

An improved unified gas-kinetic scheme and the study of shock structures

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With discretized particle velocity space, a unified gas-kinetic scheme for entire Knudsen number flows has been constructed based on the Bhatnagar–Gross–Krook (BGK) model (2010. *J. Comput. Phys.*, **229**, 7747–7764). In comparison with many existing kinetic schemes for the Boltzmann equation, besides accurate capturing of non-equilibrium flows, the unified method has no difficulty to get accurate solution in the continuum flow regime as well, such as the solution of the Navier–Stokes equations. More importantly, in the continuum flow regime, the time step used by the unified scheme is determined by the Courant–Friedrichs–Lewy condition, which can be many orders larger than the particle collision time. In some sense, the unified method overcomes the time step barrier for many kinetic methods, such as direct simulation Monte Carlo (DSMC), direct Boltzmann solver and many other kinetic solvers. The unified scheme is a multiscale method, where the macroscopic flow variables and microscopic gas distribution function are updated simultaneously. In an early approach in the unified BGK (U-BGK) scheme, the heat flux in the BGK model is modified through the update of macroscopic flow variables, then this modification feeds back into the update of non-equilibrium gas distribution function. In this paper, we are going to develop a unified scheme for the Shakhov model, the so-called unified Shakhov (U-Shk), where the heat flux is corrected directly through the modification of gas distribution function. Theoretically, it will be shown that current U-Shk is more consistent than the U-BGK for the highly non-equilibrium flow computations. The study of shock structures from low to high Mach numbers will be presented and the simulation results will be compared with DSMC solutions as well as possible experimental measurements. The result improvement of U-Shk over U-BGK is clearly achieved. Based on the simulation results, now we fully believe that the unified scheme is an accurate and efficient flow solver in all Knudsen number flow regime.

Keywords: unified scheme; shock structure; non-equilibrium flows.

1. Introduction

The classification of the various flow regimes based on the dimensionless parameter, the Knudsen number, is a measure of the degree of rarefaction of the medium. The Knudsen number Kn is defined as the ratio of the mean free path to a characteristic length scale of the system. In the continuum flow regime where $Kn < 0.001$, the Navier–Stokes (NS) equations with linear relations between stress and strain and the Fourier’s law for heat conduction are adequate to model the fluid behaviour. For flows in

the continuum–transition regime ($0.1 < Kn < 1$), the NS equations are known to be inadequate. This regime is important for many practical engineering problems, such as the simulation of microscale flows and hypersonic flow around space vehicles in low earth orbit. Hence, there is a strong desire and requirement for accurate models which give reliable solutions with lower computational costs. The Boltzmann equation describes the flow in all flow regimes: continuum, continuum–transition and free molecular. However, designing an accurate and efficient Boltzmann solver for both rarefied and continuum regimes seems to be very challenging.

One of the outstanding numerical techniques available for solving the Boltzmann equation is the direct simulation Monte Carlo (DSMC) (Bird, 1994) method. The DSMC method is a widely used technique in the numerical prediction of low-density flows. However, in the continuum–transition regime, where the density is not low enough, the DSMC requires a large number of particles for accurate simulation, which makes the technique expensive in terms of both the computation time and the memory requirement. At present, the accurate modelling of realistic configurations, such as aerospace vehicles in 3D by the DSMC method for $Kn \ll 1$, is beyond the currently available computing power. The DSMC method requires that the time step and cell size are less than the particle collision time and mean free path, which subsequently introduce enormous computational cost in the high-density regime.

The Boltzmann equation is valid from the continuum flow regime to the free molecule flow. So, theoretically a direct Boltzmann solver which is valid in the whole range of Knudsen number can be developed if the numerical discretization is properly designed. In the framework of deterministic approximation, the most popular class of methods is based on the so-called discrete velocity methods or discrete ordinate method of the Boltzmann equation (Chu, 1965; Yang & Huang, 1995; Li & Zhang, 2009; Mieussens, 2000; Aristov, 2001; Kolobov *et al.*, 2007). These methods use regular discretization of particle velocity space. Most of these methods can give accurate numerical solution for high Knudsen number flows, such as those from the upper transition to the free molecule regime. However, in the continuum flow regime, it is recognized that they have difficulty in the capturing of the NS solutions, especially for the high Reynolds number flows, where the intensive particle collisions take place. In the continuum flow regime, the requirement of time step in these methods being less than the particle collision time makes them prohibitive. In order to get unconditionally stable schemes with large time step, it is natural to use implicit or semi-implicit method for the collision part (Mieussens, 2000; Pieraccini & Puppo, 2007). However, even though a scheme could overcome the stability restriction and use large time step, there is still accuracy concern, because many of the schemes have the same numerical mechanism as flux vector splitting methods in the continuum regime, and the intrinsic numerical dissipation is proportional to time step (Xu & Li, 2001). The condition for the validity of the transport and collision splitting method is that a physical scale on the mean free path and particle collision time has been well resolved. To resolve such a scale flow physics in continuum flow regime is not practical. In the past 20 years, people have been working on the development of the asymptotic-preserving (AP) schemes (Klar, 1998; Jin, 1999; Lemou & Mieussens, 2008; Degond *et al.*, 2006; Carrillo *et al.*, 2008). One of the main target for the AP scheme is that there is no such a time step limitation and the scheme could recover the corresponding macroscopic models accurately as Knudsen number goes to zero.

