The Maxwell gas-surface interaction model for general discrete velocity framework in predictions of rarefied and multi-scale flows

Jianfeng Chen\textsuperscript{a}, Sha Liu\textsuperscript{a,b,c,*}, Chengwen Zhong\textsuperscript{a,b,c}, Yanguang Yang\textsuperscript{d}, Congshan Zhuo\textsuperscript{a,b,c}, Yong Wang\textsuperscript{a}, Dingwu Jiang\textsuperscript{d}

\textsuperscript{a}School of Aeronautics, Northwestern Polytechnical University, Xi’an, Shaanxi 710072, China
\textsuperscript{b}National Key Laboratory of Science and Technology on Aerodynamic Design and Research, Northwestern Polytechnical University, Xi’an, Shaanxi 710072, China
\textsuperscript{c}Institute of Extreme Mechanics, Northwestern Polytechnical University, Xi’an, Shaanxi 710072, China
\textsuperscript{d}Computational Aerodynamics Institute, China Aerodynamics Research and Development Center, Mianyang 621000, China

Abstract

The rarefied flow and multi-scale flow are very important for the aerodynamic design of spacecraft, ultra-low orbital vehicles and plumes. By introducing a discrete velocity space (DVS), the discrete velocity method (DVM) and unified methods can capture the complex and non-equilibrium distribution functions, and the flow behaviors are exactly described. Furthermore, the unified methods obtained the ability of predicting flows from continuum to rarefied regimes by adopting the philosophy of unified modeling, and further be extended to other multi-scale physics such as radiation heat transfer, phonon heat transfer and plasma. But the gas-gas interaction (GGI) is just one face of the flow problems, the concrete dynamic process needs also the description of gas-surface interaction (GSI). While in both DVM and unified methods, only a simple but not accurate GSI is used, which can be viewed as a Maxwell GSI with a fixed accommodation coefficient at 1 (full accommodation) at the present stage. Therefore, in order to break the bottleneck of DVM and unified methods of extending to the numerical experiment and study of real multi-scale flow physics this pa-

*Corresponding author
Email address: shaliu@nwpu.edu.cn (Sha Liu)
per mainly address the problem of precise GSI in the DVM framework, by constructing boundary conditions of concrete Maxwell GSI with an adjustable accommodation coefficient. In the constructing process, the problems of macro-conservation and micro-consistency in the DVS at boundary are well solved by reflected macroscopic flux and interpolation distribution function and interpolation error, respectively. Moreover, the multi-scale flows in the background of aeronautics and aerospace are often at supersonic and hypersonic speed, the unstructured velocity space (UVS) was proposed. For generality consideration, the GSI in this paper is forced on UVS, while the conventional structured velocity space can be viewed as a special case of UVS. Also the GSI can be used for both monatomic and diatomic gases with non-equilibrium translational and rotational temperatures (thermal non-equilibrium). By combined with the unified methods (unified gas-kinetic scheme in the paper), the effectiveness and validity of the present GSI on DVM framework are verified by a number of flow simulations including supersonic flow over sharp flat plate in slip regime, circular cylinder in transitional regime, blunt wedge in transitional regime, blunt circular cylinder in slip regime, and truncated flat plate in slip regime.

**Keywords:** Multi-scale flows, GSI, Accommodation coefficient, Unstructured velocity space

1. Introduction

A good knowledge of rarefied and multi-scale hypersonic flows is critical for the aerodynamic design of spacecraft, ultra-low orbital vehicles and plumes. Usually the degree of rarefaction of a gas is quantified by the Knudsen (Kn) number $Kn = \lambda/L$ where $\lambda$ is the gas mean free path (m.f.p.) and $L$ is the characteristic length of the object in the flow. According to $Kn$ number, the flow can be classified qualitatively into continuum flow ($Kn < 0.001$), slip flow ($0.001 < Kn < 0.1$), transitional flow ($0.1 < Kn < 10$) and free molecular flow ($Kn > 10$). Multi-scale flow is a term with a broad engineering background that refers to different flow regimes existing simultaneously. For in-
stance, while thinking about the flow of near-space vehicles and micro-/nano-electro-mechanical systems (MEMS/NEMS), several flow regimes including continuum flow, slip flow, and even free molecule flow will occur in the same computational domain and the local \( Kn \) number may fluctuate by many orders of magnitude. The gas-gas interaction (GGI) and gas-surface interaction (GSI), which are dealt with by flow solvers and boundary conditions, respectively, are essential parts of the flow process.

1.1 The numerical methods for flows for all flow regimes

In terms of flow numerical prediction, the traditional method of computational fluid dynamics based on the Navier-Stokes (N-S) equations is appropriate for continuum flow in airspace and macro scale, whereas the model molecular method based on rarefied gas dynamics represented by direct simulation Monte Carlo (DSMC) \[1\] method is excellent for rarefied flow and micro scale flow. However, each of the two methods mentioned above will have its own challenges when used to simulate multi-scale flow numerically \[1, 2, 3\]. People expect to combine the two methods through flow field zoning to address the multi-scale flow problem in light of the N-S method’s and DSMC method’s respective successes in continuum flow and rarefied flow, and the overlapping hybrid particle-continuum method is proposed \[4, 5, 6\]. The rarefied computing domain and the continuum computing domain must somewhat overlap in order to improve information transmission. To categorize the flow domain, empirical or semi-empirical criteria are typically used \[7, 8\]. The multi-scale problem can be partially resolved by the coupling approach, but it remains a highly challenging challenge to split the computational domain precisely and couple several flow regimes in a reasonable manner \[2\].

In recent years, a class of multi-scale asymptotic preserving (AP) \[9\] schemes based on kinetic theory have been developed, making it possible to solve the problem of all flow regimes using the same numerical method. With a local analytical integral solution of the kinetic model equation connected particle transport and collision in the numerical flow, the unified gas-kinetic scheme
(UGKS) developed by Xu et al. [10, 11] is a multi-scale technique. Thus, the molecular mean free path and collision time are not constraints on the size of the cell or the time step. Another multi-scale approach based on the same physical process as UGKS is the discrete unified gas-kinetic scheme (DUGKS) put forth by Guo et al. [12, 13]. The characteristic difference solution of the kinetic model equation in space and time, which couples the molecular transport and collision effects in a numerical time step, is used to reconstruct the multi-scale numerical flux at a cell interface rather than the analytical integral solution. Therefore, DUGKS can also be regarded as a special treatment of UGKS. Due to its straightforward flux reconstruction method and AP properties, DUGKS has undergone significant development [14]. DUGKS was expanded to unstructured mesh by Zhu et al. [3]. Wu et al. [15] suggested a DUGKS approach that takes outside forces into account. For the purpose of modeling the steady flow in all flow regimes, Pan et al. [16] built an implicit DUGKS. DUGKS was expanded to address the moving boundary issue by Wang et al. [17]. A simplified DUGKS was recently proposed by Zhong et al. [18, 19]. The DUGKS has so far been effectively used to solve a wide range of flow issues in several flow regimes, including turbulent flows [20, 21], micro flows [22, 23], compressible flows [13, 24], multiphase flows [25, 26], gas-solid flows [27], and gas mixture systems [28].

Because of the wide spreading of the particle velocity distribution in high speed flow and the narrow-kernel distribution function at high Kn number cases, the velocity mesh must cover a very large domain with high resolution. The storage and computational load will be unbearable if a conventional structured velocity mesh is used [30]. The usage of adaptive velocity mesh in phase space was suggested by the authors of the literature [2, 31, 32] to carry out automatic velocity mesh revision as needed. However, adaptive velocity mesh approaches are typically more challenging and call for additional steps in the solution process when compared to conventional velocity mesh approaches. Titarev et al. [30] and Yuan et al. [33] provide a comparatively easy method for producing a non-uniform unstructured velocity mesh (UVM), and Chen et al. [24, 34] soon adopted this technique for their Conserved DUGKS. The benefit of UVM is
that it enables flexible grid point placement, which lowers the number of grid points and prevents ray effects.

1.2 The modeling gas-surface interactions and the algorithms

The impact of the GSI model increases considerably as gas rarefaction increases, and it is one of the primary mechanisms that governs aerodynamic forces and heat transmission during hypersonic flight. Therefore, selecting the right model to calculate hypersonic rarefied flows is crucial. The initial and most basic explanation of the GSI model, which consists of the incidence and reflection processes, was provided by Maxwell as early as 1859. Maxwell established two classical reflection models, namely specular and diffuse reflections, which are the result of a gas molecule colliding with a perfectly reflecting or a completely accommodating solid surface, respectively. In the diffuse reflection model, the gas molecules are adsorbed close to the wall for a considerable amount of time, entirely erasing any memory of the encounter. These molecules are then uniformly reemitted to the half space above the wall at all angles after being desorbed. Based on the macroscopic properties of the solid surface (density, velocity, and temperature), the reflected velocity follows the Maxwell distribution. In the specular reflection model, a gas molecule that directly collides with a wall without being absorbed is reflected like a completely elastic sphere. The normal velocity component is reversible, but the tangential velocity component doesn’t change. The angle of reflection is therefore the same as the angle of incidence. The diffuse reflection model is frequently employed in natural settings. The time it takes for gas molecules to be adsorbed by the surface, particularly in the continuum flow problem, is typically substantially longer than for rarefied gas flow or smooth surface flow. Diffuse or specular reflection models should not be used exclusively in situations when the adsorption time is neither very long nor very short. By using the accommodation coefficient $\sigma$, Maxwell integrated the diffuse model and the specular reflection model: the incident molecules with the proportion $\sigma$ reflect diffusely, while the remaining molecules reflect in a specular manner. Because
of this interaction, the Maxwell model is a single parameter model that cannot simultaneously describe the transport of momentum and energy. Additionally, it is challenging to determine since the fraction of diffuse reflection molecules is an empirical metric that highly depends on numerous physical variables of gas and surface [46]. Cercignani and Lampis [47] developed a phenomenological model (CL model) to characterize GSI in accordance with the reciprocal law, in which two parameters pertaining to the tangential momentum and normal energy transport were incorporated. Later, Lord [48, 49] expanded and updated the CL model (known as the CLL model in the DSMC), making it a popular tool for theoretical and computational studies of rarefied gas flows. The CLL model enhances the reflected gas molecule velocity distributions and agrees well with the lobular distribution, but it does not agree well with the findings of experiments using a molecular beam. Based on the empirical parameters, some models describe the GSI by fitting with the experimental results, among which Nocilla model [50, 51] and multi-flux model [54] are the most typical models.

