of satellites and spacecrafts. For this type of rocket engine, the fluid experiences continuum, transition flow regime, which provides a necessary test for the validity of the current high order GKS method for the near continuum flow regime.

Low density nozzle flow has been measured using the electron beam fluorescence technique by Rothe, and DSMC simulations have been performed by Chung et al. The flow condition for the test case is stagnation temperature $T_0 = 300$ K, stagnation pressure $P_0 = 474$ Pa, wall temperature $T_w = 300$ K, and the Knudsen number $Kn_{\infty} = 5.2 \times 10^{-3}$. This is an axisymmetric flow problem; only one quarter part of this nozzle has been computed with $340 \times 60 \times 60$ grid points used inside the nozzle. An empirical first-order slip boundary condition is used in the current high order GKS method for the isothermal boundary condition.

Figure 3 shows the Mach contour and non-dimensional density contour inside this nozzle, where the high ratio of density from the inlet to outlet is observed. The experimental data of density and rotational temperature along the nozzle centerline are shown in Fig. 4. The current high order GKS method is validated in the near continuum flow regime as computation results provide a close match with the experimental measurement.
FIG. 3. Mach contour (left) and non-dimensional density contour (right) in the nozzle flow computations.

FIG. 4. Density and rotational temperature distributions along the central line of the nozzle, where $R_t$ is the throat radius. The measured rotational temperature is from the experiment.

C. Rarefied hypersonic flow over a flat plate

Physical phenomena occurring around spacecraft in a hypersonic rarefied gas flow are studied in order to understand these phenomena and to design a real size vehicle. Following the experiment conducted by Tsuboi and Matsumoto simulation on the hypersonic rarefied gas flow over a flat plate is implemented. The case is run 34, with the nozzle exit Mach number $Ma = 4.89$, stagnation temperature $T_0 = 670$ K, stagnation pressure $P_0 = 983$ Pa, nozzle exit temperature $T_e = 116$ K, flat plate surface temperature $T_w = 290$ K with the first-order slip boundary condition used, and the Knudsen number $Kn_{\infty} = 6.2 \times 10^{-3}$. The geometry is shown in Fig. 5, where $400 \times 200$ and $300 \times 100$ grid points above and below the flat plate are used. In this case, the shock wave and boundary layer interaction near a sharp leading edge causes a non-equilibrium effect between the translational and rotational temperature in the rarefied gas regime.

The temperature distributions in the vertical direction above the flat plate at the locations of $x = 5$ mm and $x = 20$ mm from the leading edge are shown in Fig. 6. As a comparison, the UGKS results and DSMC results are also included. As shown in Fig. 6, the current high order GKS result is comparable with the DSMC result, while the current high order GKS is more efficient than DSMC. However, UGKS results have a perfect match with the experiment measurement than the current high order GKS method and DSMC solution, which shows its great advantage for multi-scale flow simulation. Here coarse grids in physical space are used in the UGKS scheme, with $59 \times 39$ grid points above the plate and $44 \times 25$ below the plate. However, velocity space is discretized with $80 \times 60$ grid points in the UGKS scheme, so the current high order GKS method is still competitive in the near continuum flow regime considering its higher efficiency than UGKS.

D. Type IV shock-shock interaction

Shock-shock interaction is the key issue in hypersonic flow. The presence of intense shock waves’ interaction strongly affects vehicle aerodynamic performance and leads to substantial localized aerodynamic heating. Shock-shock interaction
FIG. 5. Translational (left) and rotational (right) temperature contours in the hypersonic flow over a flat plate.

FIG. 6. Rotational temperature distributions in the vertical direction at \( x = 5 \) mm (left) and \( x = 20 \) mm (right). The measured rotational temperature, current high order GKS solutions, UGKS solution, and DSMC solution are presented.

was classified by Edney into six patterns, depending on the impinging position and angle. In this paper, type IV interaction is studied, which is the most severe case to form the hot spot on the surface of the cylinder due to the supersonic jet hitting on the wall. The flow patterns of the formation of a supersonic impinging jet, a series of shock waves, expansion waves, and shear layers in a local area of interaction form a pretty challenging case for such a high-order GKS scheme.

