Ray effect in rarefied flow simulation

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ABSTRACT

Ray effect usually appears in the computation of radiative transfer when discrete ordinates method (DOM) is used. The cause and remedy for the ray effect have been intensively investigated in the radiation community. For rarefied gas flow, the ray effect is also associated with the discrete velocity method (DVM). However, few studies have been carried out in the rarefied community. In this paper, we make a detailed investigation of the ray effect in the rarefied flow simulation. Starting from a few commonly used benchmark tests, the root of the ray effect will be analyzed theoretically and validated numerically. The mitigation strategy by adjusting the discretization in the particle velocity space is studied as well. The guidelines are proposed to optimize the velocity space discretization for effectively reducing the ray effect. However, the design of optimal velocity space discretization is problem dependent and it can be hardly obtained in a highly rarefied flow simulation with complicated geometry. Due to the intrinsic self-adaptation of particle velocity, the stochastic particle method could automatically provide an optimized velocity discretization and avoid the ray effect. In the term of ray effect mitigation, the use of stochastic particle method is recommended in the numerical simulation of highly rarefied flow.

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1. Introduction

Ray effect is one of the most commonly known side effect of the discrete ordinates method (DOM) in the numerical simulation of radiative heat transfer. In 1960s, unphysical spatial distortion in the numerical solution, i.e., the so-called ray effect, was observed in solving the Boltzmann transport equation. In 1968, Lathrop [1] reported the ray effect in details. It was recognized that the cause of ray effect is associated with discrete ordinates formulation. In DOM, a specific set of discrete angular direction is employed to cover a continuous angular space, and it restricts the number of characteristic direction for photons’ streaming. Specifically, the limited discrete angular directions only have a finite capability to describe a distribution function and resolve the evolution. The error in the solution from the poorly resolved direction gets enlarged through a propagating process, especially in the optically thin region, and results in the ray effect.

In radiative transfer simulation, many remedies have been proposed to mitigate the ray effect. Lathrop [2] presented the fictitious source method to convert the discrete ordinate approximation into a spherical harmonics-like equation by introducing a fictitious source term. Originating from the modified differential approximation [3,4], the modified DOM [5–

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divides the radiation intensity into the wall-related intensity and the medium-related intensity, and computes these two components by analytic method and discrete ordinates approximation, respectively. In the modified DOM, Coelho [8] considered the ray effect caused by the sharp gradient of medium temperature. Baek et al. [9] solved the wall related intensity by the Monte Carlo method instead of adopting analytic computation. In analogy to the filtered spherical harmonics expansions [10], the discrete ordinates discretization of a filtered radiative transport equation [11,12] was presented to reduce the ray effect. From the analysis of ray effect, it is commonly agreed that increasing the number of discrete angular directions is the most straightforward way to mitigate the problem. However, for the standard quadrature sets of DOM, undesirable negative weights will occur for \( N > 12 \), which gives an upper limit on the number of angular directions and constrains the \( S_N \) method to fully remove the ray effect. Therefore, many strategies have been proposed to adjust the angular discretization and quadrature sets in order to mitigate the ray effect, such as \( T_N \) quadrature set [13], staggered and adaptive quadrature sets [14], and quadrature rotation [15,16]. In the community of radiative heat transfer, the ray effect and the mitigation strategies have been intensively investigated. Detailed analysis and discussions can be found in [2,17–19].

In rarefied flow simulation, in order to capture the non-equilibrium transport, based on the discrete distribution function many numerical schemes have been developed, where the continuous velocity space is approximated by a specific set of discrete velocity points, such as the discrete velocity method (DVM) [20,21], gas-kinetic unified algorithm (GKUA) [22], unified gas-kinetic scheme (UGKS) [23,24] and discrete UGKS (DUGKS) [25,26]. The ray effect appears in DOM in the rarefied flow simulation with the discontinuities induced by solid boundary or initial state [27,28]. For example, several plateaus were found by Brull et al. [29] in the numerical solution of Sod test case, and it was pointed out that the size of the plateaus is related to the discrete velocity interval and evolution time. In the computation of lid-driven cavity flow, diagonal wiggles were observed in the temperature distribution obtained by the DVM [30–32] and implicit UGKS [33]. Ray effect was also mentioned in the DUGKS computation [34,35]. Similar to the mitigation techniques in the radiation community, semi-analytic method [28,36] has been introduced to remove the influence of ray effect by identifying the propagation of the discontinuities. Without discretization in the velocity space, the integro-moment method (IMM) [37] does not suffer from the ray effect either. However, for highly non-equilibrium flow with complex geometry, the discrete velocities are usually employed. In comparison with discrete angular directions in radiative transfer, the discretization of the particle velocity space in rarefied flow is more flexible. Increasing the number of discrete velocities and optimizing the velocity discretization is a straightforward and effective way in DOM to mitigate the ray effect. Therefore, in the current paper we will focus mainly on the numerical discretization of the particle velocity space. Since the stochastic particle methods, such as the direct simulation Monte Carlo (DSMC) [38], unified stochastic particle (USP) method [39], unified gas-kinetic particle (UGKP) and wave-particle (UGKWP) methods [40–43], are ray effect free and can be regarded as an adaptive method in the velocity space, and the particle method will be considered as well in the present paper.

The rest of the paper is organized as follows. In Section 2, theoretical analysis is carried out on the cause and main features of the ray effect. In Section 3, the analysis will be validated by numerical tests. Different mitigation techniques are compared in Section 4. A conclusion will be drawn in the last section.