Recently, based on the gas-kinetic Bhatnagar–Gross–Krook (BGK) model, with discretized particle velocity space, a unified gas-kinetic scheme has been developed for the whole Knudsen regime (Xu & Huang, 2010). The novelty of this scheme is that the physical process of particle transport and collision is coupled in the update of both macroscopic flow variables and microscopic distribution function. Different from many other approaches, the critical step is that an integral solution of the kinetic model is used in the flux evaluation across the cell interface. The integral solution describes two-scale physical processes. One is the hydrodynamic scale through the integration of the equilibrium states over a domain

with particle collisions and the other is the kinetic scale for the particle-free transport. The weight between these two scales depends on the cell resolution and time step. Therefore, the integral solution gives an accurate representation for both continuum and free molecule flows. The weakness of many existing kinetic methods is that an operator-splitting technique is used numerically to treat the transport and collision. This decoupled numerical treatment has implicitly enforced the applicable regime of these methods in the mean particle collision time and mean free path scales, which are unrealistic for the capturing of the NS solution in the continuum flow regime. Theoretically, the Boltzmann equation is a statistical model with a continuous particle transport and collision process in space and time. There is no reason to believe that these particles which transport across the cell interface will not suffer particle collision during their movement towards the cell interface, especially when the cell size is much larger than the particle mean free path. Due to its multiscale nature of the unified scheme, the update of macroscopic flow variables makes it possible to correct the Prandtl number through the modification of heat flux. In the continuum flow regime at high Reynolds number, a standard Courant-Friedrichs-Lewy condition for the macroscopic NS equations can be used as the time step in the unified scheme, which is much larger than the particle collision time.

The unified BGK (U-BGK) scheme (Xu & Huang, 2010) fixes the heat flux, such as the unit Prandtl number in the BGK equation, through the modification of heat flux in the update of macroscopic flow variables, which subsequently affects the update of gas distribution function. Even though this kind of fix works very well in the continuum flow regime, there is still loophole in the update of microscopic gas distribution function. In this paper, we are going to improve the previous U-BGK scheme and develop a revised unified scheme based on the Shakhov model. This paper will focus on the study of shock structures using the unified gas-kinetic scheme. The shock strength has a wide range in Mach numbers from the continuum $M \sim 1$ to hypersonic one $M \sim 10$. The simulation results will be compared with the DSMC results and possible experimental measurements. This study will clearly demonstrate the validity of the unified method, which becomes a valuable alternative besides the DSMC.

This paper is arranged in the following. Section 2 reviews the unified scheme for the BGK model. Section 3 extends the method to solve the Shakhov model. Section 4 is about the numerical shock structure tests. The last section is the conclusion.

2. Unified gas-kinetic scheme

In this section, we will review the unified scheme for all Knudsen number flows. The 1D kinetic equation will be used to illustrate the idea. The 1D gas-kinetic BGK equation can be written as (Chapman & Cowling, 1990; Bhatnagar *et al.*, 1954)

$$f_t + uf_x = \frac{g - f}{\tau}, \quad (1)$$

where f is the gas distribution function and g is the equilibrium state approached by f . Both f and g are functions of space x , time t , particle velocities u and internal variable ζ . The particle collision time τ is related to the viscosity and heat conduction coefficients, i.e. $\tau = \mu/p$, where μ is the dynamic viscosity coefficient and p is the pressure. The equilibrium state is a Maxwellian distribution,

$$g = \rho \left(\frac{\lambda}{\pi} \right)^{\frac{k+1}{2}} e^{-\lambda((u-U)^2 + \zeta^2)},$$

where ρ is the density, U is the macroscopic velocity in the x direction, λ is equal to $m/2kT$, m is the molecular mass, k is the Boltzmann constant and T is the temperature. For 1D flow, the total number of

degrees of freedom K in ξ is equal to $(3 - \gamma)/(\gamma - 1)$. In this paper, only monatomic gas with $\gamma = 5/3$ will be studied and K is equal to 2 to account for the particle motion in the y and z directions. In the equilibrium state, the internal variable ξ^2 is equal to $\xi^2 = \xi_1^2 + \xi_2^2 + \dots + \xi_K^2$. The relation between mass ρ , momentum ρU and energy E densities with the distribution function f is

$$\begin{pmatrix} \rho \\ \rho U \\ E \end{pmatrix} = \int \psi_\alpha f \, d\Xi, \quad \alpha = 1, 2, 3, \tag{2}$$

where ψ_α is the component of the vector of moments

$$\psi = (\psi_1, \psi_2, \psi_3)^\top = \left(1, u, \frac{1}{2}(u^2 + \xi^2) \right)^\top$$

and $d\Xi = du \, d\xi_1 \, d\xi_2 \dots d\xi_K$ is the volume element in the phase space with $d\xi = d\xi_1 \, d\xi_2 \dots d\xi_K$. For the 1D flow, we can integrate the kinetic equation (1) in $d\xi$ first before discretization. Therefore, ξ will not appear in the following presentation. More specifically, two equations, which are obtained by integrating (1) with $d\xi$ and $\xi^2 d\xi$, will be solved for the 1D reduced distribution functions \hat{g} and \hat{h} . This technique is the same as the methods presented in Chu (1965) and Yang & Huang (1995). Since the equations for \hat{g} and \hat{h} have the similar form as the BGK equation, in the following we present the unified method for solving the equation of f which is absent from the internal variable ξ .

The physical space is divided into numerical cells with cell size Δx , and the j th cell is given by $x \in [x_{j-1/2}, x_{j+1/2}]$ with cell size $\Delta x = x_{j+1/2} - x_{j-1/2}$. The temporal discretization is denoted by t^n for the n th time step. The particle velocity space is discretized by $2N + 1$ subcells with cell size Δu , and the centre of k th velocity interval is $u_k = k \Delta u$, and it represents the average velocity u in that interval,

$$u \in \left[\left(k - \frac{1}{2} \right) \Delta u, \left(k + \frac{1}{2} \right) \Delta u \right], \quad k = -N, -(N - 1), \dots, -1, 0, 1, \dots, (N - 1), N.$$

Then, the averaged gas distribution function in cell j , at time step t^n and around particle velocity u_k is defined by

$$f(x_j, t^n, u_k) = f_{j,k}^n = \frac{1}{\Delta x \Delta u} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{u_{k-1/2} \Delta u}^{u_{k+1/2} \Delta u} f(x, t^n, u) \, dx \, du, \tag{3}$$

where Δx is the cell size and Δu is the particle velocity interval.