An experimental test has been conducted by the Office National d’Études et de Recherches Aéronautiques (ONERA) to investigate shock-shock interactions, which provides free-stream air flow properties of \( M_\infty = 10, T_\infty = 52.5 \) K, \( T_w = 300 \) K, \( Re_\infty/m = 1.66 \times 10^5 \), and the Knudsen number \( Kn_\infty = 5.5 \times 10^{-3} \). The leading edge of the shock generator is positioned at a distance \( L = 102 \) mm upstream of the cylinder and \( 53 \) mm below the axis of the cylinder, and the cylinder diameter is \( 16 \) mm. Our simulation is based on \( 250 \times 440 \) grid points around the cylinder. Configuration for the ONERA shock-shock interaction experiment and the Schlieren images by density gradient magnitude from the current computation is shown in Fig. 7. A steady state solution is obtained from the high order GKS scheme after a long time iteration with the iterative steps on the order of \( 10^5 \), and the flow structure keeps the same form.

The translational temperature contour and rotational temperature contour around the cylinder are shown in Fig. 8. These contours confirm the existence of multiple temperature for this hypersonic flow. More specifically, the Mach number and pressure in the supersonic jet region are shown in Fig. 9, which clearly show the strong jet and hot spot around the cylinder surface. Figure 10 presents two horizontal profiles of the measured rotational temperature in the experiment. One is located above the upper shock triple point at \( y = -2 \) mm, and the other is the line at \( y = -4 \) mm, which passes the transmitted shock and intersects with the surface one degree below the location of jet impingement. The high-order GKS results are close to the DSMC solution at \( y = -2 \) mm, while oscillation appears in DSMC simulation. At \( y = -4 \) mm, our computational results have a closer match with the experiment than with the DSMC solution, especially near the \( x = 0 \) mm region.
FIG. 7. Configuration for the ONERA experiment (left) and Schlieren images by density gradient magnitude (right) from the current high order GKS for type IV shock-shock interaction.

The non-dimensional pressure and heat flux along the cylindrical surface from experimental measurements, the high order GKS, and DSMC computational results are shown in Fig. 11, where $p_{c,s} = 760$ Pa and $q_{c,s} = 5.7$ W/cm$^2$ are the reference values for the undisturbed flow around the cylinder. The experimental heating data set is inadequate to define the

FIG. 8. Translational temperature contour (left) and rotational temperature contour (right) for type IV shock-shock interaction.

FIG. 9. Local Mach contour (left) and pressure (right) contour in the supersonic jet region.
peak value because of the limited spatial resolution, while the high order GKS and DSMC present the close peak position with different peak values. In terms of pressure distribution, the high order GKS outweighs DSMC results near 0°. Near the 0° region, a slightly low pressure region is found in Fig. 9, which provides confidence on the high accuracy achieved by the high-order GKS scheme.

The current high-order multi-temperature GKS focuses on high-temperature non-equilibrium flow simulation in the near-continuum flow regime efficiently without updating discrete velocity distribution. The GKS method has the similar function as the well-known regularized 13-moment equations and the nonlinear coupled constitutive relations (NCCRs) for the non-equilibrium flow study with updating macroscopic flow variables only. As to the extension of the current high-order multi-temperature GKS to rarefied flow, further investigation and improvements will be considered in future work.

V. CONCLUSION

In this paper, a high-order three-dimensional multi-temperature GKS method is implemented under the two-stage fourth-order framework. Based on the extended BGK model, the three-dimensional macroscopic governing equations for diatomic gas are derived, which provide better insight into the behavior of the multi-temperature flow. Based on the developed multiple temperature kinetic model, a corresponding high-order GKS is constructed under the two-stage fourth-order framework and the source term discretization with the fourth-order Simpson interpolation rule. For non-equilibrium multi-temperature flow computation, decaying homogeneous isotropic turbulence, nozzle flows, hypersonic rarefied flow over a plate, and type IV shock-shock interaction cases are tested. Comparisons among the numerical solutions from the current high order GKS scheme, UGKS results, DSMC solutions, and experimental measurements show the
high accuracy and quite robustness of the current numerical method. Most importantly, since the current finite volume gas-kinetic scheme updates the macroscopic flow variables only, the GKS can achieve high efficiency in comparison with UGKS and DSMC methods, especially for flow simulation in the near continuum regime.