2. Analysis of ray effect

In this section, we will give a detailed analysis of the ray effect in the rarefied flow simulation. The fundamental governing equation of the gas distribution function \( f \) for rarefied gas evolution is the Boltzmann equation,

\[
\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = \Sigma(f, f),
\]

(1)

where \( \mathbf{u} \) is the microscopic velocity of gas particles and \( \Sigma(f, f) \) denotes the full Boltzmann collision term. The macroscopic conservative variables \( \mathbf{w} \) can be obtained by taking moments of the gas distribution function,

\[
\mathbf{w} = \int f \psi \, d\mathbf{u},
\]

(2)

where \( \psi = (1, \mathbf{u}, \|\mathbf{u}\|^2/2)^T \). The vector of conservative variables \( \mathbf{w} \) denotes the densities of mass \( \rho \), momentum \( \rho \mathbf{U} \) and energy \( \rho E \). Corresponding to the conservative flow variables, the local equilibrium state is a Maxwellian distribution

\[
g(\mathbf{u}) = \rho \left( \frac{\lambda}{\pi} \right)^{d/2} \exp \left( -\lambda (\mathbf{u} - \mathbf{U})^2 \right),
\]

(3)

where \( d \) is the degree of freedoms. \( \lambda \) is related to the temperature \( T \) by \( \lambda = m_0 / 2 k_B T \), where \( m_0 \) is the molecular mass and \( k_B \) is the Boltzmann constant.

For simplicity, we will take the analysis based on a one dimensional test with an initial discontinuity in the physical space. Specifically, the initial condition is

\[
(\rho, \mathbf{U}, T) = \begin{cases} 
(\rho_l, U_l, T_l), & x < 0, \\
(\rho_r, U_r, T_r), & x > 0,
\end{cases}
\]

(4)
where \( \rho, U, T \) denote macroscopic density, velocity and temperature, respectively. This test case, i.e., the Sod shock tube problem, is widely computed in the Euler limit and in the rarefied regime at different Knudsen numbers as a benchmark to validate new designed algorithms. Since the purpose of this study is to explore the ray effect, the solution of the Sod problem in the rarefied regime is considered.

2.1. Collisionless limit

The cause of ray effect will be analyzed firstly based on the case with no particles’ interaction, and the influence of the particles’ collision will be considered in the next section. In the collisionless limit, the governing equation of gas distribution function \( f \) becomes

\[
\frac{\partial f}{\partial t} + u \cdot \frac{\partial f}{\partial x} = 0,
\]

which describes the full free transport process of gas molecules.

For the Sod problem with an initial discontinuity described in Eq. (4), the initial distribution function is given by the Maxwellian distributions \( g_l \) and \( g_r \) for the left and right states. The initial state is illustrated in the Fig. 1(a), where there is a spatial discontinuity at \( x = 0 \) for the distribution function \( f \) in the phase space. In the collisionless limit, the gas particles keep free streaming with their initial microscopic velocity in the physical space, and the distribution function will evolve into a highly non-equilibrium state which deviates far from the local Maxwellian equilibrium state. As shown in Fig. 1(b), the initial discontinuity line \( x = 0 \) evolves into a discontinuity line \( x = ut \) in the phase space at time \( t \). For each physical location point \( x \), the distribution function in the velocity space is a combination of two half Maxwellian distributions, which is split at the velocity point \( u = x/t \). Therefore, the analytic solution of the distribution function at time \( t \) is

\[
f(x, t, u) = \begin{cases} 
  g_l(u), & u > x/t, \\
  g_r(u), & u < x/t.
\end{cases}
\]

At time \( t \), the point \( u \) in the velocity space has one-to-one correspondence with the physical location \( x \). When the discontinuity of \( f \) at point \( u \) moves in space and time, it presents the distribution function in different physical locations. Fig. 2(a) and 2(b) show an example of the distribution function in the velocity space for the location points \( x_a \) and \( x_b \). For physical location \( x \), the macroscopic variables \( w \) are

\[
w(x, t) = \int_{-\infty}^{u=x/t} g_r(u') \psi du' + \int_{u=x/t}^{\infty} g_l(u') \psi du',
\]

and the variation of the macroscopic flow variables in the physical space between two arbitrary points \( x_a \) and \( x_b \) would be

\[
w(x_b) - w(x_a) = \int_{u_a}^{u_b} \left[ g_l(u') - g_r(u') \right] \psi du',
\]

which corresponds to the integration of the distribution function difference in the interval \((u_a, u_b)\), see the illustration in Fig. 2(c). As the point \( u \) gradually moves from \( u_a \) to \( u_b \) in the velocity space, it indicates a smooth transition of macroscopic flow variables from \( x_a \) to \( x_b \) in the physical space.

In rarefied gas simulation, in order to capture the highly non-equilibrium state, a finite number of discrete velocities are usually employed to describe the distribution function in the velocity space. The variation of the flow field is coming from the value change of discrete distribution function at specific velocity points. From the phase space with discrete velocity
Fig. 2. Distribution functions in the velocity space at time $t$. (a) Distribution function at $x_a = u_a t$, (b) distribution function at $x_b = u_b t$, and (c) distribution function difference between $x_a$ and $x_b$.

Fig. 3. Distribution at time $t$ for the case with discrete velocity space. (a) Distribution in the phase space, (b) discrete distribution function at $x_a$ and $x_b$ with discontinuity points $u_a$ and $u_b$ locating within one discrete velocity interval, (c) discrete distribution function at $x_a$ and $x_b$ with discontinuity points $u_a$ and $u_b$ locating in two discrete velocity intervals.

points as illustrated in Fig. 3(a), the analytic solution for the discrete distribution function at physical location $x$ can be obtained

$$ f(x, t, u_k) = \begin{cases} g_l(u_k), & u_k > x/t, \\ g_r(u_k), & u_k \leq x/t, \end{cases} \tag{9} $$

and the analytic solution of the conservative variables gives

$$ w(x, t) = \sum_{u_k \leq x/t} \psi_k g_l(u_k)\omega_k + \sum_{u_k > x/t} \psi_k g_r(u_k)\omega_k \tag{10} $$

where $\omega_k$ is the weight at the velocity point $u_k$ for numerical integration. It can be found that even though the discontinuity line $u = x/t$ is accurately captured at the discrete velocity points, such as at $u_k$ and $u_{k+1}$, since there is no discrete velocity point to distinguish the variation between $u_k$ and $u_{k+1}$, the solution between the physical location points $x_k$ and $x_{k+1}$ can not be resolved.