Due to its ease of implementation, the GSI model in DSMC has drawn a lot of attention [35, 44, 54, 55]. While in DVM, the GSI model is less typically employed [56]. Since DVM uses discrete velocity space (DVS), which is fixed in time and space, the specular reflection model can only be applied when the velocity space is symmetrical about the wall boundary. As a result, in the simplified treatment of the previous work, just the diffuse reflection is applied to the flat boundary [56, 58]. It is also incredibly difficult to build a DVS that is symmetric for all boundaries since object boundaries are not always straight. As a result, a boundary condition processing technique must be developed that is appropriate for both the general DVM framework and the general boundary shape. The approach presented in this study is based on the unstructured DVS and is directly transferable to the structured DVS (which can be regarded as a special unstructured DVS). The Maxwell GSI model, which has a straightforward shape and complies with the reciprocity principle [44], is now the most popular model in rarefied gas dynamics. By adjusting the Maxwellian accommodation coefficient, we investigate how the GSI affects the physical properties
of aerodynamic surfaces in this research. Simultaneously, an efficient solver for all flow regimes that incorporates the GSI model is created by merging UGKS with a simplified multi-scale flux.

The rest of the paper is structured as follows: in the second section, UGKS based on the Boltzmann-Shakhov and Boltzmann-Rykov model equations will be introduced. The GSI model, which is based on unstructured DVS, is introduced in the third section. The numerical simulation and comparison in the fourth section covers supersonic flow over sharp flat plate, circular cylinder, blunt wedge, blunt circular cylinder, and truncated flat plate. The fifth section is the conclusion.

2. Numerical method

2.1 Gas-kinetic models

The Boltzmann equation serves as the basis for the UGKS:

\[
\frac{\partial f}{\partial t} + \mathbf{\xi} \cdot \nabla f = \Omega
\]  

where \( f = f (\mathbf{x}, \mathbf{\xi}, \eta, e, t) \) is the velocity distribution functions for particles moving in D-dimensional physical space with velocity \( \mathbf{\xi} = (\xi_1, \ldots, \xi_D) \) at position \( \mathbf{x} = (x_1, \ldots, x_D) \) and time \( t \). Here \( \eta = (\xi_{D+1}, \ldots, \xi_3) \) is the dummy velocity (with the degree of freedom \( L = 3 - D \)) consisting of the remaining components of the translational velocity of particles in three dimensional space; \( e \) is a vector of \( K \) elements representing the internal degree of freedom of molecules; \( \Omega \) is the collision operator. Many kinetic models, including the Bhatnagar-Gross-Krook (BGK) collision model \[59\], the Shakhov model \[60\], the ellipsoidal statistical model (ES model) \[61\], and the Rykov model \[62\], have been proposed and used in the research of rarefied flows in order to simplify the collisional model of the full Boltzmann equation. To build kinetic models and create the related gas-kinetic schemes, numerous attempts have been made. Only the non-equilibrium transitional energy is taken into account when modeling monatomic gases. In addition to the three translational degrees of freedom for the diatomic molecule,
there are internal degrees of freedom. There are two degrees of freedom for rotation at room temperature. The degrees of freedom associated with vibrations begin to be aroused at temperatures higher than 1000 K. Only the degrees of freedom for translation and rotation are taken into account in this paper. The UGKS will be built using the Shakhov model for monatomic gas and the Rykov model for diatomic gas.

The following is the expression for the Boltzmann-BGK type control equation:

\[
\frac{\partial f}{\partial t} + \xi \cdot \nabla f \equiv \Omega = \frac{g^* - f}{\tau}
\]

(2)

where \( \tau \) is the relaxation time for the translational degree of freedom and can be calculated as \( \tau = \mu / p_t \), where \( \mu \) and \( p_t \) are the viscosity and pressure determined by the translational temperature \( T_t \) rather than equilibrium temperature \( T \). The energy equalization theorem is satisfied by the equilibrium temperature \( T \), the translational temperature \( T_t \), and the rotation temperature \( T_r \). And \( g^* \) are the Maxwell equilibrium distribution functions, Shakhov equilibrium distribution functions, or Rykov equilibrium distribution functions. The variable hard sphere (VHS) model is utilized in this study to determine viscosity:

\[
\tau = \frac{\mu}{p_t} = \frac{\mu}{\rho RT_t} = \frac{1}{\rho RT_t} \mu_0 \left( \frac{T_t}{T_0} \right) \omega
\]

(3)

where \( \rho \) and \( R \) are density and the specific gas constant, respectively. The viscosity of freestream flow \( \mu_0 \) is correlated with the m.f.p. \( \lambda \) in the following way:

\[
\lambda = \frac{2\mu (5 - 2\omega)(7 - 2\omega)}{15\rho(2\pi RT)^{1/2}}
\]

(4)

where \( T \) is In the nondimensional system, the \( Kn \) number is defined as:

\[
Kn = \frac{\lambda}{L_{ref}} = \frac{2\mu (5 - 2\omega)(7 - 2\omega)}{15\rho L_{ref}(2\pi RT)^{1/2}} = \sqrt{\frac{\gamma}{\pi}} \sqrt{2} (5 - 2\omega)(7 - 2\omega) \frac{Ma}{Re}
\]

(5)

where \( Ma = \frac{u}{\sqrt{2}RT} \) and \( Re = \frac{\rho u L_{ref} \mu}{\mu} \) are the Mach (\( Ma \)) number and Reynolds (\( Re \)) number, respectively, and \( L_{ref} \) is the reference length. Depending on the inter-molecular interaction model, where \( \omega \) is given as 0.5, 0.81, and 0.74 for the hard sphere model, ideal argon, and nitrogen, respectively.
2.2 Reduced gas-kinetic models

The discrete velocity space must be used to record the free transit of molecules, which is dependent only on the D-dimensional particle velocity $\xi$ and unrelated to $\eta$ and $e$ (for diatomic gas). The following reduced distribution functions are used in the current numerical scheme to prevent discretizing $\eta$ and $e$:

\[
G(t, x, \xi) = m \int f d\eta d\xi
\]

\[
H(t, x, \xi) = m \int \eta^2 f d\eta d\xi
\]

\[
R(t, x, \xi) = \int c f d\eta d\xi
\]

The physical meaning of $G$, $H$ and $R$, respectively, is the distribution of the mass, translational internal energy, and rotating energy in the dummy velocity space and rotational energy space. The quasi-linear feature of the model equation is advantageous for this condensed treatment. Only the simplified distribution functions $G$ and $H$ are required for monatomic gases. The reduced distribution function $R$ for rotational energy will also be introduced for diatomic gases. $R$ will, it should be observed, inevitably vanish in three dimensions. Then the macro quantity can be expressed as:

\[
W = \begin{pmatrix}
\rho \\
\rho u \\
\rho E \\
\rho E_r
\end{pmatrix} = \int \begin{pmatrix}
G \\
\xi G \\
\frac{1}{2} (\xi^2 G + H) + R
\end{pmatrix} d\xi
\]

where, $\rho E = \rho u^2 + \rho \varepsilon$ is the total energy density, $\rho \varepsilon = \rho c_v T$ is the inertial energy density, $\rho E_r$ is the rotational energy density. And translational, rotational, and total heat flux are expressed as:

\[
q_t = \frac{1}{2} \int c (c^2 G + H) d\xi
\]

\[
q_r = \int c R d\xi
\]

\[
q = q_t + q_r
\]
where \( \mathbf{c} = \xi - \mathbf{u} \) is the peculiar velocity. The governing equation of the reduced distribution function is:

\[
\begin{align*}
\frac{\partial G}{\partial t} + \xi \cdot \frac{\partial G}{\partial r} &= \frac{g^G - G}{\tau} \\
\frac{\partial H}{\partial t} + \xi \cdot \frac{\partial H}{\partial r} &= \frac{g^H - H}{\tau} \\
\frac{\partial R}{\partial t} + \xi \cdot \frac{\partial R}{\partial r} &= \frac{g^R - R}{\tau}
\end{align*}
\] (9)

