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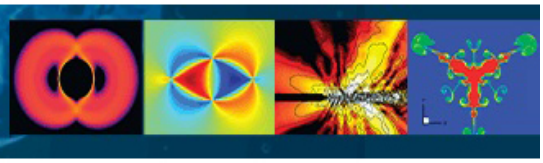

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ABSTRACT

Many kinetic relaxation models have been proposed for the study of rarefied flows. Based on the single relaxation time model, a discrete velocity method-based unified gas-kinetic scheme (UGKS) has been constructed. The UGKS models the gas dynamics on the discretized space directly on account of accumulating flow evolution from particle transport and collision within a time step. Under the UGKS framework, a unified gas-kinetic wave-particle (UGKWP) method has been further developed for non-equilibrium flow simulation, where the time evolution of the gas distribution function is composed of analytical wave and individual particles. In the highly rarefied regime, the flow evolution is mainly described by the particle transport and collision. Because of the use of single relaxation time for particle collision, there is a noticeable discrepancy between the UGKWP solution and the full Boltzmann or direct simulation Monte Carlo (DSMC) result, such as the temperature distribution inside a shock layer at high Mach numbers. In this Letter, a modification of the particle collision time according to the particle velocity will be implemented in the UGKWP. As a result, the new model greatly improves the performance of the UGKWP in the capturing of non-equilibrium flows. There is an excellent match between UGKWP and DSMC or Boltzmann solution in the highly rarefied regime. In the continuum flow regime, due to the absence of particles, the modification of the particle collision time will not take effect and the UGKWP will get back to the hydrodynamic Navier–Stokes flow solver with correct dissipative coefficients at small cell Knudsen numbers.

According to the Knudsen number, defined as the ratio of the particle mean free path over a characteristic length scale, the flow regime can be classified into the continuum, transition, and rarefied one. In many engineering applications, such as hypersonic flows around a vehicle in near space flight, multiple regimes can co-exist in a single computation, where the local Knudsen number can vary widely on many orders of magnitude.[1] The development of a multiscale method for all flow regimes becomes necessary.[2] The Boltzmann equation resolves the flow dynamics on the kinetic particle mean free path and collision time scale.[3] Many Boltzmann solvers based on the discrete velocity method (DVM) have been constructed with the requirement on the cell size and time step at the kinetic scale.[4–8] Instead of solving the complicated collision term of the Boltzmann equation, the direct simulation Monte Carlo (DSMC) mimics the Boltzmann transport and collision process using stochastical particles and achieves great success for the rarefied flow study.[9] Same as the direct Boltzmann solver, the DSMC also requires the cell size and time step to be less than the particle mean free path and collision time. In the study of rarefied flows, many kinetic relaxation models and the corresponding schemes have been proposed.[10–16]

Based on the gas-kinetic relaxation models and DVM discretization, a unified gas-kinetic scheme (UGKS) has been developed for the rarefied and continuum flows.[17,18] The evolution of the gas distribution function in the UGKS is based on the integral solution of the kinetic model equation, where the accumulating effect from particle transport and collision within a numerical time step is used in the construction of the multiscale method. The integral solution is basically composed of the hydrodynamic evolution from the integration of the equilibrium state and the kinetic

particle-free transport from the initial non-equilibrium gas distribution. The weights between dynamics of these two scales depend on the cell's Knudsen number. Therefore, the integral solution can give an accurate representation for both continuum and free molecule flows and is used in the construction of the multiscale scheme. In the continuum flow regime at a high Reynolds number, the UGKS gets back to the standard Navier–Stokes (NS) flow solver with a numerical time step being much larger than the particle collision time.[2] In order to improve the efficiency and reduce the memory cost, the DVM-based gas distribution function in the UGKS is replaced by a particle and wave formulation in the newly developed unified gas-kinetic wave-particle (UGKWP) method.[19–21] The evolution of particle transport and the hydrodynamic wave propagation in the UGKWP is still controlled by the integral solution of the kinetic relaxation model. Even though accurate solutions can be obtained from the UGKWP in all flow regimes, especially in the near continuum and continuum regimes, there are still solution discrepancies in the highly non-equilibrium flow regime, such as the temperature distribution inside the shock layer at a high Mach number. The reason for the difference mainly comes from the single relaxation time for all speed particles in the kinetic model equation, while the physical relaxation time varies in the Boltzmann collision term and the DSMC according to the particle velocity. In fact, based on the kinetic theory, the particle collision time τ is related to the mean free path ℓ and particle velocity $|\vec{v}|$, such as $\tau = \ell/|\vec{v}|$. The Bhatnagar-Gross-Krook (BGK) model with velocity-dependent collision frequency was briefly introduced in Ref. 22. With a similar idea, a generalization of the linearized BGK model with velocity-dependent collision frequency was considered in Ref. 23. The original numerical study of modifying the BGK model with velocity-dependent collision time in an explicit form was presented by Struchtrup in 1997[24] and further developed by Mieussens and Struchtrup in 2004.[25] Later in 2005, the velocity-dependent BGK model was improved further by Zheng and Struchtrup.[26] The current research is along the same line of reasoning. Due to the wave-particle decomposition in the UGKWP, in the highly rarefied regime, the flow evolution is mainly controlled by particles. Therefore, the particle collision time in the UGKWP can be easily modified according to the particle velocity. Since this only affects the free transport distance of a few very high speed particles, the mass, momentum, and energy in the scheme are fully conserved. This direct modeling on particle transport greatly improves the performance of the UGKWP in capturing the non-equilibrium solution. In the near continuum regime, the particles in the UGKWP disappear, and a continuum Navier–Stokes flow solver is recovered.