In analogy to that in the continuous velocity space, the variation of macroscopic flow variables between $x_a$ and $x_b$ would be the numerical integration of the distribution function difference over the velocity interval $(u_a, u_b)$, i.e.,

$$ w(x_b) - w(x_a) = - \sum_{u_a \leq u_k < u_b} \psi_k [g_l(u_k) - g_r(u_k)]\omega_k. \tag{11} $$

If $x_k$ locates close to $x_b$ and the corresponding discontinuity points $u_a$ and $u_b$ are in one discrete velocity interval as shown in Fig. 3(b), the discrete distribution functions given by Eq. (9) and the macroscopic variables by Eq. (10) have no difference at $x_a$ and $x_b$, and there is no discrete velocity point satisfying $u_a < u_k < u_b$ to contribute the spatial variation of flow variables. If $x_b$ is a little bit far away from $x_a$ and the corresponding discontinuity points $u_a$ and $u_b$ locate in different velocity intervals as illustrated in Fig. 3(c), the discrete distribution functions for $x_a$ and $x_b$ would be different at some specific discrete velocities (e.g., the hollow circles illustrated in Fig. 3(c)), and the spatial variations between $x_a$ and $x_b$ will be the moments of distribution function difference at these discrete velocities. As to the spatial distribution, it can be seen in Fig. 3(a) that the discrete distribution function function and macroscopic flow variables take sudden changes at the discrete-velocity-determined location points $x_k$, and keep unchanged within the spatial interval $(x_k, x_{k+1})$. As a result, the numerical solution will have stepped structures in the physical space. The analytic solutions at time $t = 0.15$ from Eq. (7) for continuous velocity space and from Eq. (10) for a discrete velocity space with uniform interval $\Delta u = 0.25$ are plotted in Fig. 4, where the initial data is $(\rho_0, U_0, T_0) = (1, 0, 2)$ and $(\rho_0, U_0, T_0) = (0.125, 0, 1.6)$. The ray effect can be clearly observed.

As mentioned, the discontinuity at $u_k$ in the discrete velocity space will cause a sudden change at $x_k = u_k t$ in the physical space, so the macroscopic variable jump at $x_k$ will be the moment of the distribution function change at $u_k$

$$ \Delta w(x_k) = \psi_k [g_r(u_k) - g_l(u_k)]\omega_k, \tag{12} $$
The length of the stepped flow structure is
\[ \Delta x_k = x_{k+1} - x_k = u_{k+1} \Delta t - u_k \Delta t = t \Delta u_k. \]  
(13)

In this paper, we will refer to the macroscopic variable jump and the length of the stepped flow structure as the jump and step of ray effect, respectively.

In addition, it could be noticed that the previous analysis is based on continuous physical space and discrete velocity space, and the distribution function at the discrete velocity point is given exactly. Therefore, the result with the ray effect has the analytic solution for the cases with discrete velocity space in the collisionless limit. From this point of view, if any discrete velocity method doesn't present numerical solution with ray effect, the method would be doubtful about its accuracy in capturing the correct discrete distribution function and its spatial resolution in resolving the stepped flow structure. This is associated with the hyperbolic property of the governing equation [44]. For the collisionless cases, with time evolution, the initial information propagates along the given discrete velocity direction without decaying, so the unresolved information with uncertainty would be extended in the whole physical space and thus may deviate its result from the analytic one with a continuous particle velocity space. For further comprehension, we may compare the ray effect with the Riemann problem of one dimensional Euler equations where three characteristics give the solution with multiple stages. Here, the difference is that the three characteristics of Riemann problem are determined by the Euler equations, while the finite number of characteristics in the discrete velocity method comes from the numerical treatment with velocity space discretization. Once the resolution of velocity space is given, it sets a highest resolution limit for the discrete velocity method, and the spatial variations in physical space induced by the velocity discretization of the distribution function cannot be avoided, even with a much refined spatial mesh. Moreover, it should be pointed out that in the radiative transfer problems, due to the special angular variable discretization on a unit sphere, ray effect is usually associated with the loss of rotational invariance [2,44,45]. Since the velocity space discretization in the discrete velocity methods is much more flexible, it has no direct relation between the ray effect and the rotational invariant property in the rarefied flow simulation. One example is the analysis of Sod test, which is a purely one dimensional case in both physical and velocity space.

2.2. Collision influence

In previous section, the cause of the ray effect has been analyzed based on the one dimensional case in the collisionless limit. In this section, the influence of particle collision will be considered. Since the evaluation of the full Boltzmann collision term is complicated, we will adopt the BGK-type kinetic model in the current paper to approximate the collision term.

The BGK-type kinetic model equation can be written as
\[ \frac{\partial f}{\partial t} + u \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{g - f}{\tau}, \]  
(14)

where \( g \) is the local equilibrium state and \( \tau \) is the mean collision time or the relaxation time. For a local constant relaxation time \( \tau \), the integral solution along the characteristic line can be obtained
\[ f(x_0, t) = \frac{1}{\tau} \int_0^t g(x', t') e^{-\frac{(t-t')}{\tau}} d t' + e^{-t/\tau} f_0(x_0 - ut), \]  
(15)

where \( f_0(\mathbf{x}) \) is the initial distribution function around \( x_0 \) at time \( t = 0 \), and \( g(x, t) \) is the equilibrium state in space and time. The initial distribution function \( f_0 \) decays exponentially with the increment of time \( t \). Thus, the initially unresolved information due to the use of discrete velocity points would have less influence in the final numerical solution after a few time-steps evolution. Specifically, the initial discontinuity of the distribution function in the velocity space for the Sod
problem will decay exponentially due to the particles’ interaction. Combined with Eq. (11), the jump of $g_l$ and $g_r$ at a discrete particle velocity $u_k$ will decay with the smearing of the discontinuity in the distribution function. Quantitatively, the jump of the ray effect would be reduced by 86.5% and 90% after 2 and 3 mean collision times.