For diatomic gas flow, the Rykov equilibrium is:

\[
\begin{align*}
G^G &= \left(1 - \frac{1}{Z_T}\right) G^t + \frac{1}{Z_r} G^r \\
H^H &= \left(1 - \frac{1}{Z_T}\right) H^t + \frac{1}{Z_r} H^r \\
R^R &= \left(1 - \frac{1}{Z_T}\right) R^t + \frac{1}{Z_r} R^r
\end{align*}
\] (10)

with

\[
\begin{align*}
G^t &= g^{eq}(T) \left[1 + \frac{c \cdot q_t}{15 p_t RT_t} \left(\frac{c^2}{RT_t} - D - 2\right)\right] \\
G^r &= g^{eq}(T) \left[1 + \omega_0 \frac{c \cdot q_r}{15 p_T RT} \left(\frac{c^2}{RT} - D - 2\right)\right] \\
H^t &= RT_t g^{eq}(T_t) (3 - D) \left[1 + \frac{c \cdot q_t}{15 p_T RT_t} \left(\frac{c^2}{RT_t} - D\right)\right] \\
H^r &= RT g^{eq}(T) (3 - D) \left[1 + \omega_0 \frac{c \cdot q_r}{15 p_T RT} \left(\frac{c^2}{RT} - D\right)\right] \\
R^t &= RT_t \left[G^t + (1 - \delta) \frac{c \cdot q_t}{p_t RT_t} g^{eq}(T_t)\right] \\
R^r &= RT \left[G^r + \omega_1 (1 - \delta) \frac{c \cdot q_r}{p_T RT} g^{eq}(T)\right]
\end{align*}
\] (11)

and \( g^{eq} \) represents the Maxwell equilibrium:

\[
g^{eq}(T) = \frac{\rho}{(2\pi RT)^{D/2}} \exp \left(-\frac{c^2}{2RT}\right)
\] (14)

Where the coefficients adopt the values \[11, 33\], \( \delta = 1/1.55 \), \( \omega_0 = 0.2354 \), \( \omega_1 = 0.3049 \) for nitrogen in the present work. \( Z_r \) is the rotational relaxation collision number accounting for the ratio of the slower inelastic translation–rotation energy relaxation relative to the elastic translational relaxation.
For monatomic gas flow, the Shakhov equilibrium is:

\[ g^G = g^{eq} + G_{Pr} \]
\[ H^G = H^{eq} + H_{Pr} \]  

(15)

with

\[ G_{Pr} = (1 - Pr) \frac{c \cdot q}{5pRT} \left( \frac{c^2}{RT} - D - 2 \right) g^{eq} \]

(16)

\[ H^{eq} = (K + 3 - D) RT g^{eq} \]

(17)

\[ H_{Pr} = (1 - Pr) \frac{c \cdot q}{5pRT} \left[ \left( \frac{c^2}{RT} - D \right) (K + 3 - D) - 2K \right] RT g^{eq} \]

(18)

where Prandtl (Pr) number equals 2/3. All the above equilibrium distribution functions can be obtained by macroscopic quantities.

2.2 UGKS with simplified multi-scale flux

The distribution function and macro quantity of the UGKS with simplified multi-scale flux are updated simultaneously in this research. Prior to updating the microdistribution function, the macroquantity is updated first, followed by the equilibrium distribution function. For traditional flow field output, on the other hand, macroquantities and other statistics are used.

\( G, H \) and \( R \) can be substituted by the new symbol \( \phi \) in the algorithm for simplicity’s sake since they share the same updating process, as seen in Eq. (9); this allows us to write the governing equation as

\[ \frac{\partial \phi}{\partial t} + \xi \cdot \nabla \phi = \Omega_{\phi} \equiv \frac{g^{\phi} - \phi}{\tau} \]

(19)

Integrating Eq. (19) into control volume \( V_j \) from time \( t_n \) to \( t_{n+1} \), it can be obtained that:

\[ \phi^{n+1}_{j} (\xi) - \phi^{n}_{j} (\xi) + \frac{\Delta t}{|V_j|} F^{n+1/2}_{j} (\xi) = \frac{\Delta t}{2} \left[ \Omega^{n+1}_{j} (\xi) + \Omega^{n}_{j} (\xi) \right] \]

(20)

where \( |V_j| \) and \( \Delta t = t_{n+1} - t_n \) denote the volume of \( V_j \) and the time interval, and \( F^{n+1}_{j} \) denotes the microflux across the cell interface as determined by:

\[ F^{n+1/2}_{j} (\xi) = \int_{\partial V_j} (\xi \cdot n_f) \phi \left( x_f, \xi, t_{n+1/2} \right) dS \]

(21)
where \( \partial V_j \) is the surface of the control volume \( V_j \), \( x_f \) and \( n_f \) are the interface’s midpoint and the external normal unit vector of \( dS \) (an infinitesimal element of \( \partial V_j \)), respectively. It should be noted that a trapezoidal rule is used for the time discretization of the collision term.

In this study, Eq. (20) is integrated into velocity space to first update the conservative variables [22, 24]:

\[
W_{n+1}^j = W_n^j - \Delta t \left| V_j \right| \int_{\partial V_j} (\xi \cdot n_f) \left( \frac{G(x_f, \xi, t_{n+1/2})}{2} + \xi G(x_f, \xi, t_{n+1/2}) + H(x_f, \xi, t_{n+1/2}) + R(x_f, \xi, t_{n+1/2}) \right) dS d\xi + S
\]

(22)

where \( S = (0,0,0,S_r)^T \) is the source term, and only the rotation term is not zero:

\[
S_r = \frac{\Delta t}{2} \int [\Omega^n + \Omega_r^{n+1}] d\xi = \frac{\Delta t}{2Z_{r\tau^n}} ([\rho RT]^n - [\rho RT_r]^n) + \frac{\Delta t}{2Z_{r\tau^{n+1}}} ([\rho RT]^{n+1} - [\rho RT_r]^{n+1})
\]

(23)

Afterward, the implied evolution Eq. (20) can be changed into the following explicit equation:

\[
\phi_{n+1}^j(\xi) = \left( 1 + \frac{\Delta t}{2\tau_j} \right)^{-1} \left[ \phi_n^j(\xi) - \frac{\Delta t}{\left| V_j \right|} F_{n+1/2}^j(\xi) + \frac{\Delta t}{2} \left( g_{j}^{\phi,n+1}(\xi) + g_{j}^{\phi,n}(\xi) - \phi_n^j(\xi) \right) \right]
\]

(24)

The evolution equations for the microscopic distribution functions and the macroscopic conservative variables are respectively Eqs. (22) and (24). The entire scheme may be established after the distribution functions \( \phi(x_f,\xi,t_{n+1/2}) \) at the cell interface are obtained.

Origin UGKS and DUGKS use analytic and numerical quadrature solutions, respectively, to obtain \( \phi(x_f,\xi,t_{n+1/2}) \). In this study, the simplified multi-scale flux is built using the numerical quadrature solution. The characteristic line (in the direction of particle velocity) is integrated using Eq. (19) from \( t_n \) to \( t_{n+1/2} \). The characteristic line comes to an end at the cell interface’s midpoint,
as shown in FIG. 1. The following equation describes this procedure:

\[
\phi(x_f, \xi, t_{n+1/2}) - \phi(x_f - \xi h, \xi, t_n) = h g^\phi(x_f, \xi, t_{n+1/2})
\]

(25)

where \( h = \Delta t / 2 \) denotes a half-time step and \( x_f \) denotes the interface’s midpoint.

Finally, the interface distribution function \( \phi(x_f, \xi, t_{n+1/2}) \) can be expressed as:

\[
\phi(x_f, \xi, t_{n+1/2}) = \frac{1}{\tau_{n+1/2}} \left[ \phi(x_f - \xi h, \xi, t_n) + \frac{h}{\tau_{n+1/2}} g^\phi(x_f, \xi, t_{n+1/2}) \right]
\]

(26)

where \( \phi(x_f - \xi h, \xi, t_n) \) can be integrated in velocity space to produce the macroscopic quantity at the new moment, which is what \( g^\phi(x_f, \xi, t_{n+1/2}) \) depends on. And \( \phi(x_f - \xi h, \xi, t_n) \) can be calculated from the following reconstruction using the Taylor expansion at the control volume:

\[
\phi(x_f - \xi h, \xi, t_n) = \phi_C(x_C, \xi, t_n) + \Psi(x_C, \xi, t_n) \nabla \phi_C(x_C, \xi, t_n) \cdot (x_f - \xi h - x_C), \quad x_f - \xi h \in V_C
\]

(27)

where \( V_C \) stands for control volume which is centered at point C (FIG. 1). If \( \xi \cdot n_f \geq 0 \), point C is P (the center the left cell) in FIG. 1, otherwise point C is Q (the center of the right cell). \( \phi_C(x_C, \xi, t_n) \) is the gradient of the auxiliary distribution functions at point C, which is calculated by the least-square method in this paper, and \( \Psi(x_C, \xi, t_n) \) is the gradient limiter used to suppress the numerical oscillations. And the Venkatakrishnan limiter [64] is chosen in this paper.