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APPENDIX: CONNECTION BETWEEN BGK AND MACROSCOPIC NON-EQUILIBRIUM MULTI-TEMPERATURE EQUATIONS IN THREE-DIMENSIONS

Derivation of the Navier-Stokes and Euler equations from the BGK model can be found in Appendix B.\textsuperscript{10} For macroscopic non-equilibrium multi-temperature equations in two-dimensions, it has been derived in previous work.\textsuperscript{12} This appendix provides the details for the derivation of macroscopic non-equilibrium multi-temperature equations in three-dimensions. In this Appendix, “Eq. (B.x)” represents the preliminary equation in Appendix B,\textsuperscript{10} which will not be rewritten in the current appendix.

Continuity equation is given by

\begin{equation}
\rho_j + (\rho U_k)_k = 0, \quad (A1)
\end{equation}

which can be used to simplify the momentum equations, the total energy equations, and the rotational energy equations.

For momentum equations, the left-hand side $L_5$ in Eq. (B2) can be grouped as

\begin{equation}
L_5 = \frac{1}{2} U_n^2 [\rho_j + (\rho U_k)_k] + \rho U_n U_{n,j} + \rho U_k U_{n,k}
+ U_k p_k + \frac{K + 3}{2} [p_j + U_k p_k] + \frac{K + 5}{2} p U_k k
+ \frac{K}{2} (p_r - p)_l + \frac{K}{2} (p_r - p U_k)_k.
\end{equation}

The first term is $\frac{1}{2} U_n^2 L_1$ which is $O(\varepsilon^2)$, and next three are $U_n L_n$ and are therefore $O(\varepsilon)$. Then $L_5$ can be rewritten as

\begin{equation}
L_5 = \frac{K + 3}{2} [p_j + U_k p_k] + \frac{K + 5}{2} p U_k k + \rho U_n L_n
+ \frac{K}{2} [(p_r)_l + (p_r U_k)_k] - [p_j + (p_r U_k)_k]. \quad (A2)
\end{equation}

Based on the Chapman-Enskog expansion up to zero order, the rotational energy equation is obtained as

\begin{equation}
(p E_r)_l + (p E_r U_k)_k = \frac{3 \rho}{2 (K + 3)} Z_{r,r} \left( \frac{1}{\lambda_r} - \frac{1}{\lambda_r} \right).
\end{equation}

which can be used to eliminate $(p_r)_l + (p_r U_k)_k$. Based on $p_r = \rho E_r$, Eq. (A2) can be rewritten as

\begin{equation}
- \frac{K + 3}{2} [p_j + U_k p_k] = \frac{K + 5}{2} p U_k k
+ \frac{K}{2} \left[ \frac{3}{2 (K + 3)} Z_{r,r} \left( \frac{1}{\lambda_r} - \frac{1}{\lambda_r} \right) \right]
- [p_j + U_k p_k] + U_n L_n + O(\varepsilon).
\end{equation}

Finally, we get

\begin{equation}
p_j + U_k p_k = - \frac{K + 3}{2} [p_j + U_k p_k] + \frac{K}{2} \left[ \frac{3}{2 (K + 3)} Z_{r,r} \left( \frac{1}{\lambda_r} - \frac{1}{\lambda_r} \right) \right] + (p_r U_k)_k + U_n L_n + O(\varepsilon).
\end{equation}

Using the fact that all odd moments in $w_k$ vanish, we get

\begin{equation}
F_{jk} = \sum (u_j u_k)_l + (u_j u_k u_l)_l
= u_j u_k U_{l,j} + \rho U_k U_{l,j} + \rho U_j U_{l,k} + \rho U_j U_{l,k}
+ \rho U_k U_{l,j} + (p_r U_k)_j + (p_r U_l)_k.
\end{equation}

The term in square brackets multiplying $U_j$ is $L_j$, i.e., it is $O(\varepsilon)$, and can therefore be ignored. Then, after gathering terms with coefficients $U_k$ and $p$, we have

\begin{equation}
F_{jk} = U_k [(p U_j)_l + (p U_l U_j)_j] + p U_k [(U_j + U_k) \delta_j]
+ \frac{1}{2} \left[ \frac{3}{2 (K + 3)} Z_{r,r} \left( \frac{1}{\lambda_r} - \frac{1}{\lambda_r} \right) \right] \delta_j.
\end{equation}