The kinetic relaxation model for the evolution of gas distribution function f is

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla_{\vec{x}} f = \frac{M-f}{\tau}, \tag{1}$$

where M is the equilibrium state, $\vec{v}$ is the particle velocity, and τ is the relaxation or collision time. For monatomic and diatomic gases, the BGK, Ellipsoidal Statistical (ES), Shakhov, and Rykov models can be formulated in the above relaxation form.[10–13] For a local constant collision time τ, the integral solution of Eq. (1) can be written as[17,27]

$$f\left(\vec{x},t,\vec{v},\vec{\xi}\right) = \frac{1}{\tau}\int_0^t e^{-(t-t')/\tau} M\left(\vec{x}',t',\vec{v},\vec{\xi}\right)dt' + e^{-t/\tau} f_0(\vec{x}-\vec{v}t), \tag{2}$$

where $\vec{\xi}$ is the internal variable and f_0 is the initial gas distribution function at $t = 0$. In both equilibrium state and initial distribution, the particle transports along characteristics $\vec{x}' = \vec{x} + \vec{v}(t'-t)$.

The UGKWP is constructed on a discretized physical space $\sum_i \Omega_i \subset \mathcal{R}^3$ and discretized time $t^n \in \mathcal{R}^+$.[19–21] Initially, at the beginning of each time step, the distributions of macroscopic flow variables and microscopic gas distribution function inside each control volume are known. The cell averaged conservative flow variables, such as $\vec{W}_i = (\rho_i, \rho_i\vec{U}_i, \rho_i E_i)$ in a physical control volume Ω_i, are defined as

$$\vec{W}_i^n = \frac{1}{|\Omega_i|}\int_{\Omega_i} \vec{W}^n(\vec{x})d\vec{x},$$

and the corresponding distribution of particles is given by f_0, with the condition

$$\vec{W}_i^n = \int f_0\vec{\psi}d\Xi,$$

where $\vec{\psi} = (1, \vec{v}, \frac{1}{2}(\vec{v}^2 + \vec{\xi}^2))^T$ is the vector of moments for the conservative flow variables and $d\Xi = d\vec{v}d\vec{\xi}$.

The UGKWP updates both the macroscopic flow variables and the gas distribution function. The macroscopic variables are updated in a conservative form as follows:

$$\vec{W}_i^{n+1} = \vec{W}_i^n + \frac{\Delta t}{|\Omega_i|}\sum_{l_s\in\partial\Omega_i} |l_s|\vec{F}_s, \tag{3}$$

where $l_s \in \partial\Omega_i$ is the cell interface with center $\vec{x}_s$ and outer unit normal vector $\vec{n}_s$. The flux function for the macroscopic variables at the cell interfaces is constructed from Eq. (2),

$$\begin{aligned}\vec{F}_s &= \frac{1}{\Delta t}\int_0^{\Delta t}\int f\left(\vec{x}_s,t,\vec{v},\vec{\xi}\right)\vec{v}\cdot\vec{n}_s\vec{\psi}d\Xi dt \\ &= \frac{1}{\Delta t}\int_0^{\Delta t}\int\left[\frac{1}{\tau}\int_0^t e^{(t'-t)/\tau} M\left(\vec{x}_s',t',\vec{v},\vec{\xi}\right)dt'\right. \\ &\quad \left. + e^{-t/\tau} f_0(\vec{x}_s-\vec{v}t)\right]\vec{v}\cdot\vec{n}_s\vec{\psi}d\Xi dt,\end{aligned} \tag{4}$$

with the characteristic line $\vec{x}_s' = \vec{x}_s + \vec{v}(t'-t)$. The equilibrium flux from the integration of Maxwellian distribution is denoted as $\vec{F}_{eq,s}$,

$$\vec{F}_{eq,s} \overset{\text{def}}{=} \frac{1}{\Delta t}\int_0^{\Delta t}\int\frac{1}{\tau}\int_0^t e^{(t'-t)/\tau} M\left(\vec{x}_s',t',\vec{v},\vec{\xi}\right)dt'\vec{v}\cdot\vec{n}_s\vec{\psi}d\Xi dt, \tag{5}$$

which can be evaluated analytically from the distribution of macroscopic flow variables $\vec{W}^n$ through the gas-kinetic formulation.[27] The flux coming from the free transport of f_0 is given by $\vec{F}_{fr,s}$,

$$\vec{F}_{fr,s} \overset{\text{def}}{=} \frac{1}{\Delta t}\int_0^{\Delta t}\int e^{-t/\tau} f_0(\vec{x}_s-\vec{v}t)\vec{v}\cdot\vec{n}_s\vec{\psi}d\Xi dt, \tag{6}$$

which is evaluated by tracking the particles from the initial distribution f_0.[19–21] Then, the updates of macroscopic variables will become

$$\vec{W}_i^{n+1} = \vec{W}_i^n + \frac{\Delta t}{|\Omega_i|}\sum_{l_s\in\partial\Omega_i}|l_s|\vec{F}_{eq,s} + \frac{\Delta t}{|\Omega_i|}\vec{W}_{fr,i}, \tag{7}$$

where $\vec{W}_{fr,i}$ is the net free streaming flow of cell i calculated by counting the particles passing through the cell interfaces during a time step. One of the outstanding features of the UGKWP is that the gas distribution function f_0 is composed of collisional particles and collisionless particles in the evolution process within a time step

Δt. The flux in $\vec{W}_{fr,i}$ from the collisional particle can be evaluated analytically. The number of collisionless particles is proportional to $e^{-\Delta t/\tau}$. In the continuum flow regime, all fluxes from f_0 can be evaluated analytically and the UGKWP will become a NS solver without particles. The detailed formulation is given next.