3. Maxwellian boundary condition in unstructured DVS

For solid wall flows, the discrete distribution functions at the wall surface should be given under the proper wall boundary conditions, such as the GSI model [14]. The most widely used model is the Maxwell model, which is based on classical thermodynamics, in which it is assumed that molecules will either reflect diffusely with complete energy accommodation, or will reflect specularly with no change in energy [35]. The fraction of molecules that will be scattered diffusely is specified by an accommodation coefficient, \( \sigma \), and the distribution
function of the reflection from the wall to the flow field is described by the following expression:

\[
\phi (\mathbf{x}_w, \xi, t^n + h) = \sigma \phi^{eq} (\xi; \rho_w, \mathbf{u}_w, T_w) + (1 - \sigma) \phi (\mathbf{x}_w, \xi, t^n + h), \quad \xi \cdot \mathbf{n}_w < 0
\]

where \( \mathbf{x}_w, \mathbf{u}_w, T_w, \) and \( \mathbf{n}_w \) are the wall’s center position, velocity, temperature, and unit normal vector, and \( \mathbf{n}_w \)’s direction is opposite to the flow field. And the distribution functions of diffuse and specular reflections are \( \phi^{eq} (\xi; \rho_w, \mathbf{u}_w, T_w) \) and \( \phi (\mathbf{x}_w, \xi, t^n + h) \), respectively.

### 3.1 Diffuse-scattering boundary condition

The diffuse reflection model, also referred to as the diffuse-scattering rule, is a general boundary condition that presupposes the distribution function for the reflected molecules follows the Maxwellian one. And the i-th reflection distribution function is given by at the half-time step \( t^n + h \):

\[
\phi (\mathbf{x}_w, \xi_i, t^n + h) = \phi^{eq} (\xi_i; \rho_w, \mathbf{u}_w, T_w), \quad \xi_i \cdot \mathbf{n}_w < 0
\]

In this case, the wall density \( \rho_w \) should be solved according to the no-penetration criterion:

\[
\sum_{\xi_i \cdot \mathbf{n}_w < 0} w_i (\xi_i \cdot \mathbf{n}) \phi^{eq} (\xi_i; \rho_w, \mathbf{u}_w, T_w) + \sum_{\xi_i \cdot \mathbf{n}_w > 0} w_i (\xi_i \cdot \mathbf{n}) \phi (\mathbf{x}_w, \xi_i, t^n + h) = 0
\]

Since Eq. (29) can be used to derive the wall incidence distribution function, it is also possible to derive the wall density.

\[
\rho_w = - \sum_{\xi_i \cdot \mathbf{n}_w > 0} w_i (\xi_i \cdot \mathbf{n}) \phi (\mathbf{x}_w, \xi_i, t^n + h) / \sum_{\xi_i \cdot \mathbf{n}_w < 0} w_i (\xi_i \cdot \mathbf{n}) \phi^{eq} (\xi_i; 1, \mathbf{u}_w, T_w)
\]

### 3.2 Specular reflection boundary condition

The fundamental principle of specular reflection states that when a gas molecule’s reflection angle equals its angle of incidence, it is reflected like an ideal sphere with its normal velocity component inverted and tangential velocity component remaining constant. When the discrete velocity mesh is asymmetric about the
wall, it will be difficult for the reflection gas molecules to land on a particular
discrete velocity mesh point for DVM. It is necessary to interpolate the dis-
btribution function in order to achieve macroscopic conservation (i.e., no mass
and energy passing through the wall) and microscopic consistency. As seen in
FIG. 2 the DVS points employed for the flow field are represented by the solid
dots. Without sacrificing generality, if the wall is horizontal (represented by the
horizontal solid line in the figure), the discrete velocity point in the incident
region (below the solid line) is the solid point (here, the point is the distribution
function of the molecules shot at the wall), and its corresponding mirror point
(corresponding to the distribution function of the mirrored reflected molecules)
is the hollow point in the reflection region (above the solid line). The incident
point \( \xi_i \) and the wall normal vector \( n_w \) can be used to determine the position
of the mirror point \( \xi'_i \) in velocity space:

\[
\xi'_i = \xi_i - 2 n_w \cdot (\xi_i \cdot n_w)
\] (32)

The incident distribution function can be found in Eq. (26); therefore, it is
possible to determine the distribution function of the solid points in the lower
half of FIG. 2. Furthermore, the distribution function of their mirror points,
or the hollow points in the upper half of the region, has a value equal to that
of the solid points. As will be covered in more detail below, the distribution
function values of the solid points of the reflection region—which are the real
velocity points of the current velocity mesh situated in the reflection region—are
obtained by reconstructing the spatial points nearby while guaranteeing the
accuracy (conservation) of the flux integral. Two workable methods are provided
in this paper because the Maxwellian bound on the DVM is first proposed.

3.2.1 Method 1 for calculating reflected macroscopic fluxes

This paper first finds a sufficient number of hollow points (distribution func-
tion unknown) close to the solid points (distribution function known) in the
reflection area. This allows for the calculation of the distribution function value
of the solid points in the reflection area, or the value of the distribution function
of the reflection. The microscopic fluxes must be numerically integrated in the DVS because the macroscopic fluxes at the interface and boundary update the cell-centered conserved values in UGKS. This raises the question of integration weights. If the weights of these hollow points are still based on the size of the velocity space mesh, there will be a problem with the non-conservation of macroscopic fluxes on the boundary, and the weights must be changed to fix this problem. The reflection distribution function is produced for the specular reflection boundary through interpolation, and its initial integral weights must be rebuilt because they are no longer relevant. It is still assumed that the wall is horizontal (horizontal solid line in the figure), that the discrete velocity point in the incident region is solid (below the solid line), and that its corresponding mirror point is hollow (in the reflection region), as shown in FIG. 3 (above the solid line). Using the law of conservation of mass, momentum, and energy, the solid point in the reflection region has been spatially interpolated to determine the value of the distribution function, and the set of weight equations for the i-th discrete velocity can be listed:

$$ \varphi_{i,o} \phi_{i,o} w_{i,o} (\xi_i \cdot n_w) = \sum_{k=1}^{n} \varphi_{i,k} \phi_{i,k} w_{i,k} (\xi_i \cdot n_w) $$

(33)

where $\varphi = [1, \xi, \frac{1}{2} \xi^2]^T$ for collision invariant and $\varphi_i \phi_i w_i$ stand for the mass, momentum, and energy of the i-th incident velocity point. The information about the hollow point (the mirror point of the incident point) and the k-th solid point (the reflected point) around the hollow point is provided by the subscripts o and k, respectively. It should be observed that in Eq. 33, the only variable that is unclear is the integral weight at the right end of the equal sign. In order to build the appropriate set of equations, it is necessary to select a sufficient number of neighboring points. The equation implies that the contribution of a single mirror point (incident point) is equal to the contribution of a number of reflected points. The integral weights of the reflected points must then be added once all mirror points (incident points) have been decomposed equally.
3.2.2 Method 2 for calculating reflected macroscopic fluxes

Additionally, for specular reflections, the incident distribution function flux information in conjunction with the wall physical parameters can be used directly to provide an accurate and reliable estimate of the macroscopic flux of the reflected molecules. The velocity space weights must be uniform throughout the flow field without further weight modification. The moments of the incident distribution function are used to determine the incident fluxes of mass, momentum, and energy. The reflected fluxes are then obtained directly using the conservation of mass, momentum, energy, constant tangential momentum flux, and reverse normal momentum flux of the specular reflection condition. This is another method for solving for the wall reflected macroscopic flux. If $F^I$ and $F^R$, respectively, stand in for the macroscopic incident flux and reflected flux, then we have:

\[
\begin{align*}
F^I_\rho &= -F^R_\rho \\
F^I_\rho E &= -F^R_\rho E \\
F^I_{\rho U} &= -\left[\left(1 - 2n_x^2\right) F^R_{\rho U} + (-2n_x n_y) F^R_{\rho V}\right] \\
F^I_{\rho V} &= -\left[(-2n_x n_y) F^R_{\rho U} + \left(1 - 2n_y^2\right) F^R_{\rho V}\right]
\end{align*}
\]

where the fluxes of mass, energy, x- and y-directional momentum are denoted by $F_\rho$, $F_{\rho E}$, $F_{\rho U}$, and $F_{\rho V}$, respectively. Method 2 is obviously preferred over Method 1 since Method 1 requires the solution of a system of equations, whereas Method 2 does not.

3.2.3 Micro-consistency

It is particularly interesting that both Methods 1 and 2 are based on the constancy of the macroscopic fluxes. The distribution function of the reflection region is interpolated in velocity space at the microscopic level, which results in an interpolation error:

\[
\phi_{int} = \phi_{re} + \phi_{err}, \, \xi_i \cdot \mathbf{n}_w < 0
\]

where the interpolated distribution function, denoted as $\phi_{int}$, is the sum of the actual reflection distribution function, denoted as $\phi_{re}$, and the deviation distri-
bution function, denoted as $\phi_{err}$. The divergence of the interpolation distribution function causes the microscopic fluxes of the wall cells to vary, which in turn causes the cell-centered distribution function (a microscopic update produced by updating the next step) to vary. Since the conserved flux strictly complies with the specular reflection boundary condition, the cell-centered macroscopic variables can be used to adjust the cell-centered distribution function and ensure the conservation:

$$f^{n+1} = \mathcal{F}^{n+1} + g(W^{n+1}) - g(W^{n+1})$$

where $\mathcal{W}^{n+1}$ is the conserved quantity determined poorly by integrating the cell-central distribution function and $W^{n+1}$ is the conserved quantity determined by accurately updating the conserved flux. During numerical simulations of the supersonic flow across a cylinder, it was found that if the distribution function interpolation error correction was not applied, the computer would crash immediately. However, after the correction, precise results could be obtained.