The coefficient of $U_k$ is $L_j$, according to Eq. (B7), and can therefore be neglected. To eliminate $p_j$, from the last term, we use Eq. (A2) for $L_5$. Finally, decompose the tensor $U_{k,j}$ into its dilation and shear parts in the usual way, which gives

\begin{equation}
F_{jk} = \sum (u_k u_j)_{l,l} + \rho U_k [(U_j + U_k) \delta_j]
+ \frac{1}{2} \left[ \frac{3}{2 (K + 3)} Z_{r,r} \left( \frac{1}{\lambda_r} - \frac{1}{\lambda_r} \right) \right] \delta_j.
\end{equation}

Analogy to deriving the Navier-Stokes total energy equation, we write

\begin{equation}
N_k = \sum (u_k^2 + \xi^2_{r,r})_l + \rho u_k \left[ \frac{1}{2} u^2_k + \frac{1}{2} \xi^2_{r,r} \right]_l,
\end{equation}

which can be written as

\begin{equation}
N_k = N_k^{(1)} + N_k^{(2)},
\end{equation}

where

\begin{equation}
N_k^{(1)} = \sum (u_k^2 + \xi^2_{r,r})_l + \rho u_k \left[ \frac{1}{2} u^2_k + \frac{1}{2} \xi^2_{r,r} \right]_l,
\end{equation}

and

\begin{equation}
N_k^{(2)} = \sum (u_k^2 + \xi^2_{r,r})_l + \rho u_k \left[ \frac{1}{2} u^2_k + \frac{1}{2} \xi^2_{r,r} \right]_l.
\end{equation}

For $N_k^{(1)}$, we have

\begin{equation}
N_k^{(1)} = \sum \left[ \frac{1}{2} \langle u_k^2 + \xi^2_{r,r} \rangle_0 + \frac{1}{2} \langle u_k^2 + \xi^2_{r,r} \rangle_0 \right]_l
+ \frac{1}{2} \rho U_k^2 + \frac{K + 3}{2} p \langle U_k \rangle_0 + \left[ U_k \left( \frac{3}{2} \rho U_k^2 + \frac{K + 3}{2} p \right) \right]_0
+ \frac{K}{2} (p_r - p)_l U_{k,l} + \frac{1}{2} \rho U_k^2 + \frac{1}{2} \rho U_k^2 (p_r - p) U_{k,l}.
\end{equation}
The coefficient of $U_k$ in the equation above is $L_5$ and therefore can be dropped, and the remaining terms can be rewritten as

$$N_k^{(1)} = \frac{1}{2} U_p^2 + \frac{K+3}{2} \frac{p}{\rho}[U_{k,t} + U_k U_{k,l}] + p U_{k,l}. \tag{A4}$$

According to Eq. (B7) to eliminate $U_{k,t}$, we get

$$N_k^{(1)} = -\frac{1}{2} U_p^2 + \frac{K+3}{2} \frac{p}{\rho} p_k + p U_{k,l}$$
$$+ \frac{K}{2}(p_r-p)U_k + \frac{K}{2} U_l(p_r-p)U_{k,l}. \tag{A6}$$

For $N_k^{(2)}$, remembering that moments odd in $w_k$ vanish, we have

$$N_k^{(2)} = \langle U_{n,w_k, w_k} \rangle + \langle U_{n,w_k, w_k} \rangle$$
$$+ \frac{1}{2} \langle U_{n,w_k, w_k} \rangle + \frac{1}{2} \langle U_{n,w_k, w_k} \rangle$$
$$= (p U_{k,t}) + (p U_{k,t}) + \frac{1}{2} \langle U_{n,p}_k \rangle$$
$$+ \frac{K+5}{2} \frac{p^2}{\rho} + \frac{K}{2} \frac{(p_r-p)}{\rho} \frac{U_l}{U_{k,l}}. \tag{A7}$$