The evolution of particle $P_k(m_k, \vec{x}_k, \vec{v}_k, e_k, t_{f,k})$ is represented by its mass m_k, position coordinate $\vec{x}_k$, velocity coordinate $\vec{v}_k$, internal energy e_k, and free streaming time $t_{f,k}$. The particle evolution follows the same integral solution as Eq. (2) of the kinetic model equation, which results in

$$f\left(\vec{x}, t, \vec{v}, \vec{\xi}\right) = \left(1 - e^{-t/\tau}\right) M^+\left(\vec{x}, t, \vec{v}, \vec{\xi}\right) + e^{-t/\tau} f_0(\vec{x} - \vec{v}t). \tag{8}$$

The above M^+ is named as the hydrodynamic distribution function with analytical formulation, i.e., the wave formulation of the gas distribution function. The initial particle distribution f_0 has a probability of $e^{-t/\tau}$ to free streaming and a probability of $(1 - e^{-t/\tau})$ to colliding with other particles, and the post-collision distribution follows the distribution $M^+(\vec{x}, t, \vec{v}, \vec{\xi})$. The time for the free streaming to stop and follow the distribution M^+ is called the first collision time t_c. The cumulative distribution function of the first collision time is

$$F(t_c < t) = 1 - \exp(-t/\tau), \tag{9}$$

from which t_c can be sampled as $t_c = -\tau \ln(\eta)$ with η generated from a uniform distribution $U(0, 1)$. For a particle P_k, the free streaming time is given by

$$t_{f,k} = \begin{cases} -\tau \ln(\eta), & \text{if } -\tau \ln(\eta) < \Delta t \\ \Delta t, & \text{if } -\tau \ln(\eta) \geq \Delta t, \end{cases} \tag{10}$$

where Δt is the time step. In a numerical time step from t^n to t^{n+1}, all simulating particles in the UGKWP method can be categorized into two groups: the **collisionless particle** P^f and the **collisional particle** P^c. The categorization is based on the relation between the free streaming time t_f and the time step Δt. Specifically, the collisionless particle is defined as the particle whose free streaming time t_f is longer than or equal to the time step Δt, and the collisional particle is defined as the particle whose free streaming time t_f is shorter than Δt. For the collisionless particle, its trajectory is fully tracked during the whole time step. For the collisional particle, the particle trajectory is tracked until t_f. Then, the particle's mass, momentum, and energy are merged into macroscopic quantities in that cell, and the simulation particle gets eliminated. Those eliminated particles may get re-sampled once the updated total macroscopic quantities $\vec{W}^{n+1}$ and the fraction from the eliminated particles $\vec{W}^{n+1,h}$ are obtained.

Now, the particle will take free streaming for a period of $t_{f,k}$,

$$\vec{x}_k^{n+1} = \vec{x}_k^n + \vec{v}_k t_{f,k}. \tag{11}$$

The net free streaming flow of cell i within a time step Δt can be calculated by counting the particles passing through the cell interface, which can be written as

$$\vec{W}_{fr,i} = \frac{1}{\Delta t}\left(\sum_{k \in P_{\partial\Omega_i^+}} \vec{W}_{P_k} - \sum_{k \in P_{\partial\Omega_i^-}} \vec{W}_{P_k}\right), \tag{12}$$

where $\vec{W}_{P_k} = \left(\omega_k m_k, \omega_k m_k \vec{v}_k, \frac{1}{2} m_k\left(\omega_k \vec{v}_k^2 + \kappa_k e_k\right)\right)^T$, $P_{\partial\Omega_i^+}$ is the index set of the particles streaming into cell Ω_i during a time step, and $P_{\partial\Omega_i^-}$ is the index set of the particles streaming out of cell Ω_i. Then, the update of the total macroscopic flow variables in Eq. (7) is fully determined. The updated hydrodynamic flow variables originating from the eliminated particles are

$$\vec{W}_i^{n+1,h} = \vec{W}_i^{n+1} - \vec{W}_i^{n+1,p},$$

where $\vec{W}_i^{n+1,p}$ is macroscopic flow quantities of all remaining particles in the cell i, which can be evaluated by adding their mass, momentum, and energy together.

Theoretically, we can go to the next time step by sampling particles from the distribution M^+ with a total mass, momentum, and energy of $\vec{W}^{n+1,h}$ and get the particle representation of f_0 with the condition $\vec{W}_i^{n+1} = \int f_0 \vec{\psi} d\Xi$ again for the next time step evolution. This is the so-called unified gas-kinetic particle (UGKP) method.[19,20] In the UGKP, the initial distribution f_0 in cell i is composed of the newly sampled particles and the remaining particles from the previous time step. However, the UGKWP is further developed from the UGKP in the following. Not all particles from $\vec{W}_i^{n+1,h}$ need to be sampled because some sampled particles will become collisional hydro-particles in the next time step from t^{n+1} to t^{n+2} and disappear again by collision. Therefore, only collisionless hydro-particles from $\vec{W}_i^{n+1,h}$ need to be sampled with $t_{f,k} = \Delta t$. Based on the cumulative distribution function of the first collision time in Eq. (9), the collisionless hydro-particles sampled from $M^+(\vec{W}_i^{n+1})$ take a total mass of $e^{-\Delta t/\tau_i}|\Omega_i|\rho_i^{n+1,h}$. The collisional hydro-particles have a total mass $(1 - e^{-\Delta t/\tau_i})|\Omega_i|\rho_i^{n+1,h}$ with a corresponding distribution M^+. The flux contribution in f_0 from collisional hydro-particles can be evaluated analytically, which is denoted as $\vec{F}_{fr,s}^h$.[19] Therefore, the flux contribution from f_0 in Eq. (6) can be evaluated as