The BGK equation (1) can be written as

$$f_t = -u f_x + \frac{g - f}{\tau}. \tag{4}$$

Integrating the above equation in a control volume $\int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t^n}^{t^{n+1}} (\dots) \, dx \, dt / \Delta x$, the differential equation becomes an integral equation

$$f_j^{n+1} = f_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} (u \hat{f}_{j-1/2}(t) - u \hat{f}_{j+1/2}(t)) \, dt + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} \frac{g - f}{\tau} \, dx \, dt, \tag{5}$$

where $\hat{f}_{j+1/2}$ is the gas distribution function at the cell interface $x_{j+1/2}$. The above equation is exact and there is no numerical error introduced yet. For a kinetic scheme, two terms on the right-hand side of the above equation have to be numerically evaluated.

With the discretization of space x_j , time t^n and particle velocity u_k , the finite-volume scheme based on the integral solution of (5) is

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta x} \int (u_k \hat{f}_{j-1/2,k} - u_k \hat{f}_{j+1/2,k}) dt + \frac{1}{\Delta x} \int \int \frac{g-f}{\tau} dx dt, \quad (6)$$

where $f_{j,k}^n$ is the averaged distribution function in the j th cell $x \in [x_{j-1/2}, x_{j+1/2}]$ at the particle velocity u_k . Instead of using upwind scheme for the evaluation of the distribution function at a cell interface, the solution $\hat{f}_{j+1/2,k}$ in the above equation is constructed from an integral solution of the BGK model (1),

$$\begin{aligned} \hat{f}_{j+1/2,k} &= f(x_{j+1/2}, t, u_k) = \frac{1}{\tau} \int_{t^n}^t g(x', t', u_k) e^{-(t-t')/\tau} dt' \\ &\quad + e^{-(t-t^n)/\tau} f_{0,k}^n(x_{j+1/2} - u_k(t-t^n), t^n, u_k), \end{aligned} \quad (7)$$

where $x' = x_{j+1/2} - u_k(t-t')$ is the particle trajectory and $f_{0,k}^n$ is the initial gas distribution function of f at time $t = t^n$ around the cell interface $x_{j+1/2}$ at the particle velocity u_k , i.e. $f_{0,k}^n = f_0^n(x, t^n, u_k)$. The gas distribution function $\hat{f}(x_{j+1/2}, t, u_k)$ at the discretized particle velocity u_k can be expressed as

$$\hat{f}_{j+1/2,k}(0, t) = \tilde{g}_{j+1/2,k} + \tilde{f}_{j+1/2,k}, \quad (8)$$

where $\tilde{g}_{j+1/2,k}$ is all terms related to the integration of the equilibrium state g and $\tilde{f}_{j+1/2,k}$ is the terms from the initial condition f_0 (Xu, 2001). The use of the above integral equation is important in designing a unified scheme for all flow regimes, where \tilde{g} term is related to the drifting of a Maxwellian distribution on the hydrodynamic scale and \tilde{f} represents the kinetic scale for the particle-free transport. The detailed formulation can be found in Xu & Huang (2010).

In order to discretize the collision term in (6) efficiently and accurately, a multiscale unified formulation is the following. Let us first take moment ψ on (6). Due to the vanishing of the particle collision term for the conservative variables, we have

$$\begin{aligned} W_j^{n+1} &= W_j^n + \frac{1}{\Delta x} \int \int_{t^n}^{t^{n+1}} u (\tilde{g}_{j-1/2} - \tilde{g}_{j+1/2}) \psi dt du \\ &\quad + \frac{1}{\Delta x} \sum_k \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) \psi dt, \end{aligned} \quad (9)$$

where $\tilde{g}_{j+1/2}$ has the same expression as $\tilde{g}_{j+1/2,k}$ but is integrated in a continuous particle velocity space $u_k = u$. The integration of the equilibrium part \tilde{g} can be evaluated analytically (Xu & Huang, 2010) and the integration of the non-equilibrium part \tilde{f} can be done using quadrature. Due to the BGK model, in the above update of conservative variables, the heat transfer $q_{j+1/2}$ in the energy flux F_E across a cell interface has a corresponding unit Prandtl number. In order to fix the heat flux, we can modify the heat flux by replacing the original energy flux F_E in (9) with a new one,

$$F_E^{\text{new}} = F_E + \left(\frac{1}{\text{Pr}} - 1 \right) q_{j+1/2}, \quad (10)$$

where $q_{j+1/2}$ is the original heat flux in (9).

In general, based on the above updated conservative variables, we can immediately obtain the equilibrium gas distribution function $g_{j,k}^{n+1}$ inside each cell; therefore, based on (6), the unified kinetic scheme for the update of gas distribution function becomes

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta x} \left(\int_{t^n}^{t^{n+1}} u_k (\tilde{g}_{j-1/2,k} - \tilde{g}_{j+1/2,k}) dt + \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) dt \right) + \frac{\Delta t}{2} \left(\frac{g_{j,k}^{n+1} - f_{j,k}^{n+1}}{\tau^{n+1}} + \frac{g_{j,k}^n - f_{j,k}^n}{\tau^n} \right), \quad (11)$$

where the trapezoidal rule has been used for the time integration of collision term. So, from the above equation, the unified multiscale scheme for the update of gas distribution function is

$$f_{j,k}^{n+1} = \left(1 + \frac{\Delta t}{2\tau^{n+1}} \right)^{-1} \left[f_{j,k}^n + \frac{1}{\Delta x} \left(\int_{t^n}^{t^{n+1}} u_k (\tilde{g}_{j-1/2,k} - \tilde{g}_{j+1/2,k}) dt + \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) dt \right) + \frac{\Delta t}{2} \left(\frac{g_{j,k}^{n+1}}{\tau_j^{n+1}} + \frac{g_{j,k}^n - f_{j,k}^n}{\tau_j^n} \right) \right]. \quad (12)$$

The particle collision times τ_j^n and τ_j^{n+1} are defined based on the temperature and pressure in the cell, i.e. $\tau_j^n = \mu(T_j^n)/p_j^n$ and $\tau_j^{n+1} = \mu(T_j^{n+1})/p_j^{n+1}$, which are known due to the updated macroscopic flow variables in (9).