For the kinetic equation with full Boltzmann collision term, the particles’ interaction is also to erase the initial information of the distribution function, so the influence of the particles’ collision on the ray effect is similar. Qualitatively, the ray effect would be released with the increment of collision frequency. According to this property, mitigation strategies can be developed, such as the filtered discrete ordinates method [11,12].

3. Numerical validation

In this section, numerical tests including Sod problem, Rayleigh flow, and lid-driven cavity flow are computed to show the ray effect in the rarefied flow simulation. The theoretical analysis in the previous section will be validated by the numerical result. Without special statement, the reference values to normalize the flow variables are chosen as $T_0 = 273$ K and $U_0 = \sqrt{2k_B T_0/m_0}$. The unified gas-kinetic scheme (UGKS) [23,24] is employed to provide the numerical solutions of discrete velocity method. For the collisionless cases, UGKS will give the same results as other discrete velocity method; while for collisional cases at smaller Knudsen numbers, UGKS couples the gas particle transport and collision in the flux evaluation. Very fine meshes in the physical space will be used in the following cases, which ensures that the results can be recovered by any other discrete velocity method under such a fine mesh condition.

3.1. Sod test case

The Sod shock tube problem is computed to validate the quantitative analysis of the ray effect in the previous section. The initial condition is

$$\begin{cases}
(\rho, U, p) = (1, 0, 1), & x < 0, \\
(0.125, 0, 0.1), & x > 0,
\end{cases}$$

where $p$ is pressure. In the collisionless limit at $Kn \to \infty$, the velocity space is discretized by 61 velocity points in the range of $[-10, 10]$. In order to clearly show the ray effect, a uniform mesh with 1000 cells is used in the physical space. The numerical solutions at time $t_e = 0.15$ are presented in Fig. 5. It can be easily found that the step $\Delta x_k$ of the ray effect is about 0.05, which is consistent with the analytic result $\Delta x_k = t_e \Delta u$ in Eq. (13). Besides, the numerical solutions obtained by trapezoidal rule and Newton–Cotes method for velocity space integration are compared. It can be seen that the results obtained by these two methods have the same step but different jumps of the ray effect, because at the same discontinuity point $u_k$, the integration weights are different for these two methods. As predicted in Eq. (12), the density jumps are supposed to be

$$\Delta \rho(x_k) = |g_l(x_k/t_e) - g_r(x_k/t_e)| \omega_k.$$

In order to give a quantitative demonstration, we pick up the density jumps and compare with the discontinuity of the distribution function between the left and right states. As shown in Fig. 6, the density jumps of the trapezoidal solutions with $\omega_k = \Delta u$ are equal to the discontinuity in distribution function. The normalized jumps in the Newton–Cotes solutions by $|g_l(x_k/t_e) - g_r(x_k/t_e)| \Delta u$ give 

\[
\begin{array}{cccc}
28 & 64 & 64 & 28 \\
45 & 45 & 45 & 45
\end{array}
\]

which correspond to the coefficients in the composite integration. Hence, the theoretical analysis in Eq. (12) and Eq. (13) are numerically validated in a quantitative way.
in time, the ray shown decaying with the wall function being.

The analytic solutions are compared with the discrete velocity method, and the results are shown in Fig. 7(b).

3.2. Rayleigh flow

The Rayleigh flow is computed at different Knudsen numbers to explore the ray effect in the rarefied flow simulation. The Rayleigh flow is an unsteady gas flow around a vertical plate. The initial argon gas flow around the plate is stationary with an initial temperature 273 K, and the plate moves with a constant vertical velocity 30 m/s and a higher temperature 373 K. The computational domain is 1 meter long, which is used to define the Knudsen number with the variable hard sphere model. The dynamic viscosity is computed by the power law $\mu = \mu_0(T/T_0)\omega$ with $\omega = 0.81$.

The computational domain is discretized by $10^4$ uniform cells to approximate the case of a continuous physical space. The trapezoidal rule with $40 \times 40$ discrete velocity points covering a range of $[-4, 4] \times [-4, 4]$ is employed for the velocity space integration. In the collisionless limit at $K_n \to \infty$, the numerical solutions at time $t_e = 0.2$ are given in Fig. 7. It can be found that the step of the ray effect is $\Delta x_t = t_e \Delta t = 0.04$ as predicted by the theoretical analysis. Here the distribution function at the physical location point $x$ at time $t_e$ is a combination of the initial half Maxwellian distribution $g_0$ and the wall reflected half Maxwellian distribution $g_w$ as shown in Fig. 8(c). Therefore, the jump of the ray effect at $x_t = u_k t_e$ would be the numerical integration of the distribution function difference along the discontinuity line $u = u_k$. The analytic distribution function differences are plotted in Fig. 8(d), 8(e) and 8(f) for evaluation of the ray effect jumps. In Fig. 8(d), with increment of $u$, the distribution function difference $|g_0 - g_w|$ decreases to zero first, and then slightly increases before decaying to zero again, which agree with the variations of the density jumps shown in Fig. 7(a). Similarly in Fig. 8(e) and 8(f), the distribution function differences $|u(g_0 - g_w)|$ and $|v(g_0 - g_w)|$ exactly indicate the velocity jumps of ray effect shown in Fig. 7(b).