$$\sum_s |l_s| \vec{F}_{fr,s} = \sum_s |l_s| \vec{F}_{fr,s}^h + \vec{W}_{fr,i}^p,$$

where $\vec{W}_{fr,i}^p$ is the flux contribution of all the remaining particles from the previous time step and the newly sampled collisionless particles,

$$\vec{W}_{fr,i}^p = \frac{1}{\Delta t}\left(\sum_{k \in P_{\partial\Omega_i^+}} \vec{W}_{P_k} - \sum_{k \in P_{\partial\Omega_i^-}} \vec{W}_{P_k}\right).$$

So, in the UGKWP, the macroscopic flow variables in Eq. (7) evolve as

$$\vec{W}_i^{n+1} = \vec{W}_i^n + \frac{\Delta t}{|\Omega_i|}\left(\sum_{l_s \in \partial\Omega_i} |l_s| \vec{F}_{eq,s} + \sum_{l_s \in \partial\Omega_i} |l_s| \vec{F}_{fr,s}^h + \vec{W}_{fr,i}^p\right). \tag{13}$$

In the UGKWP, the number of particles used in the evolution depends on the cell Knudsen number $Kn_c = \tau/\Delta t$ and takes a fraction of macroscopic variables $e^{-1/Kn_c}\vec{W}$ inside each control volume. In the continuum flow regime with $\Delta t \gg \tau$, the particle will gradually disappear, and the UGKWP will become a gas-kinetic scheme for the Navier–Stokes equations.[27]

The above UGKWP is based on the single relaxation time kinetic model τ, even though the viscosity and heat conduction

coefficients can be correctly defined through the Shakhov or Rykov models. In physical reality, the particle mean free path ℓ has a clear definition, such as the hard sphere molecule,[9]

$$\ell = \frac{16}{5}\left(\frac{m}{2\pi kT}\right)^{1/2}\frac{\mu}{\rho},$$

where μ is the dynamic viscosity coefficient, ρ is the density, and T is the temperature. The particle collision time is related to the particle velocity $|\vec{v}|$ through $\ell/|\vec{v}|$. In order to incorporate this physical reality, a direct modification of the particle collision time in the UGKWP can be constructed along a similar idea in Ref. 25. For those particles with a relative high velocity, the newly modeled τ^* has the following form:

$$\tau_* = \begin{cases} \tau & \text{if } |\vec{v}-\vec{U}| \le b\sigma \\ \dfrac{1}{1+a^*|\vec{v}-\vec{U}|/\sigma}\tau & \text{if } |\vec{v}-\vec{U}| > b\sigma, \end{cases} \tag{14}$$

where $\sigma = \sqrt{RT}$ and a and b are two parameters to be determined. Based on numerical experiments, the values of $a = 0.1$ and $b = 5$ give satisfactory results in all cases we tested at different Knudsen and Mach numbers. These fixed values are used in all numerical examples in this paper. After the determination of τ_*, for the particle, the free streaming time is still determined by $t_f = -\tau_* \ln(\eta)$. For high speed particles, the collision time will be reduced according to their velocity. For other particles, the free steaming time remains the same, and their dynamics has been taken into account properly by the kinetic relaxation model, such as recovering the viscosity and heat conduction coefficients. The above modification of the particle collision time will not affect the conservation of the scheme. For a specific particle, its mass, momentum, and energy will remain the same, and the only modification is about the distance it travels. The modification of the particle-free streaming time can be done directly in the UGKWP. This simple modification only takes effect on the high speed particle in the highly rarefied regime. The equilibrium flux remains the same as the original UGKWP method. For the flow in the continuum regime, the particles in the UGKWP will disappear without any effect from the above modification on the particle collision time, and accurate NS solutions with correct transport coefficients can be obtained. The idea of τ_* modification in the UGKWP has also a similar consideration to the previous effort for generalization of the Chapman–Enskog expansion in the non-equilibrium flow study.[28]

The above UGKWP is tested in both 1D and 2D cases at different Mach and Knudsen numbers. One of the simplest and most fundamental non-equilibrium gas-dynamic phenomena that can be used for the model validation is the internal structure of a normal shock wave. There are mainly two reasons for this. First, the shock wave represents a flow condition that is far from thermodynamic equilibrium. Second, the shock structure is unique and it separates fluid dynamics from the effect of the boundary condition. Since the 1950s, the computation of the shock structure has played a dominant role in validating kinetic theory and numerical schemes in the non-equilibrium flow study.[29,30] In order to validate the UGKWP modeling, the shock structure at different Mach numbers for monatomic and diatomic gases will be calculated. In the shock structure calculations, the reference length is the upstream mean free path, and the computational domain is $[-25, 25]$ with 100 cells. Besides the density and temperature distributions, the stress and heat flux are presented in some cases as well and compared with the reference solutions of the Boltzmann equation and DSMC. In the following calculations, the viscosity coefficient is given by

$$\mu = \mu_{ref}\left(\frac{T}{T_{ref}}\right)^{\omega}, \tag{15}$$

with the reference value

$$\mu_{ref} = \frac{15\sqrt{\pi}}{2(5-2\omega)(7-2\omega)}\frac{\ell}{L}, \tag{16}$$

where L is the characteristic length and ω is the temperature-dependent index.