This result can be written as

$$N_k^{(2)} = p(U_{k,l} + U_{k,l} + U_{k,l} + U_{k,l})$$
$$+ U_{k,l} + U_{k,l} + \frac{1}{2} U_{n,p}_k + \frac{K+5}{2} \frac{p^2}{\rho} + \frac{K}{2} \frac{(p_r-p)}{\rho} \frac{U_l}{U_{k,l}}. \tag{A8}$$

To eliminate the first order time derivative, we can rearrange the above equality as

$$N_k^{(2)} = p(U_{k,l} + U_{k,l} + U_{k,l} + U_{k,l})$$
$$+ U_{k,l} + U_{k,l} + \frac{1}{2} U_{n,p}_k + \frac{K+5}{2} \frac{p^2}{\rho} + \frac{K}{2} \frac{(p_r-p)}{\rho} \frac{U_l}{U_{k,l}}. \tag{A9}$$

$U_{k,t}$ can be eliminated by Eq. (B7), and $p_{r} + U_{p,l}$ can be eliminated by Eq. (A4).

Hence

$$N_k^{(2)} = p(U_{k,l} + U_{k,l} - \frac{p_k}{\rho} + U_{k,l})$$
$$+ U_{k,l} - \frac{5}{2} U_{n,p}_l - \frac{K}{(K+3)Z_{r} \tau} (p - p_r)$$
$$+ \frac{K}{2} \frac{(p_r-p)}{\rho} \frac{U_l}{U_{k,l}}. \tag{A7}$$

For $N_k$, sum up $N_k^{(1)}$ and $N_k^{(2)}$ together, obtaining

$$N_k = p(U_{k,l} + U_{k,l} - \frac{2}{3} U_{k,l}) - \frac{K}{(K+3)Z_{r} \tau} (p - p_r)$$
$$+ \frac{K+5}{2} \frac{p}{\rho} + \frac{K}{2} \frac{(p_r-p)}{\rho} \frac{U_l}{U_{k,l}}$$
$$+ \frac{K}{2} U_l(p_r-p)U_{k,l} + \frac{K}{2} \frac{(p_r-p)}{\rho} \frac{U_l}{U_{k,l}}. \tag{A8}$$

 Eliminate $U_{k,t}$ by Eq. (B7) again, leading to

$$N_k = p(U_{l}(U_{k,l} + U_{k,l}) - \frac{2}{3} U_{k,l}) - \frac{K}{(K+3)Z_{r} \tau} (p - p_r)$$
$$+ \frac{K}{2} \frac{(p_r-p)}{\rho} + \frac{5}{2} \frac{p}{\rho} \frac{U_l}{U_{k,l}}. \tag{A8}$$

For rotational energy equation, multiplying the continuity equation [Eq. (A1)] by $\frac{K}{4 \lambda_t}$ and the subtracting the result from Eq. (A3) give

$$L_6 = \rho(K_{4 \lambda_t}) + p U_{k} - \frac{3}{4} \rho \frac{K}{4Z_{r} \tau} (1 - 1) + O(\epsilon^2). \tag{A9}$$

Unfolding $R_6$ leads to

$$R_6 = \frac{\partial}{\partial u_k} \{ \frac{1}{2} \rho_{k} \rho_{u_k} \}$$
$$= \{ \rho_{u_k} \} + (\rho U_{k} U_{l} + p_{d_{k,l}})$$
$$+ p U_{k} \frac{K}{4 \lambda_t} + (\frac{K}{4 \lambda_t}) \rho_{u_k} U_{l} + p_{d_{k,l}} \}.$$ 

The term in square brackets is $L_6$, i.e., $O(\epsilon)$, and can be dropped. Gathering terms with coefficients $U_k$ and $p$, and eliminating $\rho(U_{k,l}) + p_{d_{k,l}}$ by Eq. (A9), we have

$$R_6 = \frac{\partial}{\partial u_k} \{ \frac{1}{2} (\rho U_{k}) + (\rho U_{k} U_{l} + p_{d_{k,l}}) \}$$
$$+ (\frac{K}{4 \lambda_t}) \rho_{u_k} U_{l} + p_{d_{k,l}} \}.$$ 

Above equations can be rewritten in the form of Eq. (10).