We also compute the Rayleigh flow at different Knudsen numbers to explore the influence of particles’ collision on the ray effect. As shown in Fig. 9, the jumps decrease for the cases with collisions at smaller Knudsen numbers. After 4 collision time, i.e., $t > 4\tau$, the ray effect is hardly observed. For quantitative study, we plot the time evolution solutions for the case of $\tau = 0.05$ in Fig. 10. The local density jumps due to the discontinuity of distribution function at $u_k = 0.3$ are shown in details. By fitting the extracted data of density jumps, we find that the jump decays exponentially. Quantitatively, the
Fig. 8. Analytic distribution function in velocity space for Rayleigh flow at $\text{Kn} \to \infty$. (a) Initial Maxwellian distribution $g_0(u, v)$; (b) reflected Maxwellian distribution $g_w(u, v)$ from the wall; (c) distribution function $f(u, v)$ at physical location $x$ which is a combination of $g_0$ and $g_w$ at $u = x/t$; (d) (e) and (f): distribution function difference between $g_0$ and $g_w$ for evaluation of ray effect jumps.

Fig. 9. Numerical solutions at time $t_\varepsilon = 0.2$ for Rayleigh flow at different Knudsen numbers.

decay rate is $e^{-59.123x} = e^{-59.123u/t} \approx e^{-t/0.056}$. Since the relaxation time in the enlarged local region is about $\tau \approx 0.053$, the analysis of the decay rate $e^{-t/\tau}$ in Section 2.2 has been numerically demonstrated.

3.3. Cavity flow

The lid-driven cavity flow is studied in rarefied regime to show the ray effect in the two dimensional case. The stationary gas in the cavity is driven by the moving lid with a constant horizontal velocity $U_w = 100$ m/s. The initial temperature $T_0$ is 273 K for the monatomic argon gas. Isothermal boundary condition with a fixed temperature of $T_w = 273$ K is applied to all side walls. The Knudsen number is defined with respect to the length of the side wall.

In the computation, the physical space and velocity space are discretized by the uniform meshes with $65 \times 65$ cells and $60 \times 60$ discrete velocity points, respectively. The integration weight for each velocity point is $0.18 \times 0.18$. In the collisionless
Fig. 10. Time evolution of the Rayleigh flow for \( \tau = 0.05 \). (a) Time accurate density distribution and local enlargement of density jumps; (b) decay of the density jumps.

Fig. 11. Cavity flow in the collisionless limit. (a) Density; (b) temperature; (c) magnitude of velocity and streamlines. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

Fig. 12. Composition of the distribution function for arbitrary location point in the cavity at Kn \( \to \infty \). \( g_M \) denotes the reflected Maxwellian distribution function.

In the collisionless limit, the flow field is shown in Fig. 11, where obvious ray effect can be observed. In details, two main phenomena are observed: (a) the ray effect shows radial pattern originated from the top corners; (b) the ray effect looks more severe along the diagonal directions. In the following, we will give the explanation.
In Fig. 12, we draw a diagram to illustrate the distribution function at an arbitrary location point. It can be found that the distribution function is formed by the reflected particles from the solid boundaries. The velocity space is divided into four sections according to which wall the reflected particles come from. Specifically, with the isothermal boundary condition, the distribution function is given by

\[ f(\theta) = g_M(\rho_w(\theta), U_w, T_w), \]

(18)

where \( g_M \) is the reflected Maxwellian distribution function, and \( \rho_w(\theta) \) is obtained by the non-penetration solid boundary condition with zero mass flux. Since the three stationary walls \( B_1, B_2 \) and \( B_3 \) have the same temperature \( T_w \) and velocity \( U_w \), and the flow field variations near these boundaries are small, the reflected Maxwellian distribution from \( B_1, B_2 \) and \( B_3 \) would be almost the same. Therefore, the discontinuities of the distribution function among the sections \( S_1, S_2 \) and \( S_3 \) in the velocity space would be mild. However, the top boundary has a constant velocity and the density and temperature around the top two corners are quite different from those along the other three solid walls. The reflected Maxwellian distribution function from the top corners especially the top right one will lead to strong discontinuities in the velocity space. As shown in Fig. 13, the distribution functions at different locations are plotted. Since the discontinuity exists along the radial direction in the velocity space, the ray effect occurs due to the low resolution along circumferential direction, which results in the spatial distortions with radial patterns as observed in Fig. 11(b).

Eq. (11) shows that each jump in the ray effect is due to the difference in the distribution function at the velocity points along the line with discontinuities. For the Rayleigh flow case, the same number of discrete velocity points make contributions to the ray effect jumps, i.e., as shown in Fig. 8(c) when the discontinuity line moves along \( u \) direction, the same number of discrete velocity points (the number of velocity discretization in \( v \) direction) go across the discontinuity line accounting for each jump. However, for the two dimensional cavity flow, since the discontinuity lines are along the radial direction \( \theta \), there are different numbers of discrete velocity points lying on the discontinuity line along different \( \theta \) direction for the case with rectangular grid points in the velocity space. There are more points lying in the directions of \( \theta = 0^\circ, 45^\circ \) and \( 90^\circ \) with jumps than those on the other directions. As a result, the ray effect appears severely along the diagonal, horizontal and vertical directions, which can be observed in Fig. 11(b) in the central domain and the region near the top boundary. Actually, this can be interpreted as that with regular discrete velocity points along the directions of \( 0^\circ, 45^\circ \) and \( 90^\circ \) the local angular resolution \( \Delta \theta \) in the velocity space is lower than that in the other irregular directions. For comparative study, the cavity flow with an unstructured discretization in velocity space is computed. As shown in Fig. 14(a), the distribution function at the location \((0.5, 0.5)\) is plotted for the case with unstructured mesh points in the velocity space, where the areas of the triangles are basically equal to those in the previous uniform mesh and the integration weight \( \omega \) is almost the same. Since the angular resolution is approximately homogeneous for the unstructured velocity space, the enhanced ray effect along the diagonal directions and near the top boundary disappears, i.e., the results in Figs. 14(b) and 14(c). In addition, in order to get rid of the influence of the geometry in the studies, we present the solutions for cavities with different widths and heights for comparisons. It can be found that the ray effect is still enhanced in the directions of \( 45^\circ, 0^\circ \) and \( 90^\circ \) instead of along the geometric diagonal direction. This observation confirms the enhancement of the ray effect in specific directions is due to the rectangular discretization of the velocity space instead of the geometric configuration of computational domain in physical space. In Fig. 15, from the flow field in the bottom region of the deep cavity, we can find that the spatial resolution degrades more than that in the squared cavity, because the discontinuity from the unresolved solution due to the discrete velocity space from the top corners are further amplified after long distance propagation. In contrast, the shallow cavity has more severe ray effect (Fig. 16).