First, the shock structure of a monatomic gas is presented. Comparisons of the UGKWP results are made with the solutions computed by Ohwada,[31] where the full Boltzmann equation for the hard sphere molecule was solved. For the hard sphere molecule, ω is set to be 0.5. Figure 1 shows the density, temperature, stress, and heat flux inside a shock layer at Mach number M = 3 computed by both the current and the original single relaxation time UGKWP, where better agreement has been obtained from the updated UGKWP.

Figure 2 shows the argon shock structures for a viscosity coefficient of $\mu \sim T^{0.72}$ at Mach number 9, where the comparisons are among the original, current UGKWP, and DSMC solutions. Good agreement has been obtained between the UGKWP and DSMC solutions.

In addition to the monatomic gas, the shock structure in a diatomic gas is presented as well. The diatomic gas UGKWP method is presented in Ref. 21. For the diatomic gas, besides the translational relaxation, the rotational relaxation is included as well. The relaxation time between the rotational and translation energy exchange is determined by the rotational collision number Z_{rot}. For the nitrogen gas, the viscous coefficient follows Eqs. (15) and (16) with the temperature-dependent index $\omega = 0.74$. The rotational collision number used in the UGKWP is $Z_{rot} = 2.4$. The normalized temperature and density comparisons between UGKWP and DSMC at M = 1.53, 4.0, 5.0, and 7.0 are plotted in Fig. 3. With the modification of the particle collision time, the UGKWP avoids the early temperature rising problem and presents good agreement with the DSMC results. In comparison with the Rykov model-based UGKS results,[32] significant improvement has been observed.

As tested in Ref. 25, the plane Couette flow was calculated here as well for argon gas with $\omega = 0.81$. The Knudsen number is defined by $\mathrm{Kn} = \mu_0\sqrt{2\pi RT_0}/(2p_0L)$ with the reference temperature $T_0 = 273$ K, viscosity $\mu_0 = 2.1173 \times 10^{-5}\mathrm{Ns/m^2}$, pressure $p_0 = \rho_0 RT_0$, and characteristic length $L = 1$ m. With a fixed bottom wall, the top wall moves at a speed $u_w = 1000$ m/s in the horizontal direction. The temperatures at the bottom and top walls are fixed at $T_w = T_0 = 273$ K. The cases with $Kn = 0.01199, 0.1199$, and 1.199 are computed. The initial temperature of the gas in all cases is set to be T_0, and the initial density is set as ρ_0. In the computation, the physical domain is $[0, 1]$ with 200 cells in the y direction. The velocity and temperature profiles calculated by the UGKWP and DSMC are shown in Fig. 4. Reasonable agreements have obtained between the

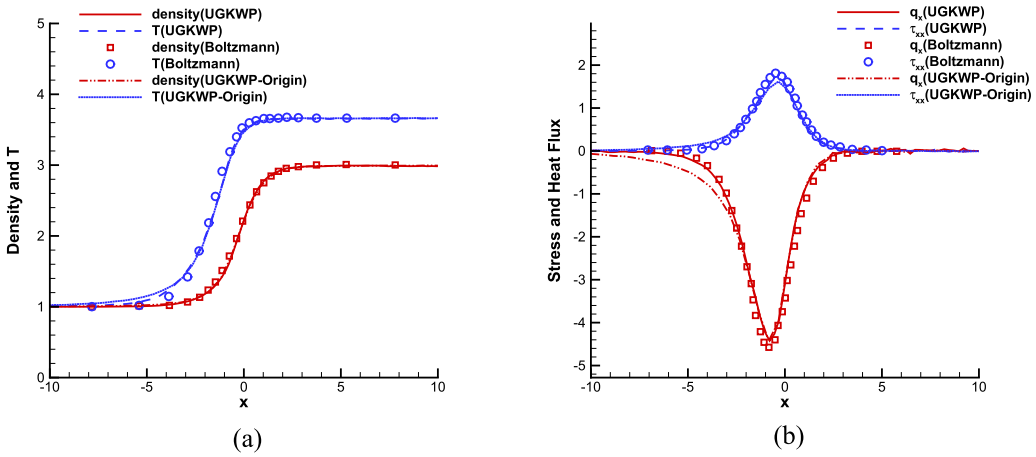

FIG. 1. M = 3 shock structure for a hard sphere molecule calculated by the original UGKWP, the updated UGKWP, and the direct Boltzmann solver. The x-coordinate is normalized by ℓ. The symbols are the results from Ref. 31. (a) Density and temperature distributions; (b) stress and heat flux.