In the above U-BGK scheme, the fix of Prandtl number is through the correction of heat flux in the update of macroscopic variables in (9), then effects the construction of the equilibrium state g^{n+1} in the collision term in (11), and the update of gas distribution function f^{n+1} . The above approach is only partially correct because the fluxes $u_k \tilde{g}$ and $u_k \tilde{f}$ in (11) still have intrinsic unit Prandtl number. Theoretically, these fluxes should also be modified to have a correct Prandtl number. This is the main reason that we develop a new unified scheme based on the Shakhov model.

3. Unified scheme for Shakhov model

In the previous section, we present the unified scheme for the BGK model. The unit Prandtl number is corrected through the heat flux modification for the update of macroscopic flow variables. Then, this modification affects the update of non-equilibrium distribution function. In order to fix the Prandtl number, many generalized BGK-type kinetic models have been developed. Two of the well-known ones are Ellipsoidal and Shakhov models. The Shakhov model can be written as (Shakhov, 1968)

$$f_t + u f_x = (f^+ - f)/\tau,$$

where

$$f^+ = g \left[1 + (1 - \text{Pr}) \mathbf{c} \cdot \mathbf{q} \left(\frac{c^2}{RT} - 5 \right) / (5pRT) \right],$$

with random velocity $c = u - U$ and the heat flux q . In the above model, the Prandtl number is automatically fixed by choosing the value Pr.

A unified scheme can be developed for the above model as well. The update of the distribution function is the same as the previous scheme,

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta x} \int (u_k \hat{f}_{j-1/2,k} - u_k \hat{f}_{j+1/2,k}) dt + \frac{1}{\Delta x} \int \int \frac{f^+ - f}{\tau} dx dt. \quad (13)$$

However, the solution $\hat{f}_{j+1/2,k}$ in the above equation is constructed from the integral solution of the Shakhov model using the method of characteristics,

$$\begin{aligned} \hat{f}_{j+1/2,k} = f(x_{j+1/2}, t, u_k, \zeta) &= \frac{1}{\tau} \int_{t^n}^t f^+(x', t', u_k, \zeta) e^{-(t-t')/\tau} dt' \\ &+ e^{-(t-t^n)/\tau} f_{0,k}^n(x_{j+1/2} - u_k(t - t^n), t^n, u_k, \zeta), \end{aligned} \quad (14)$$

where $x' = x_{j+1/2} - u_k(t - t')$ is the particle trajectory and $f_{0,k}^n$ is the initial gas distribution function of f at time $t = t^n$ around the cell interface $x_{j+1/2}$ at the particle velocity u_k , i.e. $f_{0,k}^n = f_0^n(x, t^n, u_k)$. The gas distribution function $\hat{f}(x_{j+1/2}, t, u_k)$ at the discretized particle velocity u_k can be expressed as

$$\hat{f}_{j+1/2,k}(0, t) = \tilde{g}_{j+1/2,k}^+ + \tilde{f}_{j+1/2,k}, \quad (15)$$

where $\tilde{g}_{j+1/2,k}^+$ is all terms related to the integration of the ‘equilibrium’ state f^+ and $\tilde{f}_{j+1/2,k}$ is the term from the initial condition f_0 . For the Shakhov model, the term $\tilde{g}_{j+1/2,k}^+$ is related to the BGK solution $\tilde{g}_{j+1/2,k}$ in (8), which can be approximated as

$$\tilde{g}_{j+1/2,k}^+ = \tilde{g}_{j+1/2,k} + (1 - e^{-t/\tau}) g \left[(1 - \text{Pr})(u - U) q \left(\frac{(u - U)^2}{RT} - 3 \right) \right] / (5pRT), \quad (16)$$

where q is the heat flux.

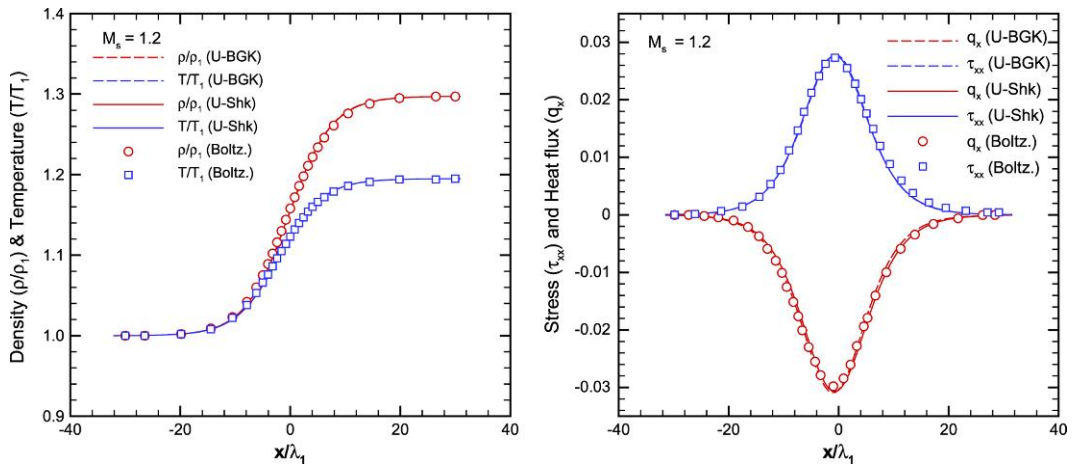


FIG. 1. $M = 1.2$ argon shock structure calculated by the unified schemes and the direct Boltzmann solver.