Its basic logic is the interpolation of the reflection distribution function while ensuring the conservation of macroscopic fluxes and the consistency of microscopic fluxes. The Maxwellian boundary condition has been applied to unstructured velocity space.

4. Numerical experiment

In this part, a series of examples, including monatomic and diatomic flows, are used to demonstrate the extended application of the GSI model to the unstructured DVS.

4.1 Verification of monatomic flows

4.1.1 Supersonic flow over a sharp flat plate

In order to confirm the accuracy of the GSI model in monatomic UGKS, the first numerical simulation in this work is a monatomic gas supersonic flow
passing a flat plate. Despite the fact that the simulated gas utilized in this configuration is now a hard spherical gas, it is based on the wind tunnel test run34 by Tsuboi and Matsumoto. FIG. 4(a) depicts the physical mesh utilized for calculation as well as the flat plate’s geometric shape. The flat plate’s front end has a sharp angle of 30 degrees, a thickness of 15 mm, and an upper surface length of 100 mm. The flat plate’s surface temperature is 290K, whereas the freestream is hypersonic flow of the argon gas at a \( Ma \) number 4.89 with a temperature of 116 K., respectively. The \( Kn \) number for the freestream with the length of plate as reference length is 0.0078. The simulation’s unstructured velocity mesh, which has 896 cells, is shown in FIG. 4(b).

When \( \sigma \) is 1, indicating completely diffuse reflection, as shown in FIG. 5, the distribution of pressure, shear stress, and heat flux on the wall, the results of the calculations in this study very closely match those of DS2V. The horizontal coordinate in the comparison of the variables on the solid wall for the flat plate arithmetic example is S. The trailing edge of the flat plate’s upper surface serves as the S coordinate’s starting point. The distribution of pressure, shear stress, and heat flux on the wall at \( \sigma \)=0.8 is shown in FIG. 6. The distribution of pressure, shear stress, and heat flux on the wall at \( \sigma \)=0, or complete specular reflection, is shown in FIG. 7. The Maxwell-GSI model based on the unstructured discrete velocity mesh in this paper is found to be accurate and fits well with the combination of DS2V calculations from the comparison of these calculation results. To further examine the impact of the GSI model during the change from complete diffuse reflection to complete specular reflection, FIG. 8 provides the distribution of physical quantities on the flat plate’s surface for \( \sigma \) values of 1, 0.8, 0.6, 0.4, 0.2, and 0, respectively.

4.1.2 Mach 5 rarefied gas flow over a circular cylinder

The second simulation, which simulates a hypersonic flow through a circular cylinder, is intended to demonstrate the GSI model’s applicability to curved surface boundaries. The freestream has a \( Ma \) number and \( Kn \) number of 5.0 and 1.0, respectively. Argon serves as the working gas, and a variable hard
sphere molecular model is employed. The specific heat ratio and Prandtl number are 5/3 and 2/3, respectively. The temperature of freestream is 273 K, and the velocity is 1539.3 m/s as a result. Freestream has a dimensionless density, temperature, and velocity of 1.0, 1.0, and 4.56, respectively, while the wall’s dimensionless temperature remains constant at 1.0. The computational domain is discretized into 64x61 control bodies and is a circular region with a (0,0) circle center and a 15 radius. The wall mesh quality must meet specific criteria in order to accurately depict the heat flux on the cylindrical surface. The circular surface’s first mesh height in this illustration is 0.01. FIG. 9 depicts the unstructured discrete velocity mesh used in this example, which has 2391 cells.

On the stationary line in front of the cylinder, shown in FIG. 10, is the distribution of density, pressure, temperature, and horizontal velocity when \(\sigma\) is 1. As can be seen, the outcomes of UGKS and DSMC are in excellent agreement with all of the current calculations. The distribution of temperature on the stationary line is, as a result of the Shakhov model, somewhat higher than the DSMC results prior to the bow shock, which is consistent with the phenomenon described in the literature [66] in the case of the shock wave structure. When \(\sigma\) is 1, FIG. 11 shows how the pressure, shear stress, and heat flux are distributed across the cylinder’s surface. All of the calculated results are in perfect agreement with those of UGKS and DSMC. On the stationary line in front of the cylinder, shown in FIG. 12, is the distribution of density, pressure, temperature, and horizontal velocity when \(\sigma\) is 0.8. When \(\sigma\) is 0.8, FIG. 13 shows how the pressure, shear stress, and heat flux are distributed across the cylinder’s surface. On the stationary line in front of the cylinder, shown in FIG. 12, is the distribution of density, pressure, temperature, and horizontal velocity when \(\sigma\) is 0. When \(\sigma\) is 0, FIG. 13 shows how the pressure, shear stress, and heat flux are distributed across the cylinder’s surface. As can be observed, the computed outcomes under various \(\sigma\) closely correspond to the outcomes of the DSMC. The distribution of pressure, shear stress, and heat flux across the cylinder’s surface is shown in FIG. 16 at various \(\sigma\). It is discovered that the results of the hypersonic cylinder flow are affected to varying degrees by the GSI model.
accommodation coefficients. The wall does not alter the tangential motion of the gas molecules when the GSI model is treated as total specular reflection, much like the non-viscous flow. The pressure at the front of the cylinder at $\sigma=0$ is higher than the pressure at $\sigma=1$, despite the fact that the wall does not alter the tangential motion of the gas molecules. This is because the normal motion of the gas molecules is completely reflected back, which is similar to the wall applying a stronger force to the gas molecules than when it is completely diffuse reflection. The comparison of the drag coefficients at various $\sigma$ is shown in Table 1. The drag coefficients calculated in the paper and the DS2V calculation are very similar. Pressure and friction together produce the drag force on the cylinder. The drag coefficient of the cylinder in the current arrangement does not change much under varied $\sigma$ because, despite the fact that the wall pressure increases with decreasing $\sigma$, the wall shear stress decreases with lowering $\sigma$. Later research will continue to examine the impact of the GSI model on the cylinder’s resistance at various $Kn$.

4.1.3 Hypersonic flow over a blunt wedge

It is crucial to accurately predict the hypersonic bottom flow in near-space vehicle flow prediction, particularly when Reaction Control System (RCS) is applied on the bottom of some vehicles. It is essential to assess the effectiveness of the RCS and the reach of the jet’s effects. The current evaluates the effectiveness of the approach in the research for the high supersonic dilute expansion
flow by simulating the hypersonic flow over a blunt wedge with reference to the configuration in the literature [67]. FIG. 17 depicts the geometry of the blunt wedge. The blunt wedge has a length of \( L = 120 \text{ mm} \), a head radius of \( R = 20 \text{ mm} \), a bottom height of \( H = 74.72 \text{ mm} \), and a body slope of \( \theta = 10^\circ \). A VHS model is used, with argon as the working gas. The \( Ma \) number of freestream is 8.1, the angle of attack is 0\(^\circ\), the temperature is 189 K (equivalent to an altitude of 85 Km), the wall temperature is 273 K, and the \( Kn \) number with \( R \) and \( H \) the as the reference length is are 0.338 and 0.090, respectively. The simulation’s unstructured physical mesh, which has 11905 cells, and unstructured velocity mesh, which has 3056 cells, are shown in FIGS. 18(a) and 18(b), respectively.

The pressure, shear stress, and heat flux distribution over the surface of the blunt wedge at \( \sigma = 1 \) are shown in FIG. 19 and the results are contrasted with those of UGKS and DS2V. Where \( 0 < s < 27.9 \) denotes the wedge’s head arc, \( 27.9 < s < 132.9 \) denotes the wedge’s body, and \( 132.9 < s < 170.3 \) denotes the wedge’s bottom. The comparative results show that the findings of this research and those of the UGKS and DS2V coincide quite well. Even the variables at the bottom of the wedge, which are two or three orders of magnitude lower than the stationary location, may be predicted with high precision. The results of pressure, shear stress, and heat flux on the blunt wedge surface with DS2V for 0.8 and 0, respectively, are shown in FIGS. 20 and 21. As can be observed, the simulation findings in this article are in good agreement with those of DS2V. The results of the calculations at different \( \sigma \) are combined and compared as shown in FIG. 22 in order to investigate the impact of the GSI model on the physical properties of the blunt wedge object surface. It is discovered that the impact of the GSI model on the shear stress and heat flux in the blunt wedge head is more significant.