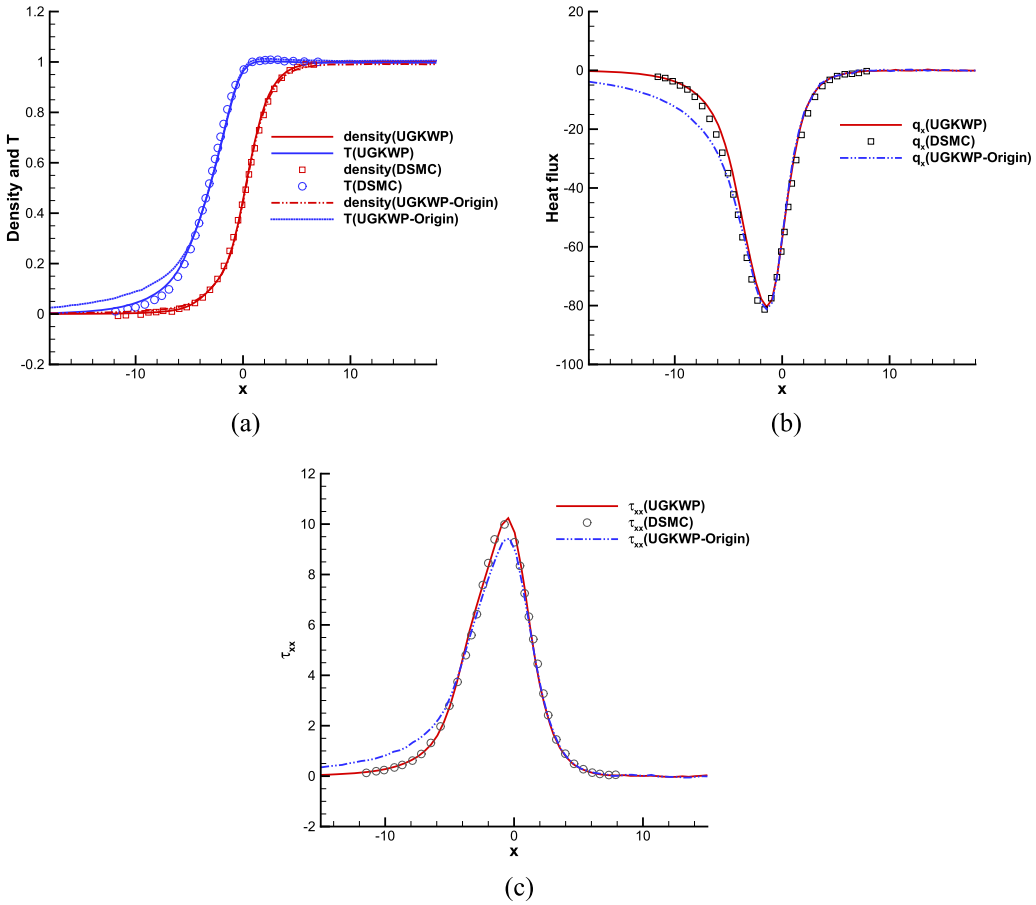

FIG. 2. M = 9 shock structure for argon gas calculated by the original and updated UGKWP and the DSMC. The x-coordinate is normalized by ℓ. The symbols are the results from Ref. 30. (a) Density and temperature distributions; (b) heat flux; (c) stress.

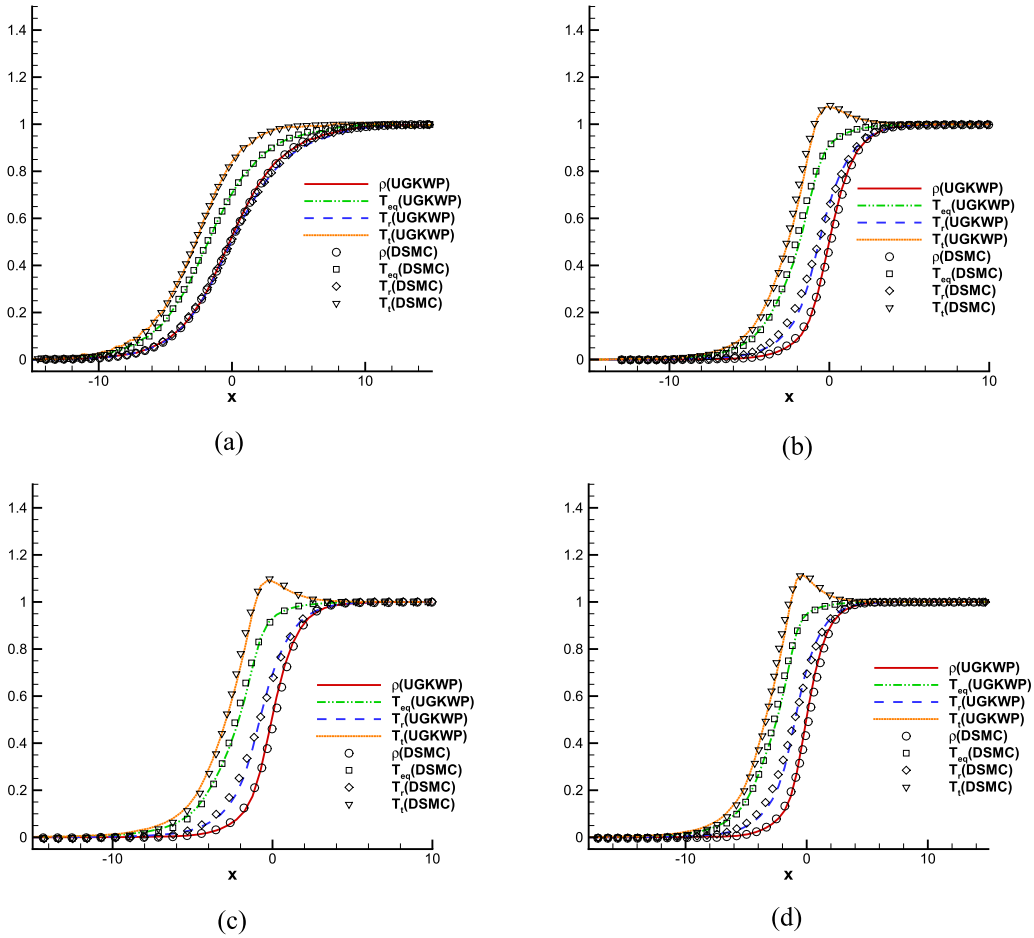

FIG. 3. Comparison of the UGKWP and DSMC results of nitrogen shock wave at different Mach numbers for nitrogen gas. (a) M = 1.53; (b) M = 4.0; (c) M = 5.0; (d) M = 7.0. The x-coordinate is normalized by ℓ. The symbols are the results from Ref. 32.