At smaller Knudsen numbers with increased particle collisions, the cavity flow at \( Kn = 0.5 \) is computed. In Fig. 17, it can be seen that the ray effect is much reduced due to particles’ collision which gradually smears the reflected discontinuities from the wall.

4. Mitigation solutions

Here, we rewrite the formula to compute the jump in the ray effect, i.e., the numerical integration of differences in the distribution function along the corresponding discontinuity line,

\[ W(x_m) = \sum_{h_m(u_i) = 0} \psi_k \Delta g_k \omega_k, \]

(19)

where \( h_M(u) = 0 \) denotes the \( m \)-th discontinuity line in the velocity space, for example, \( u = u_m \) for Sod and Rayleigh cases and \( \theta (u) = \theta_m \) for cavity flows. \( x_m \) is the physical location where the jump in the ray effect occurs due to the sudden change of the distribution function \( \Delta g_k \) on the \( m \)-th discontinuity line.

From the previous analysis and numerical validation, we know that the cause of ray effect is due to low resolution in velocity space. According to Eq. (19), we could obtain several principles for adjusting the discretization of velocity space to effectively mitigate the ray effect. These are summarized as follows.

A. Increase the number of velocity points and refine the grids in the velocity space to reduce the integration weights \( \omega_k \), especially for the regions where the moments of distribution function differences \( \psi_k \Delta g_k \) are large.
Fig. 13. Distribution function in the velocity space at different points in physical space. The white lines denote the discontinuities induced by the top corners.

B. Arrange more discrete velocity points in the direction across the discontinuity line in the velocity space, i.e., perpendicular to the discontinuity line $h_m(u) = 0$, which is helpful to reduce the step in the ray effect and meanwhile to decrease the jumps by increasing the resolution corresponding to a smaller $\omega_k$.

C. Reduce the number of discrete velocity points lying simultaneously on (across) the discontinuity line $h_m(u) = 0$ in the velocity space, to diminish their contributions to the macroscopic flow variable jumps in Eq. (19).

Similar discussions can be found in radiative transfer in the discretization of angular variable [18]. In addition, the mitigation methods which are equivalent to obtaining the solutions with more discrete velocities can be employed as well, such as taking averaged solutions over multiple times of computations on different sets of velocity space discretization [14–16].

Based on the above analysis, it is clear that the refinement of the velocity discretization can substantially reduce the ray effect. However, considering practical numerical simulation, there are other factors which could influence the ray effect in the numerical solution, such as the spatial discretization, accuracy of numerical scheme, particle collision, and the integration method. Since the ray effect comes from the enlargement of unresolved information in the particles' free trans-
Fig. 14. Cavity flow using unstructured mesh in velocity space. (a) Distribution function at \((x, y) = (0.5, 0.5)\); (b) density; (c) temperature.

Fig. 15. Flow in a deep cavity using uniform mesh in velocity space.

Fig. 16. Flow in a wide cavity using uniform mesh in velocity space.

port, and the particle collision always reduces the ray effect, only the collisionless cases will be considered in the following discussion. Different integration methods, such as trapezoidal rule and Newton–Cotes method, just provide different jumps through their different integration coefficients, and they will present the similar ray effect. Therefore, we will not further consider the difference between integration methods. With the same discretization in the physical space, different DVM will use different approach in capturing particles' streaming and collisions, which will subsequently influence the numerical solution. The influence of the spatial treatment has been discussed [46] for discrete ordinates methods in the radiative transfer problems. For the simulation of rarefied flow, the upwind scheme is commonly employed in the traditional DVM. Without special statement, the second order upwind scheme is used in the following discussion. Considering the discretization in the physical space, visual observation of ray effect can be attributed to the incompatibility between low resolution in the
velocity space and high resolution in the physical space. Therefore, if the requirement for spatial resolution is not too high, employing coarser mesh would be a very effective way to avoid the spatial distortion induced by inadequate resolution in the velocity space. Similarly, low-order accurate numerical scheme can be used as well to reduce the spatial resolution, smear the discontinuity in the phase space, and to get smoother results.

In the following, we will present some numerical results obtained by the discrete velocity method with the inclusion of several mitigation techniques. The solutions obtained by stochastic particle method will be discussed as well. Since only collisionless cases are considered, the numerical schemes based on discrete velocities, such as the DVM, GKUA, UGKS and DUGKS will give the same results; all the stochastic particle methods such as DSMC, USP, UGKP and UGKWP will become the same particle tracking schemes.

4.1. Sod test case

For the Sod test case, the mitigation techniques for the ray effect are employed to give better numerical solutions. For this case, a uniform mesh with 1000 cells is used in the physical space and 61 discrete velocity points are used to cover the velocity space $[-10, 10]$ and take trapezoidal integration method. The time step is $5 \times 10^{-5}$ and the output time is $t_e = 0.15$.

In Fig. 18, we show the results of the Sod test at $Kn \to \infty$ on a refined velocity mesh, where uniform meshes with 81 and 241 discrete velocity points and a nonuniform mesh with 81 points refined near $u_k = 0$ are employed. It shows that the ray effect is effectively reduced by a fine mesh with 241 discrete points in the velocity space. Since the difference in the distribution function has larger values around the zero velocity point, the local refinement around $u_k = 0$ can mitigate the density jump as well. However, it should be noted that for higher order moments of the distribution function, such as the velocity and temperature, the moments of the distribution function are different from the density jump evaluation, so the local refinement around the zero velocity point is less effective for the high order quantities in the ray effect.