4.2 Verification of diatomic flows

4.2.1 Supersonic flow around a blunt circular cylinder

The test of diatomic gas flow will now begin, taking into account the de-
degrees of freedom for translation and rotation of molecules. The accuracy of the GSI model in the diatomic UGKS is confirmed by this simulation. With an freestream $Ma$ number of 5.0 and a $Kn$ number of 0.1 (considering the cylinder’s radius as the reference length), a supersonic flow around a blunt circular cylinder was simulated. The temperature of freestream is 273 K, and the velocity is 1684.6 m/s as a result. The physical mesh and the unstructured discrete velocity mesh used in the simulation are shown in FIG. 23 with 9480 cells and 1620 cells, respectively. A semicircle with a radius of 1.0 and center coordinates $(0,0)$ makes up the front end of the obtuse body. The initial mesh layer is 0.005 in height, and the semicircle is divided into 100 and 79 cells in the circumferential and radial directions, respectively. The working gas for this simulation is nitrogen and a VHS model is used. The freestream dimensionless density, temperature and velocity are 1.0, 1.0 and 4.1833, respectively, and the wall dimensionless temperature is 1.0.

The distributions of pressure, shear stress, and heat flux over the object’s surface at $\sigma=1$, 0.8, and 0, respectively, are shown in FIGS. 24, 25, and 26. It is discovered that the results of this study closely match those of DS2V. The distribution of physical quantities on the surface of the object at various $\sigma$ is shown in FIG. 27, and once more it is discovered that the GSI model significantly affects the distribution of shear stress and heat flux on the wall.

4.2.2 Rarefied hypersonic flow over a truncated flat plate

The comparison of experimental results will help to confirm the effectiveness of the method in this paper since the previous instances in it are compared with numerical results. Rarefied hypersonic flow over flat plates has been studied theoretically, experimentally, and numerically by many authors, e.g., [68, 69, 70]. The simplicity of the geometry and the experimental results precision makes this case particularly useful for numerical validation. In this section, we focus on the study of the rarefied hypersonic flow over a flat plate with a truncated leading edge.

Allegre et al. [69] initially carried out this experiment with freestream con-
ditions shown in Table 2. In this experimental study, a truncated flat plate was positioned at a distance from a nozzle producing a nitrogen (The gas constant of nitrogen is \( R_N = 297 \text{ J/(kg} \cdot \text{K) \) flow with a freestream \( Ma \) number of 20.2 and temperature of 13.32 K. The plate was 100 mm long, 100 mm wide, 5 mm thick and the wall temperature was maintained at 290 K. Two angles of attack (0° and 10°) were examined in this experiment. The experimental measurements of pressure, heat flux, and density were found to have respective errors of 15%, 10%, and 10% \cite{71}. By using the VHS (\( \omega = 0.74 \)) model, the m.f.p. becomes:

\[
\lambda_\infty = \frac{1}{\sqrt{2\pi a_{ref}^2}} \left( \frac{T_\infty}{T_{ref}} \right)^{\omega - 1/2} \tag{37}
\]

The molecular diameter and relative molecular mass of nitrogen are 4.17 \( \times \) 10^{-10} m and 4.65 \( \times \) 10^{-26} g, respectively. As a result, the molecular m.f.p. and the number density are 0.00169 m and 3.713 \( \times \) 10^{20} \( \text{m}^3 \), respectively. The corresponding \( Kn \) number is 0.0169 using the length of the plate (100 mm) as the reference length. The reference physical quantities and dimensionless physical quantities are displayed in Tables 3 and 4, respectively.

The unstructured physical and velocity mesh, each consisting of 8055 and 3186 cells, are depicted in FIG. 28(a) and FIG. 28(b) for the numerical experiments. To examine how the GSI model affects the simulation results in this example, the accommodation coefficient was given only the two values of 1 and 0.8 (This value corresponds to literature prescriptions for a nitrogen flow over a steel plate at temperature \( T_w = 300 \text{ K} \) \cite{72, 73, 74}). FIG. 29 and 30, respectively, show the simulated pressure and heat flux distribution on the lower surface of the flat plate at 0 and 10 degrees of attack angle. To research the effects of the GSI model, both the DSMC and the present method simulate two states with \( \sigma \) of 1 and 0.8, respectively. The results obtained by both methods when taking \( \sigma = 0.8 \) at 0 degree attack angle are more consistent with the experimental results than the results with \( \sigma = 1 \), and the simulation results of the current method agree with the experimental results more favorably than the DSMC results. But for the 10 degree attack angle, things are a little different. Although the results of the current method at \( \sigma = 0.8 \) are closer to the experimental values.
Table 2: Freestream conditions for flat-plate simulations.

| Parameter     | Value     | Unit  |
|---------------|-----------|-------|
| Velocity($V_\infty$) | 1503      | m/s   |
| Temperature($T_\infty$)  | 13.32     | K     |
| Density($\rho_\infty$)   | $1.727 \times 10^{-5}$ | kg/m |
| Pressure($p_\infty$)     | 0.0683    | Pa    |

Table 3: Reference physical quantities.

| Parameter     | Value     | Unit  |
|---------------|-----------|-------|
| Velocity($V_{ref}$) | $\sqrt{2R_N T_\infty}$ | m/s   |
| Temperature($T_{ref}$) | $T_\infty$ | K     |
| Density($\rho_{ref}$) | $\rho_\infty$ | kg/m |
| Length($L_{ref}$)    | 1         | mm    |

than those at $\sigma=1$, the DSMC results for the pressure distribution are in better agreement with the experimental values. The current method, however, more closely matches the experimental value for the heat flux distribution for a $\sigma=1$ at the leading edge of the plate than for a $\sigma=0.8$, and vice versa at the following edge of the plate. In overall, the results for this numerical experiment show that the GSI model with an adjustable adaption factor should be used since they are more reasonable and required and are closer to the experimental values than the results for a $\sigma=1$.

5. Conclusion

The specular reflection boundary (which is a crucial component of the GSI model) is resolved in this article, and the Maxwell GSI model is applied for the first time to the DVM framework, extending its application to all flow regimes. Because the velocity mesh is not symmetric about the wall boundary for every geometry shape, it is difficult to calculate the values of the specular reflection distribution functions and check that the reflection macroscopic flux satisfies
Table 4: Dimensionless physical quantities.

| Parameter    | Value |
|--------------|-------|
| Velocity($V$) | 16.9  |
| Temperature($T$) | 1     |
| Density($\rho$) | 1     |
| Pressure($p$) | 0.5   |
| Length($p$)   | 100   |

the specular reflection requirement. Two methods are used to calculate the reflected macroscopic flux in order to ensure macro-conservation, while interpolation distribution function and interpolation error correction are used to ensure micro-consistency. Additionally, the method in the research was directly developed with the unstructured DVS because it is essential for hypersonic flow. Numerous numerical simulations show the method in the paper to be accurate and valid. The weight of complete diffuse reflections and specular reflections, or the accommodation coefficient $\sigma$ in the GSI model, was found to have a significant impact on the aerodynamic forces and heat transfer of the flow in numerical predictions. The use of completely diffuse reflection boundary conditions is not accurate enough, especially for rarefied and multi-scale flows.

The examples presented thus far are all 2D, but the main idea of the method can be used in any case; the application of 3D will be discussed in more detail later.

Acknowledgments

The authors thank Prof. Kun Xu in Hong Kong University of Science and Technology and Prof. Zhaoli Guo in Huazhong University of Science and Technology for discussions of the UGKS, the DUGKS and multi-scale flow simulations. Jianfeng Chen thanks Dr. Ruifeng Yuan in Northwestern Polytechnical University for useful discussions on the unstructured velocity space. Sha Liu thanks Prof. Fang Ming, Prof. Bi Lin and Prof. Tu Guohua in the China
Aerodynamics Research and Development Center for discussions of effective boundary condition in rarefied flows. This work was supported by the National Natural Science Foundation of China (Grant Nos. 12172301, 11902266, 12072283, and 11902264) and the 111 Project of China (Grant No. B17037).
Figure 1: Sketch of two neighboring cells and the characteristic-line.

References

[1] G. A. Bird, Molecular gas dynamics and the direct simulation of gas flows, Molecular gas dynamics and the direct simulation of gas flows (1994).

[2] S. Chen, K. Xu, C. Lee, Q. Cai, A unified gas kinetic scheme with moving mesh and velocity space adaptation, Journal of Computational Physics 231 (20) (2012) 6643–6664.

Figure 2: Templates for distribution function interpolation (Solid points represent discrete velocity points, and hollow points represent mirror points of discrete velocity points).
Figure 3: Templates for integral weight (Solid points represent discrete velocity points, and hollow points represent mirror points of discrete velocity points).

![Reflection zone](image)

- Incident zone

(a) Unstructured physical mesh
(b) Unstructured velocity mesh

Figure 4: Physical mesh and velocity mesh used for supersonic flow passing a flat plate ($Ma=4.89$, $Kn=0.0078$, $T_{\infty}=116$ K, $T_w=290$ K).

(a) Pressure
(b) Shear stress
(c) Heat flux

Figure 5: Physical quantity distribution on a flat plate surface: $\sigma=1$ ($Ma=4.89$, $Kn=0.0078$, $T_{\infty}=116$ K, $T_w=290$ K).
Figure 6: Physical quantity distribution on a flat plate surface: $\sigma=0.8$ ($Ma=4.89$, $Kn=0.0078$, $T_\infty=116$ K, $T_w=290$ K).

Figure 7: Physical quantity distribution on a flat plate surface: $\sigma=0$ ($Ma=4.89$, $Kn=0.0078$, $T_\infty=116$ K, $T_w=290$ K).