Then, we can take moment ψ on (13). Due to the vanishing of the particle collision term for the conservative variables, we have

$$\begin{aligned} W_j^{n+1} &= W_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int u (\tilde{g}_{j-1/2}^+ - \tilde{g}_{j+1/2}^+) \psi \, dt \, du \\ &+ \frac{1}{\Delta x} \sum_k \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) \psi \, dt. \end{aligned} \quad (17)$$

Different from the previous unified scheme for the BGK model, we do not need to modify the heat flux in the above equation and the Prandtl number will be correct due to the Shakhov model itself. For the macroscopic variables update W^{n+1} , the above formulation based on the Shakhov model will be the same as the modification of heat flux (10) of the previous approach. Then, based on the above updated conservative variables, we can immediately obtain the equilibrium gas distribution function $g_{j,k}^{n+1}$, which is the same as U-BGK scheme. With the reconstruction of the slopes of the conservative variables W^{n+1} at the next time level, we can uniquely determine the state $f^{+(n+1)}$. Therefore, based on (13), a unified kinetic scheme for the shakhov model becomes

$$\begin{aligned} f_{j,k}^{n+1} &= f_{j,k}^n + \frac{1}{\Delta x} \left(\int_{t^n}^{t^{n+1}} u_k (\tilde{g}_{j-1/2,k}^+ - \tilde{g}_{j+1/2,k}^+) dt + \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) dt \right) \\ &+ \frac{\Delta t}{2} \left(\frac{f_{j,k}^{+(n+1)} - f_{j,k}^{n+1}}{\tau^{n+1}} + \frac{f_{j,k}^{+n} - f_{j,k}^n}{\tau^n} \right), \end{aligned} \quad (18)$$

where again the trapezoidal rule has been used for the time integration of collision term. So, from the above equation, the unified multiscale scheme for the update of gas distribution function can be constructed. There will be no iteration in the determination of the non-equilibrium distribution function f^{n+1} . The differences between the U-BGK and the above unified Shakhov (U-Shk) scheme is that \tilde{g} is replaced by \tilde{g}^+ and g^{n+1} is replaced by $f^{+(n+1)}$. As a result, the heat flux in the update of the gas distribution function is corrected in both the transport term across a cell interface and the collision term inside each cell.

To take conservative moments on (18), the collision terms will disappear. For the update of conservative variables, the unified scheme will become identical to the BGK-NS method (Xu, 2001) in the continuum flow regime ($\tau \ll \Delta t$). The BGK-NS has the order of accuracy $O(\tau (\Delta t)^2)$ (Ohwada, 2002) to approximate the NS solutions, which means that the unified scheme is an AP method.

4. Shock structure computation

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, shock wave phenomena is unique in that it allows one to separate the differential equations of fluid motion from the boundary conditions that would be required to complete a well-posed problem. The boundary conditions for a shock wave are simply determined by the Rankine–Hugoniot relations. Thus, in the study of shock structure, one is able to isolate effects due to the differential equations themselves. Since 1950s, the computation of shock structure had played an important and critical role in validating many theories and numerical schemes in the study of non-equilibrium flow.

In order to validate the unified schemes, such as U-BGK and U-Shk, we apply them to the shock structure calculations from low Mach number cases, where the NS equations are valid, to the high Mach number cases, where the highly non-equilibrium effect appears. Besides the density and temperature distributions inside the shock layer, the stress and heat flux will also be presented in some cases. The solutions based on the unified scheme are compared with the Boltzmann solution (Ohwada, 1993), DSMC results (Bird, 1970) and possible experimental measurements (Alsmeyer, 1976; Steinhilper, 1972).

First, we present test cases on the shock structure for a monatomic gas with the non-equilibrium limited to the translational energy mode. Comparisons of our results are made with the solution of the full Boltzmann equation which were obtained by Ohwada (1993) for the hard sphere molecules at Mach numbers 1.2, 2 and 3. For the hard sphere molecules, the viscosity coefficient $\tau \sim \mu \sim T^{0.5}$, where the

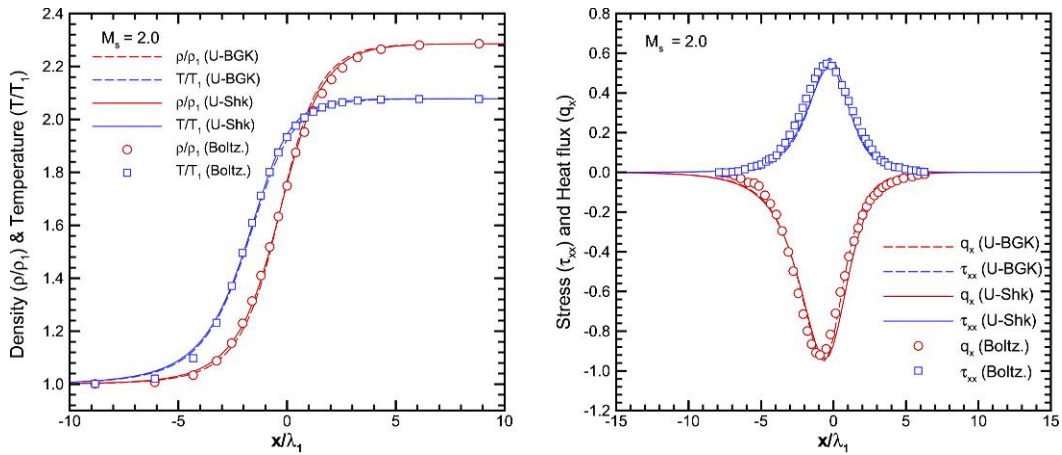


FIG. 2. $M = 2.0$ argon shock structure calculated by the unified schemes and the direct Boltzmann solver.

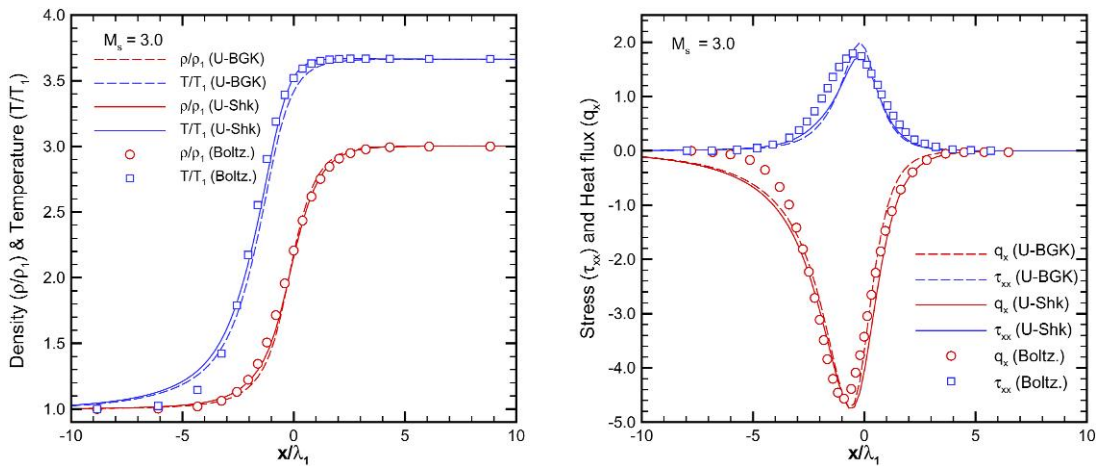


FIG. 3. $M = 3.0$ argon shock structure calculated by the unified schemes and the direct Boltzmann solver.