UGKWP and DSMC except for the temperature profile in the case of Kn = 1.199, where deviation has been observed.

In order to further validate the current UGKWP method in the high speed rarefied flow regime, the flow of argon gas passing through a circular cylinder at Mach number 20 and Knudsen number Kn = 0.1 is calculated. The Knudsen number is defined as the ratio of the mean free path over the cylinder radius. The radius of the cylinder is given by $R = 0.01$ m. The incoming argon gas has a velocity $U_\infty = 6155.174$ m/s, temperature $T_\infty = 273$ K, molecular number density $n_\infty = 1.2944 \times 10^{21}/\text{m}^3$, and reference viscosity $\mu_\infty = 2.117 \times 10^{-5}\text{Ns/m}^2$. The viscosity is calculated by Eq. (15) with $\omega = 0.81$. The cylinder has a constant surface temperature $T_w = 273$ K, and the diffusive boundary condition is adopted here. The simulation results from the current UGKWP are compared with the solutions of the DSMC and the UGKS-Shakhov.[33] Figure 5 shows the density, x-velocity, and temperature along the central symmetric line in front of the stagnation point, where both UGKWP and UGKS-Shakhov solutions agree well with the DSMC solutions, except that the temperature in UGKS-Shakhov solutions rises a little bit earlier. The comparisons of the heat flux, shear stress, and pressure along the surface of the cylinder are shown in Fig. 6, where better agreement between the solutions from the current UGKWP and the DSMC is obtained.

In this Letter, a newly modified UGKWP method has been proposed for modeling and computation of non-equilibrium flows. The main idea is to adjust the particle collision time according to the particle velocity, which is more consistent with the kinetic theory than the single relaxation time kinetic models. The modeling in the current UGKWP is more physically realistic than that in the traditional BGK-type kinetic models. With the implementation of the particle velocity-dependent collision time, accurate non-equilibrium solution can be obtained, such as the shock structure. Based on the simulation results, no obvious discrepancy between the UGKWP and DSMC results can be observed. Since the dynamic effect from most particles around the average velocity has been taken into account in the kinetic model equation, only the collision time for these particles with extremely relative high speed needs to be modified. The UGKWP method is fully conservative. The only modification is the distance traveled by the very high-speed particles. In the continuum flow regime, the UGKWP will automatically recover the

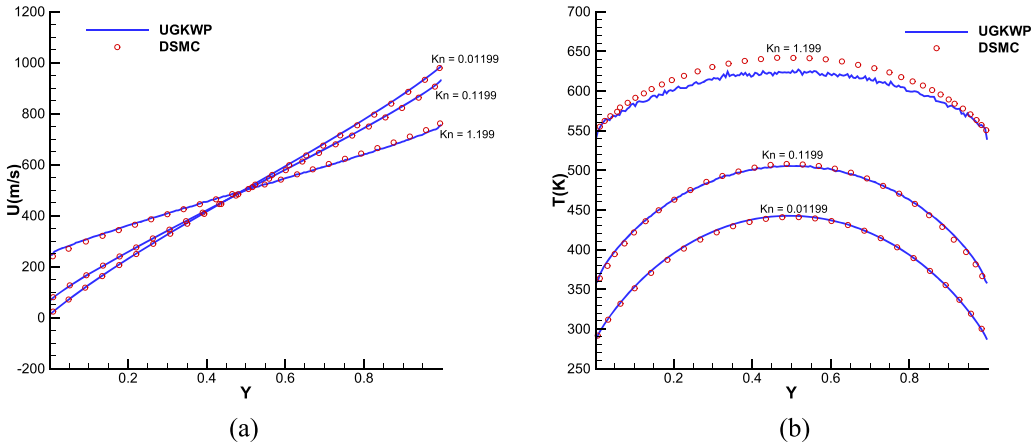

FIG. 4. Couette flow solutions from UGKWP and DSMC at different Knudsen numbers. The symbols are the DSMC results from Ref. 25. (a) Velocity distributions; (b) temperature distributions.