Figure 8: Physical quantity distribution on a flat plate surface at different $\sigma$ ($Ma=4.89$, $Kn=0.0078$, $T_\infty=116$ K, $T_w=290$ K).
Figure 9: Velocity mesh used for supersonic flow over a cylinder ($Ma=5.0$, $Kn=1.0$, $T_\infty=273$ K, $T_w=273$ K).

[3] L. Zhu, Z. Guo, K. Xu, Discrete unified gas kinetic scheme on unstructured meshes, Computers & Fluids 127 (2016) 211–225.

[4] T. E. Schwartzentruber, I. D. Boyd, A hybrid particle-continuum method applied to shock waves, Journal of Computational Physics 215 (2) (2006) 402–416.

[5] T. E. Schwartzentruber, L. C. Scalabrin, I. D. Boyd, Hybrid particle-continuum simulations of hypersonic flow over a hollow-cylinder-flare geometry, AIAA journal 46 (8) (2008) 2086–2095.

[6] J. M. Burt, I. D. Boyd, A hybrid particle approach for continuum and rarefied flow simulation, Journal of Computational Physics 228 (2) (2009) 460–475.

[7] Q. Sun, I. D. Boyd, G. V. Candler, A hybrid continuum/particle approach for modeling subsonic, rarefied gas flows, Journal of Computational Physics 194 (1) (2004) 256–277.
Figure 10: Physical quantity distribution on the stationary line in front of the cylinder at $\sigma=1$ ($Ma=5.0$, $Kn=1.0$, $T_\infty=273$ K, $T_w=273$ K).

Figure 11: Physical quantity distribution on cylinder surface at $\sigma=1$ ($Ma=5.0$, $Kn=1.0$, $T_\infty=273$ K, $T_w=273$ K).
Figure 12: Physical quantity distribution on the stationary line in front of the cylinder at \( \sigma = 0.8 \) (\( Ma = 5.0, Kn = 1.0, T_\infty = 273 \text{ K}, T_w = 273 \text{ K} \)).

Figure 13: Physical quantity distribution on cylinder surface at \( \sigma = 0.8 \) (\( Ma = 5.0, Kn = 1.0, T_\infty = 273 \text{ K}, T_w = 273 \text{ K} \)).
Figure 14: Physical quantity distribution on the stationary line in front of the cylinder at $\sigma=0$ ($Ma=5.0$, $Kn=1.0$, $T_\infty=273$ K, $T_w=273$ K).

Figure 15: Physical quantity distribution on cylinder surface at $\sigma=0$ ($Ma=5.0$, $Kn=1.0$, $T_\infty=273$ K, $T_w=273$ K).
Figure 16: Physical quantity distribution on cylinder surface at different $\sigma$ ($Ma=5.0$, $Kn=1.0$, $T_{\infty}=273$ K, $T_w=273$ K).

Figure 17: Geometric of blunt wedge (half-model).

Figure 18: Physical mesh and velocity mesh used for hypersonic flow passing a blunt wedge ($Ma=8.1$, $Kn=0.338$, $T_{\infty}=189$ K, $T_w=273$ K).
Figure 19: Physical quantity distribution on blunt wedge surface at $\sigma=1$ ($Ma=8.1$, $Kn=0.338$, $T_\infty=189$ K, $T_w=273$ K).

Figure 20: Physical quantity distribution on blunt wedge surface at $\sigma=0.8$ ($Ma=8.1$, $Kn=0.338$, $T_\infty=189$ K, $T_w=273$ K).
Figure 21: Physical quantity distribution on blunt wedge surface at $\sigma=0$ ($Ma=8.1$, $Kn=0.338$, $T_{\infty}=189$ K, $T_w=273$ K).

Figure 22: Physical quantity distribution on blunt wedge surface at different $\sigma$ ($Ma=8.1$, $Kn=0.338$, $T_{\infty}=189$ K, $T_w=273$ K).
Figure 23: Physical mesh and velocity mesh used for hypersonic flow passing a blunt circular cylinder ($Ma=5.0$, $Kn=0.1$, $T_\infty=273 \text{ K}$, $T_w=273 \text{ K}$).

Figure 24: Physical quantity distribution on blunt circular cylinder surface at $\sigma=1$ ($Ma=5.0$, $Kn=0.1$, $T_\infty=273 \text{ K}$, $T_w=273 \text{ K}$).

Figure 25: Physical quantity distribution on blunt circular cylinder surface at $\sigma=0.8$ ($Ma=5.0$, $Kn=0.1$, $T_\infty=273 \text{ K}$, $T_w=273 \text{ K}$).
Figure 26: Physical quantity distribution on blunt circular cylinder surface at $\sigma=0$ ($Ma=5.0$, $Kn=0.1$, $T_\infty=273$ K, $T_w=273$ K).

Figure 27: Physical quantity distribution on blunt circular cylinder surface at different $\sigma$ ($Ma=5.0$, $Kn=0.1$, $T_\infty=273$ K, $T_w=273$ K).

Figure 28: Physical mesh and velocity mesh used for rarefied hypersonic flow over a flat plate ($Ma=20.2$, $Kn=0.0169$, $T_\infty=13.32$ K, $T_w=290$ K).
Figure 29: Distribution of pressure and heat flux on the plate’s lower surface at a 0 degree angle of attack ($Ma=20.2$, $Kn=0.0169$, $T_\infty=13.32$ K, $T_w=290$ K).

Figure 30: Distribution of pressure and heat flux on the plate’s lower surface at a 10 degree angle of attack ($Ma=20.2$, $Kn=0.0169$, $T_\infty=13.32$ K, $T_w=290$ K).
[8] T. E. Schwartzentruber, L. C. Scalabrin, I. D. Boyd, A modular particle–continuum numerical method for hypersonic non-equilibrium gas flows, Journal of Computational Physics 225 (1) (2007) 1159–1174.

[9] S. Jin, Efficient asymptotic-preserving (ap) schemes for some multiscale kinetic equations, SIAM Journal on Scientific Computing 21 (2) (1999) 441–454.

[10] K. Xu, J.-C. Huang, A unified gas-kinetic scheme for continuum and rarefied flows, Journal of Computational Physics 229 (20) (2010) 7747–7764.

[11] K. Xu, Direct modeling for computational fluid dynamics: construction and application of unified gas-kinetic schemes, Vol. 4, World Scientific, 2014.

[12] Z. Guo, K. Xu, R. Wang, Discrete unified gas kinetic scheme for all knudsen number flows: Low-speed isothermal case, Physical Review E 88 (3) (2013) 033305.

[13] Z. Guo, R. Wang, K. Xu, Discrete unified gas kinetic scheme for all knudsen number flows. ii. thermal compressible case, Physical Review E 91 (3) (2015) 033313.

[14] Z. Guo, K. Xu, Progress of discrete unified gas-kinetic scheme for multiscale flows, Advances in Aerodynamics 3 (1) (2021) 1–42.

[15] C. Wu, B. Shi, Z. Chai, P. Wang, Discrete unified gas kinetic scheme with a force term for incompressible fluid flows, Computers & Mathematics with Applications 71 (12) (2016) 2608–2629.

[16] D. Pan, C. Zhong, C. Zhuo, An implicit discrete unified gas-kinetic scheme for simulations of steady flow in all flow regimes, Communications in Computational Physics 25 (5) (2019) 1469–1495.

[17] Y. Wang, C. Zhong, S. Liu, et al., Arbitrary lagrangian-eulerian-type discrete unified gas kinetic scheme for low-speed continuum and rarefied flow
simulations with moving boundaries, Physical Review E 100 (6) (2019) 063310.

[18] M. Zhong, S. Zou, D. Pan, C. Zhuo, C. Zhong, A simplified discrete unified gas kinetic scheme for incompressible flow, Physics of Fluids 32 (9) (2020) 093601.

[19] M. Zhong, S. Zou, D. Pan, C. Zhuo, C. Zhong, A simplified discrete unified gas–kinetic scheme for compressible flow, Physics of Fluids 33 (3) (2021) 036103.

[20] P. Wang, L.-P. Wang, Z. Guo, Comparison of the lattice boltzmann equation and discrete unified gas-kinetic scheme methods for direct numerical simulation of decaying turbulent flows, Physical Review E 94 (4) (2016) 043304.

[21] R. Zhang, C. Zhong, S. Liu, C. Zhuo, Large-eddy simulation of wall-bounded turbulent flow with high-order discrete unified gas-kinetic scheme, Advances in Aerodynamics 2 (1) (2020) 1–27.

[22] H. Liu, Y. Cao, Q. Chen, M. Kong, L. Zheng, A conserved discrete unified gas kinetic scheme for microchannel gas flows in all flow regimes, Computers & Fluids 167 (2018) 313–323.

[23] L. Zhu, Z. Guo, Numerical study of nonequilibrium gas flow in a microchannel with a ratchet surface, Physical Review E 95 (2) (2017) 023113.

[24] J. Chen, S. Liu, Y. Wang, C. Zhong, Conserved discrete unified gas-kinetic scheme with unstructured discrete velocity space, Physical Review E 100 (4) (2019) 043305.

[25] C. Zhang, K. Yang, Z. Guo, A discrete unified gas-kinetic scheme for immiscible two-phase flows, International Journal of Heat and Mass Transfer 126 (2018) 1326–1336.
[26] Z. Yang, C. Zhong, C. Zhuo, et al., Phase-field method based on discrete unified gas-kinetic scheme for large-density-ratio two-phase flows, Physical Review E 99 (4) (2019) 043302.