x -coordinate is normalized by $\sqrt{\pi}l_0/2$ and l_0 is the mean free path of the gas molecules at the upstream condition. Figures 1–3 show the density, temperature, stress and heat flux inside a shock layer by both schemes. Comparisons of the unified schemes are made with the solutions of the Boltzmann equation. For all the Mach numbers presented, the results from the direct Boltzmann solver and the current unified schemes have good agreement. At Mach number 1.2, the local Knudsen number, which is defined as the local mean free path over the density variation scale $l/(\rho/\nabla\rho)$, is less than 0.02. As expected, both the Boltzmann and the unified solutions are very close to the standard NS solution. Also, at low Mach numbers, the U-BGK and U-Shk present almost identical results.

For the Mach 8 argon shock structure, Bird's (1970) DSMC solution with $\mu \sim T^{0.68}$ gave a good agreement with the experimental data. Here, we only compare the results from the unified scheme and the DSMC method. Figure 4 shows the solution of temperature, density, heat flux and stresses from the unified schemes and that from DSMC solutions. For this Mach 8 case, the shock thickness and the separation distance between the density and temperature profiles by the unified schemes compare well

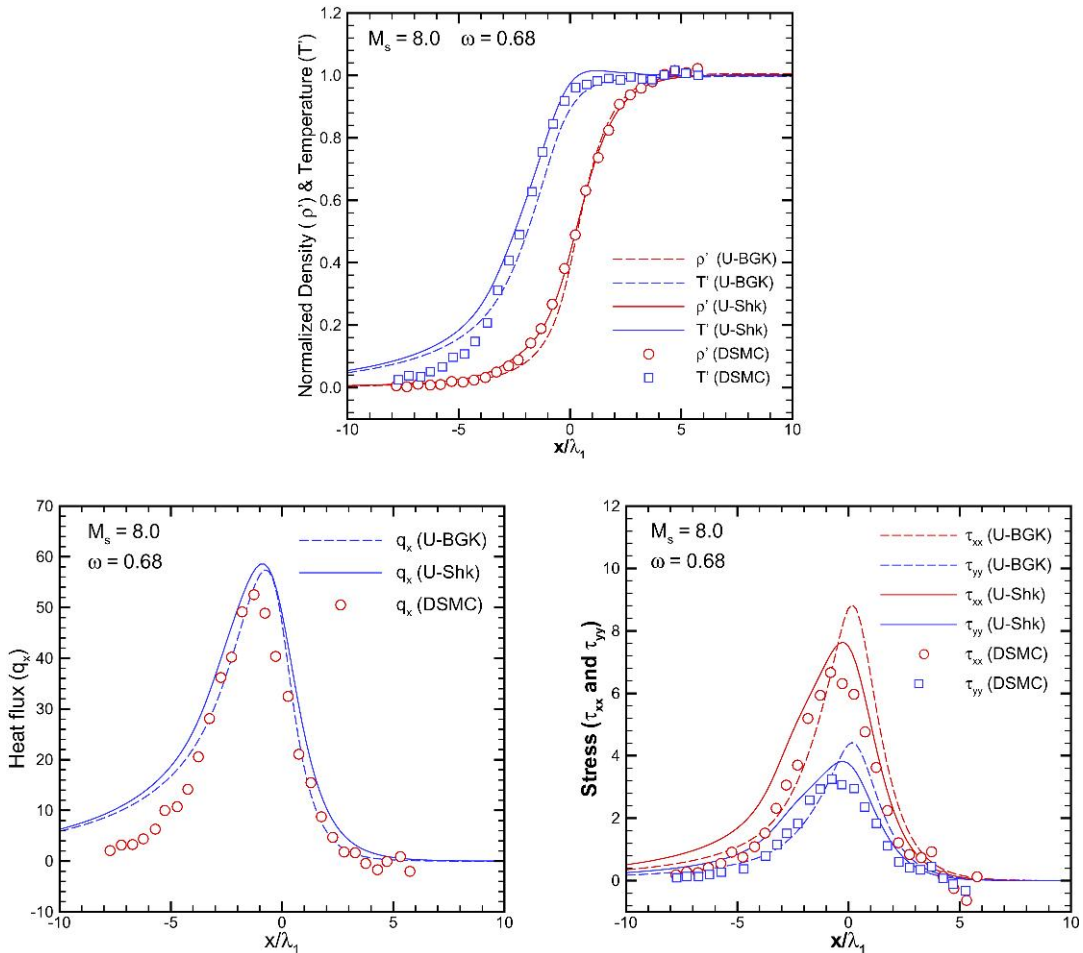


FIG. 4. $M = 8.0$, $\omega = 0.68$ argon shock structure calculated by the unified schemes and the DSMC solutions.

with those of DSMC solution. The peak values of the stress profile by the DSMC method are lower than the current unified solutions. The shock thickness from U-Shk is slightly wider than that from U-BGK.

Figures 5 and 6 show the argon shock structures for a viscosity coefficient of $\mu \sim T^{0.72}$ at Mach numbers 8.0 and 9.0 by both U-BGK and U-Shk, where the experimental measurements are used as benchmark solutions (Alsmeyer, 1976; Steinhilper, 1972). As shown in this figure, the solutions from the unified schemes match the experimental data very well in the density distributions. Again, at high Mach numbers the U-BGK presents a thinner shock thickness and narrower temperature–density distance than that of U-Shk.