With lower numerical resolution in the physical space, the ray effect can be mitigated visually on the coarse meshes with 50 and 200 cells as shown in Fig. 19, where the 80 velocity points are employed in the velocity space. Theoretically, using a low spatial resolution is a passive way to mitigate the ray effect because it does not solve the problem essentially, but smears the distorted flow structure. However, in terms of numerical simulation, as long as the numerical solutions with low spatial resolution are acceptable, using coarser mesh is a very effective way to reduce the ray effect and the computational
efficiency can be improved. As pointed out, the limited resolution on the sub-scale between grid points in the velocity space will result in uncertainty in the physical space on the scale of \( t \Delta u \). The detailed flow structure within \( t \Delta u \) cannot be resolved even with a fine mesh in the physical space. Thus, for the numerical simulations of highly rarefied flow, compatible discretization of velocity space and physical space are required, such as \( \Delta x \geq t_e \Delta u \) or \( \Delta u \leq \Delta x / t_e \).

Similar to using a coarse mesh in the physical space, it is helpful to reduce the ray effect as well by adopting a lower order numerical scheme. The solutions obtained by the first-order and second-order numerical schemes are plotted in Fig. 20. It can be found that the first-order scheme obtains smoother result than that from the second-order one, especially in reducing the jumps away from the initial discontinuity, because the finite volume averaging process, such as the constant state inside each cell from the first scheme, widens the discontinuity line. It should be pointed out that this remedy does not work at the point \( u_k = 0 \), i.e., the jump at \( x = 0 \), because the distribution function discretized at \( u_k = 0 \) has no contribution in the time evolution of numerical solutions, and the jump caused by the discontinuity at \( u_k = 0 \) remains. Therefore, for numerical simulations with discrete distribution function, it is better not to include the zero velocity points, not only because of the reason given above, but also due to the fact that the transport property of the low speed particles with both positive and negative microscopic velocities cannot be represented on the average by the evolution of the distribution function exactly at \( u_k = 0 \).

4.2. Rayleigh flow

The Rayleigh flow in the collisionless limit is re-calculated by implementing the mitigation techniques for the ray effect. The default setup is the same as that given in Section 3.2.

Fig. 21 shows the result of the Rayleigh flow with refined velocity space. The solution obtained with \( 120 \times 40 \) discrete velocity points seems better than that with \( 40 \times 40 \) points. We also shift the \( 40 \times 40 \) discrete velocity points in \( u \) direction by \( -\Delta u / 3 \), \( 0 \) and \( \Delta u / 3 \). It shows that the averaged solutions from the shifted discrete velocity points are identical to those with refined velocity space because more discrete velocity points are equivalently considered in the final averaged solution. In [37], it is claimed that the ray effect cannot be eliminated by simply increasing the number of discrete velocity points, since with the decreasing of the oscillation amplitude the frequency may be increased. However, from the analysis and observation, we would like to regard the ray effect as spatial distortions rather than oscillations because the solution does not vibrate in space and time. Therefore, the description and analysis using the frequency is not fully appropriate. Ray effect is more like the discrete velocity induced mosaic in the physical space; therefore, the ray effect is mitigated with the
Fig. 21. Rayleigh flow at $\text{Kn} \to \infty$ with refined velocity space. The red dashed lines denote the averaged solution on three different sets of velocity space discretization, which are obtained by shifting the discrete velocity points with $-\Delta u/3$, 0 and $\Delta u/3$.

Fig. 22. Rayleigh flow at $\text{Kn} \to \infty$ on coarser meshes.

Fig. 23. Rayleigh flow at $\text{Kn} \to \infty$ obtained by particle method, where the blue solid line is the averaged solution over 100 times of computations and the red dashed line denotes the noise-filtered solution.

step getting smaller when increasing the number of discrete velocity points. The numerical solutions will approach to the analytic solution once a continuous velocity space is being recovered in the grid refinement process.

The solutions on the coarse meshes with 50 and 200 cells are given in Fig. 22. As expected, the ray effect can be merely observed on the coarse mesh with 50 uniform cells.

We also compute the numerical solution by the particle method. Initially, the number of particles in each cell is 1600, the same as the number of discrete velocities in previous calculations. In the collisionless case, the particles can be accurately tracked. Mostly, the ray effect happens more severely in the velocity space where the distribution functions and their differences have large values. For particle method, more particles will be sampled in the velocity space at the place where the value of the distribution function is high. Therefore, the principle A is satisfied for stochastic method automatically. The random discretization in the velocity space from the particle method could give more discrete velocity points in the direction across the discontinuity line, and principles B and C are satisfied as well. In terms of the velocity discretization,
the particle method provides an optimal strategy in velocity space adaptation to overcome the ray effect. However, in the numerical simulation of unsteady flows, the statistical noise becomes dominant and the influence of ray effect can be neglected in this case. The numerical solutions averaged over 100 times of computations are plotted in Fig. 24. From the noise-filtered results, the typical characters of ray effect, such as stepped structures, have not been observed.