[27] S. Tao, H. Zhang, Z. Guo, L.-P. Wang, A combined immersed boundary and discrete unified gas kinetic scheme for particle–fluid flows, Journal of Computational Physics 375 (2018) 498–518.

[28] Y. Zhang, L. Zhu, R. Wang, Z. Guo, Discrete unified gas kinetic scheme for all knudsen number flows. iii. binary gas mixtures of maxwell molecules, Physical Review E 97 (5) (2018) 053306.

[29] L. Mieussens, A survey of deterministic solvers for rarefied flows, in: AIP Conference Proceedings, Vol. 1628, American Institute of Physics, 2014, pp. 943–951.

[30] V. Titarev, Numerical modeling of high-speed rarefied gas flows over blunt bodies using model kinetic equations, European Journal of Mechanics-B/Fluids 64 (2017) 112–117.

[31] C. Baranger, J. Claudel, N. Hérouard, L. Mieussens, Locally refined discrete velocity grids for deterministic rarefied flow simulations, in: AIP Conference Proceedings, Vol. 1501, American Institute of Physics, 2012, pp. 389–396.

[32] R. R. Arslanbekov, V. I. Kolobov, A. A. Frolova, Kinetic solvers with adaptive mesh in phase space, Physical Review E 88 (6) (2013) 063301.

[33] R. Yuan, C. Zhong, A conservative implicit scheme for steady state solutions of diatomic gas flow in all flow regimes, Computer Physics Communications 247 (2020) 106972.

[34] J. Chen, S. Liu, Y. Wang, C. Zhong, A compressible conserved discrete unified gas-kinetic scheme with unstructured discrete velocity space for multi-scale jet flow expanding into vacuum environment, Commun. Comput. Phys 28 (2020) 1502–1535.
[35] M. O. Hedahl, R. G. Wilmoth, Comparisons of the maxwell and cll gas/surface interaction models using ds mc, Tech. rep. (1995).

[36] F. Hurlbut, Particle surface interaction in the orbital context- a survey, Rarefied gas dynamics: Space-related studies (1988) 419–450.

[37] G. M. Whitesides, A. D. Stroock, et al., Flexible methods for microfluidics, Phys. Today 54 (6) (2001) 42–48.

[38] P. A. Thompson, M. O. Robbins, Origin of stick-slip motion in boundary lubrication, Science 250 (4982) (1990) 792–794.

[39] R. Pit, H. Hervet, L. Leger, Direct experimental evidence of slip in hexadecane: solid interfaces, Physical review letters 85 (5) (2000) 980.

[40] Y. Zhu, S. Granick, Rate-dependent slip of newtonian liquid at smooth surfaces, Physical review letters 87 (9) (2001) 096105.

[41] S. Succi, Mesoscopic modeling of slip motion at fluid-solid interfaces with heterogeneous catalysis, Physical review letters 89 (6) (2002) 064502.

[42] W. Santos, M. Lewis, Ds mc calculations of rarefied hypersonic flow over power law leading edges with incomplete surface accommodation, in: 34th AIAA Fluid Dynamics Conference and Exhibit, 2004, p. 2636.

[43] E. H. Kennard, et al., Kinetic theory of gases, Vol. 483, McGraw-hill New York, 1938.

[44] X. Jin, B. Wang, X. Cheng, Q. Wang, F. Huang, The effects of maxwellian accommodation coefficient and free-stream knudsen number on rarefied hypersonic cavity flows, Aerospace Science and Technology 97 (2020) 105577.

[45] J. C. Maxwell, Vii. on stresses in rarified gases arising from inequalities of temperature, Philosophical Transactions of the royal society of London (170) (1879) 231–256.
[46] B.-Y. Cao, J. Sun, M. Chen, Z.-Y. Guo, Molecular momentum transport at fluid-solid interfaces in mems/nems: a review, International journal of molecular sciences 10 (11) (2009) 4638–4706.

[47] C. Cercignani, M. Lampis, Kinetic models for gas-surface interactions, Transport theory and statistical physics 1 (2) (1971) 101–114.

[48] R. Lord, Some extensions to the cercignani–lampis gas–surface scattering kernel, Physics of Fluids A: Fluid Dynamics 3 (4) (1991) 706–710.

[49] R. Lord, Some further extensions of the cercignani–lampis gas–surface interaction model, Physics of Fluids 7 (5) (1995) 1159–1161.

[50] S. Nocilla, The surface re-emission law in free molecule flow (1962).

[51] F. Hurlbut, F. Sherman, Application of the nocilla wall reflection model to free-molecule kinetic theory, The Physics of Fluids 11 (3) (1968) 486–496.

[52] F. G. Collins, E. Knox, Determination of wall boundary conditions for high-speed-ratio direct simulation monte carlo calculations, Journal of Spacecraft and Rockets 31 (6) (1994) 965–970.

[53] F. G. Collins, E. Knox, Parameters of nocilla gas/surface interaction model from measured accommodation coefficients, AIAA journal 32 (4) (1994) 765–773.

[54] D. C. Wadsworth, D. B. VanGilder, V. K. Dogra, Gas-surface interaction model evaluation for dsmc applications, in: AIP Conference Proceedings, Vol. 663, American Institute of Physics, 2003, pp. 965–972.

[55] N. Yamanishi, Y. Matsumoto, K. Shobatake, Multistage gas–surface interaction model for the direct simulation monte carlo method, Physics of Fluids 11 (11) (1999) 3540–3552.

[56] Y.-D. Zhang, A.-G. Xu, G.-C. Zhang, Z.-H. Chen, Discrete boltzmann method with maxwell-type boundary condition for slip flow, Communications in Theoretical Physics 69 (1) (2018) 77.
[57] T. T. Pham, Q. D. To, G. Lauriat, C. Léonard, V. Van Hoang, Effects of surface morphology and anisotropy on the tangential-momentum accommodation coefficient between pt (100) and ar, Physical Review E 86 (5) (2012) 051201.

[58] C. Lim, C. Shu, X. Niu, Y. Chew, Application of lattice boltzmann method to simulate microchannel flows, Physics of fluids 14 (7) (2002) 2299–2308.

[59] P. L. Bhatnagar, E. P. Gross, M. Krook, A model for collision processes in gases. I. small amplitude processes in charged and neutral one-component systems, Physical review 94 (3) (1954) 511.

[60] E. Shakhov, Generalization of the krook kinetic relaxation equation, Fluid dynamics 3 (5) (1968) 95–96.

[61] L. H. Holway Jr, New statistical models for kinetic theory: methods of construction, The physics of fluids 9 (9) (1966) 1658–1673.

[62] V. Rykov, A model kinetic equation for a gas with rotational degrees of freedom, Fluid Dynamics 10 (6) (1975) 959–966.

[63] J. Yang, J. Huang, Rarefied flow computations using nonlinear model boltzmann equations, Journal of Computational Physics 120 (2) (1995) 323–339.

[64] V. Venkatkrishnan, Convergence to steady state solutions of the euler equations on unstructured grids with limiters, Journal of Computational Physics 118 (1) (1995) 120–130.

[65] N. Tsuboi, Y. Matsumoto, Experimental and numerical study of hypersonic rarefied gas flow over flat plates, AIAA journal 43 (6) (2005) 1243–1255.

[66] S. Liu, C. Zhong, Investigation of the kinetic model equations, Physical Review E 89 (3) (2014) 033306.

[67] D. Jiang, M. Mao, J. Li, X. Deng, An implicit parallel ugks solver for flows covering various regimes, Advances in Aerodynamics 1 (1) (2019) 1–24.
[68] J. Davis, J. Harvey, Comparison of the direct simulated method with experiment for rarefied flat plate flow, Progress in Astronautics and Aeronautics (1963) 335–348.

[69] J. Allegre, M. Raffin, A. Chpoun, L. Gottesdiener, Rarefied hypersonic flow over a flat plate with truncated leading edge, Rarefied gas dynamics: Space science and engineering (1994) 285–295.

[70] N. Tsuboi, H. Yamaguchi, Y. Matsumoto, Direct simulation monte carlo method on rarefied hypersonic gas flow around flat plates, Journal of spacecraft and rockets 41 (3) (2004) 397–405.

[71] R. C. Palharini, C. White, T. J. Scanlon, R. E. Brown, M. K. Borg, J. M. Reese, Benchmark numerical simulations of rarefied non-reacting gas flows using an open-source dsmc code, Computers & Fluids 120 (2015) 140–157.

[72] D. J. Rader, J. N. Castaneda, J. R. Torczynski, T. W. Grasser, W. M. Trott, Measurements of thermal accommodation coefficients., Tech. rep., Sandia National Laboratories (SNL), Albuquerque, NM, and Livermore, CA . . . (2005).

[73] W. M. Trott, J. N. Castañeda, J. R. Torczynski, M. A. Gallis, D. J. Rader, An experimental assembly for precise measurement of thermal accommodation coefficients, Review of scientific instruments 82 (3) (2011) 035120.

[74] M. Schouler, Y. Prévereaud, L. Mieussens, Survey of flight and numerical data of hypersonic rarefied flows encountered in earth orbit and atmospheric reentry, Progress in Aerospace Sciences 118 (2020) 100638.