Figure 7 presents the helium shock structure calculations at Mach number 25. Instead of the shock structure, we present the gas distribution functions directly at different locations inside the shock layer

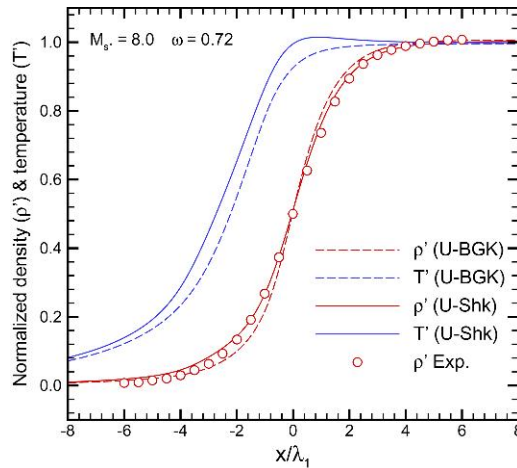


FIG. 5. $M = 8.0$ argon shock structure calculated by the unified schemes and the comparison with the experimental measurements.

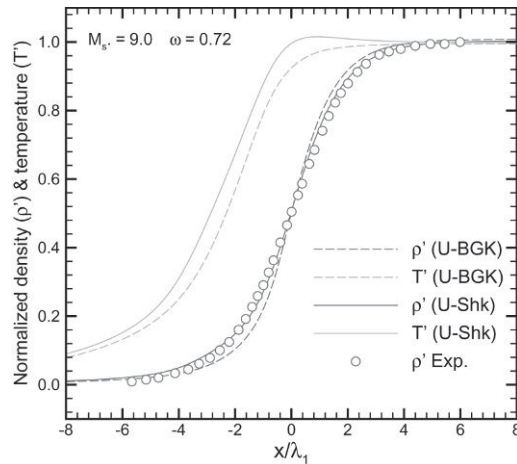


FIG. 6. $M = 9.0$ argon shock structure calculated by the unified scheme and the comparison with the experimental measurements.

(Pham-Van-Diep *et al.*, 1989; Erwin *et al.*, 1991). With the normalized density $\hat{\rho} = (\rho - \rho_1)/(\rho_2 - \rho_1)$, the locations for the distribution function presentation are at $\hat{\rho} = 0.291, 0.332$ and $\hat{\rho} = 0.610, 0.636$. In Fig. 7, the direct simulation results from U-Shk are compared with the experimental data in Pham-Van-Diep *et al.* (1989). It seems that the distribution functions are not too sensitive to the locations inside the shock layer. From Fig. 7, the validity of the unified scheme for the description of non-equilibrium flow has been proved.

Figure 8 presents the reciprocal thickness versus Mach numbers from 1 to 9 for argon gas with $\omega = 0.72$. Both experimental data (Alsmeyer, 1976) and DSMC solutions are also included. From the results, we can clearly observe that near the continuum low Mach number limit, the unified scheme

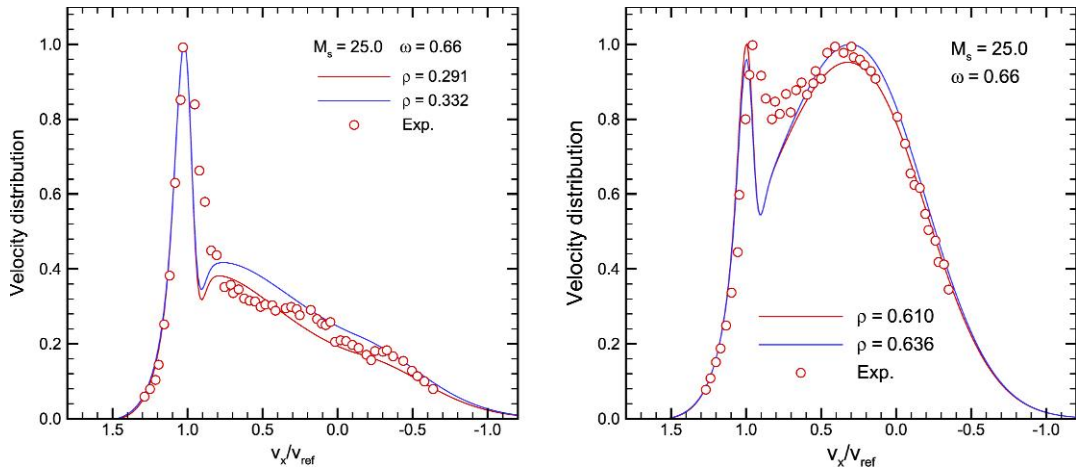


FIG. 7. Gas distribution functions from both U-Shk and experiment measurements inside $M = 25.0$ helium shock layer (Pham-Van-Diep *et al.*, 1989) at different locations with normalized densities (0.291, 0.332) and (0.610, 0.636).

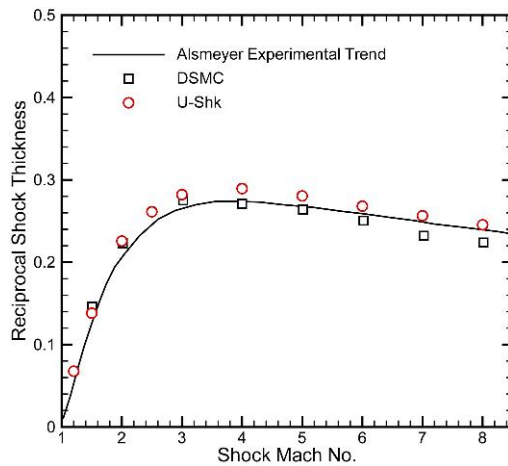


FIG. 8. Reciprocal shock thickness versus Mach numbers for argon gas from both the unified and the DSMC solutions.

presents a better match with the experimental data. This is not surprised because the unified scheme will present an accurate NS solution in the continuum regime.