4.3. Non-stationary initial discontinuity

A one-dimensional case similar to Sod test with a non-stationary initial discontinuity is computed here. The main difference from Sod case is that the initial velocity is not zero. The initial condition gives

$$ (\rho, U, T) = \begin{cases} 
(1, 2, 1), & x < 0, \\
(1, -2, 1), & x > 0.
\end{cases} $$ (20)

For this case, the computational domain is discretized by a uniform mesh with 2000 cells in physical space, and 61 discrete velocity points for covering the range of [-12, 12] in the velocity space. The solution in the collisionless limit at time $t_c = 0.1$ is presented in Fig. 24, where as expected ray effect is observed in the numerical solution due to discrete velocity space. When we employ a finer uniform mesh with 241 discrete points in the velocity space, the ray effect is much mitigated as shown in Fig. 25. In the previous Rayleigh case, by adjusting the distribution of the discrete velocities near the zero velocity point, a better solution can be obtained with reduced ray effect. However, for this case it takes no obvious effect on the results in Fig. 26, which non-uniform 61 velocity points are used. As shown in Fig. 27, the distribution function difference in the velocity space is plotted for the current case, and the required mesh refinement regions are around the velocity points $u_k = \pm 2$ in this case instead of $u_k = 0$ in the previous one. Therefore, the method through adjusting discrete velocity space to mitigate the ray effect is problem dependent, and the velocity mesh refinement around the zero velocity point doesn't always give better solutions. While, for the discontinuities induced by a stationary boundary, the region with large difference in distribution function usually locates near the zero velocity point, so the discrete velocity space refinement in the low speed region may work for such cases.
The cavity flows are recomputed by employing the mitigation techniques, including using coarse mesh in the physical space, adopting non-uniform mesh in the velocity space, employing the stochastic particle method, and using a special designed velocity space discretization. The results of temperature distribution based on different remedy are shown in Fig. 28.

For the result in Fig. 28(a), the uniform mesh with $21 \times 21$ cells is used for the spatial discretization, which is about 3 times coarser than those in the other computations. It can be found that the wiggle in the flow structure is much reduced, but the solution is less accurate due to the lower spatial resolution. For the solution in Fig. 28(b), the original $60 \times 60$ uniform discrete velocity points are shrunk near the zero velocity point, which use smaller integration weights for the low speed region, see Fig. 29(a). The ray effect is effectively mitigated, however, since too many discrete velocity points are lying on the 45° discontinuity line, the enhanced wiggles along the diagonal direction can be still observed. This refinement in velocity space doesn’t consider the principles B and C, so only jumps of ray effect are reduced, but the enhancement along the diagonal direction are not well removed. For stochastic particle method, we employ 3600 particles in each cell and take 5000 steps in averaging for the steady state solution. In Fig. 28(c), we can hardly see the ray effect. Now, we give a well designed discretization of the velocity space as shown in Fig. 29(b). This discretization satisfies all the principles for adjusting the discrete velocity points. For third quadrant of the discrete velocity space shown in Fig. 29(c), we discretize the radial direction into 25 rings where $\Delta r$ increases from the center to outside so that the integration weights in the low speed region are smaller. The number of the discrete angular directions increases from 12 to 60 from the center to outside, which gives a finer resolution in the angular direction than that with regular Cartesian mesh. Different numbers of discrete angular directions at different rings could avoid multiple discrete velocities lying on the same discontinuity line. Therefore, it gives the best numerical solution without ray effect in Fig. 28(d). However, since the optimal discretization of the velocity space is quite problem dependent, it requires special design case by case. For steady flows, due to the adaptive property and irregular discretization in the velocity space, the particle method satisfies all principles for velocity discretization automatically and could provide the same good results without ray effect. For numerical simulations with complex configurations, special discretization of the velocity space becomes difficult, so the particle methods provide a better and easy resolution to avoid the ray effect in rarefied flow simulation.
Fig. 28. Cavity flow recomputed by (a) using coarse mesh in physical space; (b) adopting nonuniform velocity points in the velocity space; (c) employing stochastic particle method; (d) using a special designed discretization of velocity space.

5. Conclusion

In this paper, a detailed analysis and numerical computation of the ray effect have been conducted in the collisionless limit for the discrete velocity method. The ray effect arises from the use of a finite number of discrete velocity points to approximate a continuous velocity space, where the limited resolution cannot resolve the possible discontinuity in the velocity space. As a result, the unresolved information is enlarged with the propagation under free transport mechanism, accompanied with the resolution reduction in the physical space. The analysis shows that the jump in the flow variables in the physical space from the ray effect is proportional to the resolution in the velocity space, which are equal to the moments of the differences of the distribution functions with discontinuity at the velocity points. For unsteady flow computation, the limited resolution $\Delta u$ in the velocity discretization results in unresolved flow structure in the physical space on the scale of $\tau \Delta u$. In practical computation, the compatible discretization of the physical space and velocity space, i.e., $\Delta x \geq \tau \Delta u$ or $\Delta u \leq \Delta x / \tau$, is required for the simulation of highly rarefied flow. With the inclusion of particle collision, the jumps of ray effect decay exponentially with time evolution by $e^{-t/\tau}$. The theoretical analysis has been quantitatively validated in the numerical computation.

Several mitigation techniques have been investigated in reducing the ray effect, such as using coarse computational mesh, employing lower order flux solver to reduce the spatial resolutions, and adjusting the discrete velocity points to improve the resolution in the velocity space. Three principles are proposed as guidelines to adjust the velocity space discretization in
order to mitigate the ray effect. Specifically, the discrete velocity points should be refined in the region where the moments of differences of the distribution functions are large; more discrete velocity points should be arranged in the direction perpendicular to the discontinuity line in the velocity space so as to increase the resolutions; and fewer discrete velocity points are allocated on the discontinuity line to reduce the contribution to ray effect jumps. The mitigation techniques have been applied in the numerical tests and the effectiveness of different approaches have been compared. Employing coarse computational mesh and low-order flux solver could reduce the ray effect, but provide lower accurate results. Adjusting the velocity discretization is very effective, especially with the optimal designed discretization in the velocity space. However, the design is quite problem dependent, and the optimal choice is hard to be obtained in complex geometry.

As a special velocity space discretization, results from stochastic particle method are also provided. Due to the self-adaptive property and irregular discretization in the velocity space, all three guidelines for velocity adjustment are automatically satisfied by the particle method. For unsteady flows, the error introduced by ray effect can be ignored because of large statistical noises. For steady flow computation with averaged processes, the particle method can provide the same good results as the optimized discrete velocity method. The adaptive property in the discretization of velocity space from particle method makes it a better choice for general highly rarefied flow computation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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