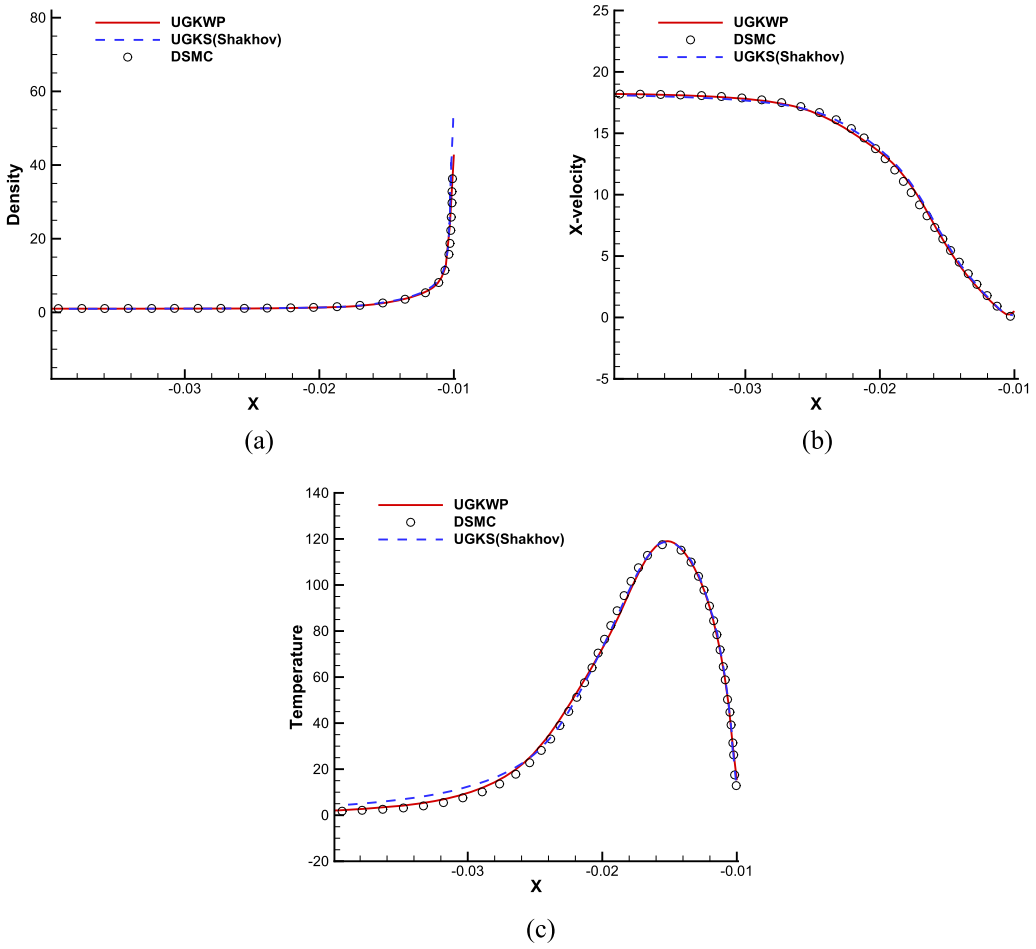

FIG. 5. Flow distributions for argon gas along the central symmetric line in front of the stagnation point at M = 20 and Kn = 0.1. (a) Density; (b) x-velocity; (c) temperature.

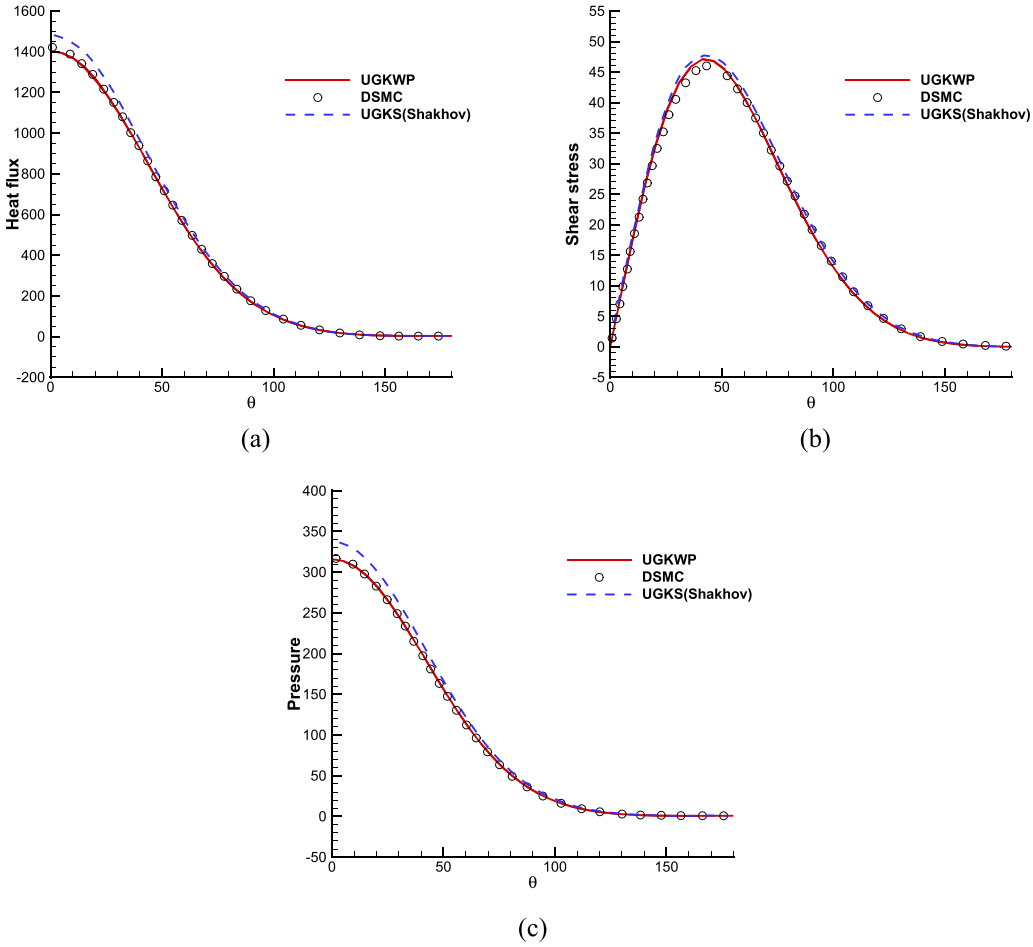

FIG. 6. Flow distributions along the surface of the cylinder for argon gas at M = 20 and Kn = 0.1. (a) Heat flux; (b) shear stress; (c) pressure.

gas-kinetic scheme for the Navier–Stokes solutions in the absence of particles. For the flow simulation with the co-existing multiple flow regimes, the UGKWP method can achieve high efficiency and present accurate solution in all flow regimes.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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