5. Conclusions

In this paper, we present unified kinetic schemes for both the BGK and the Shakhov models for shock structure simulation from low to high Mach numbers. The critical step is that the integral solution of the kinetic equation is used in the flux evaluation across the cell interface. This integral solution covers both hydrodynamic and kinetic scales, which subsequently gives an accurate representation in both continuum and free molecule flows when going to different limits of the integral solution. The weakness for the most existing kinetic methods is that a purely upwind technique is used for the flux evaluation, which is equivalent to solving the collisionless Boltzmann equation and this solution is only a partial solution of the integral solution used in the unified scheme. In other words, most current existing kinetic schemes only have the kinetic scale in their underlying numerical model. Even in the continuum flow regimes, these methods try to resolve the physics within the mean free path or mean particle collision time. Therefore, they have limited usage in this regime. Due to its multiscale nature of the unified scheme, in the continuum flow regime, the unified scheme can use a large time step in comparison with particle collision time. At the same time, the accurate NS solutions can be obtained.

The shock structure study in this paper validates the unified scheme as an accurate flow solver for both continuum and rarefied flows. The capturing of highly non-equilibrium gas distribution function inside high Mach number shock layer demonstrates clearly that the unified scheme can be safely applied to engineering rarefied gas dynamics problems. The unified scheme works accurately for flow computations in the entire Knudsen number.

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REFERENCES

- ALSMEYER, H. (1976) Density profiles in argon and nitrogen shock waves measured by the absorption of an electron beam. *J. Fluid Mech.*, **74**, 497.
- ARISTOV, V. V. (2001) *Direct Methods for Solving the Boltzmann Equation and Study of Nonequilibrium Flows*. The Netherlands: Kluwer Academic Publishers.
- BHATNAGAR, P. L., GROSS, E. P. & KROOK, M. (1954) A model for collision processes in gases I: small amplitude processes in charged and neutral one-component systems. *Phys. Rev.*, **94**, 511–525.
- BIRD, G. A. (1970) Aspects of the structure of strong shock waves. *Phys. Fluids*, **13**, 1172–1177.
- BIRD, G. A. (1994) *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. New York: Oxford University Press.
- CARRILLO, J. A., GOUDON, T., LAFITTE, P. & VECIL, F. (2008) Numerical schemes of diffusion asymptotics and moment closures for kinetic equations. *J. Sci. Comput.*, **36**, 113–149.
- CHAPMAN, S. & COWLING, T. G. (1990) *The Mathematical Theory of Non-uniform Gases*. New York: Cambridge University Press.
- CHU, C. K. (1965) Kinetic-theoretic description of the formation of a shock wave. *Phys. Fluids*, **8**, 12.
- DEGOND, P., LIU, J.-G. & MIEUSSENS, L. (2006) Macroscopic fluid models with localized kinetic upscaling effects. *Multiscale Model. Simul.*, **5**, 940–979.

- ERWIN, D. A., PHAM-VAN-DIEP, G. C. & MUNTZ, E. P. (1991) Nonequilibrium gas flows. I: a detailed validation of Monte Carlo simulation for monatomic gases. *Phys. Fluids A*, **3**, 697–705.
- JIN, S. (1999) Efficient asymptotic-preserving (AP) schemes for some multiscale kinetic equations. *SIAM J. Sci. Comput.*, **21**, 441–454.
- KLAR, A. (1998) An asymptotic-induced scheme for nonstationary transport equations in the diffusive limit. *SIAM J. Numer. Anal.*, **35**, 1073–1094.
- KOLOBOV, V. I., ARSLANBEKOV, R. R., ARISTOV, V. V., FROLOVA, A. A. & ZABELOK, S. A. (2007) Unified solver for rarefied and continuum flows with adaptive mesh and algorithm refinement. *J. Comput. Phys.*, **223**, 589–608.
- LEMOU, M. & MIEUSSENS, L. (2008) A new asymptotic preserving scheme based on micro-macro formulation for linear kinetic equations in the diffusion limit. *SIAM J. Sci. Comput.*, **31**, 334–368.
- LI, Z. H. & ZHANG, H. X. (2009) Gas-kinetic numerical studies of three-dimensional complex flows on spacecraft re-entry. *J. Comput. Phys.*, **228**, 1116–1138.
- MIEUSSENS, L. (2000) Discrete-velocity models and numerical schemes for the Boltzmann-BGK equation in plane and axisymmetric geometries. *J. Comput. Phys.*, **162**, 429–466.
- OHWADA, T. (1993) Structure of normal shock waves: direct numerical analysis of the Boltzmann equation for hard-sphere molecules. *Phys. Fluids A*, **5**, 217–234.
- OHWADA, T. (2002) On the construction of kinetic schemes. *J. Comput. Phys.*, **177**, 156–175.
- PHAM-VAN-DIEP, G. C., ERWIN, D. A. & MUNTZ, E. P. (1989) Nonequilibrium molecular motion in a hypersonic shock wave. *Science*, **245**, 624.
- PIERACCINI, S. & PUPPO, G. (2007) Implicit-explicit schemes for BGK kinetic equations. *J. Sci. Comput.*, **32**, 1–28.
- SHAKHOV, E. M. (1968) Generalization of the Krook kinetic equation. *Fluid Dyn.*, **3**, 95.
- STEINHILPER, E. A. (1972) Electron beam measurements of the shock wave structure: part 1, the inference of intermolecular potential from shock structure experiments. *Ph.D. Thesis*, California Institute of Technology, Pasadena, CA.
- XU, K. (2001) A gas-kinetic BGK scheme for the Navier-Stokes equations and its connection with artificial dissipation and Godunov method. *J. Comput. Phys.*, **171**, 289–335.
- XU, K. & HUANG, J. C. (2010) A unified gas-kinetic scheme for continuum and rarefied flows. *J. Comput. Phys.*, **229**, 7747–7764.
- XU, K. & LI, Z. W. (2001) Dissipative mechanism in Godunov-type schemes. *Int. J. Numer. Meth. Fluids*, **37**, 1–22.
- YANG, J. Y. & HUANG, J. C. (1995) Rarefied flow computations using nonlinear model Boltzmann equations. *J. Comput. Phys.*, **120**, 323–339.