

## Continuum Formulation for Non-Equilibrium Shock Structure Calculation

Kun Xu<sup>1,\*</sup> and Eswar Josyula<sup>2</sup>

<sup>1</sup> *Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

<sup>2</sup> *Air Force Research Laboratory, 2210 Eighth Street, Wright-Patterson AFB, OH 45433, USA.*

Received 11 June 2005; Accepted (in revised version) 10 December 2005

---

**Abstract.** Are extensions to continuum formulations for solving fluid dynamic problems in the transition-to-rarefied regimes viable alternatives to particle methods? It is well known that for increasingly rarefied flow fields, the predictions from continuum formulation, such as the Navier-Stokes equations lose accuracy. These inaccuracies are attributed primarily to the linear approximations of the stress and heat flux terms in the Navier-Stokes equations. The inclusion of higher-order terms, such as Burnett or high-order moment equations, could improve the predictive capabilities of such continuum formulations, but there has been limited success in the shock structure calculations, especially for the high Mach number case. Here, after reformulating the viscosity and heat conduction coefficients appropriate for the rarefied flow regime, we will show that the Navier-Stokes-type continuum formulation may still be properly used. The equations with generalization of the dissipative coefficients based on the closed solution of the Bhatnagar-Gross-Krook (BGK) model of the Boltzmann equation, are solved using the gas-kinetic numerical scheme. This paper concentrates on the non-equilibrium shock structure calculations for both monatomic and diatomic gases. The Landau-Teller-Jeans relaxation model for the rotational energy is used to evaluate the quantitative difference between the translational and rotational temperatures inside the shock layer. Variations of shear stress, heat flux, temperatures, and densities in the internal structure of the shock waves are compared with, (a) existing theoretical solutions of the Boltzmann solution, (b) existing numerical predictions of the direct simulation Monte Carlo (DSMC) method, and (c) available experimental measurements. The present continuum formulation for calculating the shock structures for monatomic and diatomic gases in the Mach number range of 1.2 to 12.9 is found to be satisfactory.

**Key words:** Non-equilibrium flow; bulk viscosity; kinetic scheme; shock structure.

---

\*Correspondence to: Kun Xu, Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong. Email: [makxu@ust.hk](mailto:makxu@ust.hk)

## 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  $\text{Kn}$  is defined as the ratio of the mean free path to a characteristic length scale of the system. In the continuum flow regime where  $\text{Kn} < 0.001$ , the Navier-Stokes equations with linear relations between stress and strain and the Fourier's law for heat conduction are adequate to model the fluid behavior. For flows in the continuum-transition regime ( $0.1 < \text{Kn} < 1$ ), the Navier-Stokes equations are known to be inadequate. This regime is important for many practical engineering problems, such as the simulation of microscale flows [12] and hypersonic flow around space vehicles in low earth orbit [15]. 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.

The numerical techniques available for solving the Boltzmann equation can be classified into particle methods and continuum methods. The direct simulation Monte Carlo (DSMC) [7] falls in the category of particle methods. 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 both in terms of the computation time and memory requirement. At present, the accurate modeling of realistic configurations, such as aerospace vehicles in three dimensions by the DSMC method for  $\text{Kn} \ll 1$ , is beyond the currently available computing power. Alternative methods, which solve the Boltzmann or model equations directly with the discretization of the phase space [3, 18], have attracted attentions in recent years.

Among continuum solution methodologies, there are primarily two approaches: (1) the Chapman-Enskog method [9], and (2) the method of moments [13]. In the Chapman-Enskog method, the phase density is expanded in powers of the Knudsen number, the zeroth-order expansion yielding the Euler equations, the first-order results in the equations of Navier-Stokes and Fourier, the second order the Burnett equations, and the third order expansion the so-called super-Burnett equations. It is well recognized that the equations of Navier-Stokes and Fourier cease to be accurate for Knudsen number above 0.1, and one might theorize that the Burnett and Super-Burnett equations are valid for larger Knudsen numbers. Unfortunately, the higher-order equations are shown to be linearly unstable for processes involving small wavelengths, or high frequencies, and thus cannot be used in numerical simulations [8]. In recent years, several authors presented augmented forms of the Burnett equations containing additional terms of the super-Burnett order as a way of stabilizing the Burnett equations [35], the BGK-Burnett equations [4], or the regularized hyperbolic equations through relaxation, reproducing the Burnett equations when expanded in  $\text{Kn}$  [16].

In the method of Grad, the Boltzmann equation is replaced by a set of moment equations which are the first order partial differential equations for the moments of the dis-

tribution function. The actual number of moments needed depends on the process being considered, but experience shows that the number of moments had to be increased with increasing Knudsen number [23]. Since the moment equations are hyperbolic, the Grad method leads to a shock structure with spurious sub-shocks for Mach numbers greater than 1.65. It is interesting to note that a close connection between the Grad's moments method and the Burnett and Super-Burnett equations has been established. [29]. Further, Struchtrup and Torrilhon regularized Grad's 13 moment equations with the help of the Burnett equations and successfully applied the method to the shock structures up to Mach 3 of a monatomic gas [21]. However, at the current stage of research, a systematic development of a continuum method for monatomic and diatomic gas for the highly non-equilibrium flow inside the shock structure is not in place. For the solution of the structure of the shock wave, the following statement in [23] may still be true: *"this is a long-standing problem in gas dynamics and it has been 'proved' several times that the method of moments cannot solve it, because the smooth shock structure breaks down at finite Mach numbers"*.

The goal of this study is to develop a continuum formulation for low density rarefied gas flows. The continuum model developed in the present study will be used to solve non-equilibrium shock structures for monatomic and diatomic gases in the Mach number range of 1.2 to 12.9. In what follows, Section 2 provides details on the construction of the current continuum model and Section 3 presents the numerical method for solving this model. This is followed by the results and discussion of the shock structure calculations presented in Section 4. This final section of the paper are the concluding remarks.

## 2 Equilibrium and non-equilibrium continuum models

### 2.1 Translational and rotational temperature equilibrium model

The Boltzmann equation expresses the behavior of a many-particle kinetic system in terms of the evolution equation for a single particle gas distribution function. The simplification of the Boltzmann equation given by the BGK model is formulated as

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{f^{eq} - f}{\tau}, \quad (2.1)$$

where  $f$  is the number density of molecules at position  $\mathbf{x}$  and particle velocity  $\mathbf{u}$  at time  $t$ . The left hand side of the above equation represents the free streaming of molecules in space, and the right side denotes the collision term. If the distribution function  $f$  is known, macroscopic variables, such as mass, momentum, energy and stress, can be obtained by integration over the moments of molecular velocity. In the BGK model, the collision operator involves simple relaxation to a state of local equilibrium, the distribution function given by  $f^{eq}$  with a characteristic time scale  $\tau$ . The equilibrium state is given by a Maxwellian,

$$f^{eq} = \rho \left( \frac{\lambda}{\pi} \right)^{\frac{K+3}{2}} e^{-\lambda((\mathbf{u}-\mathbf{U})^2 + \xi^2)},$$

where  $\rho$  is the density,  $\mathbf{U}$  the macroscopic fluid velocity, and  $\lambda = m/2kT$ , where  $m$  is the molecular mass,  $k$  the Boltzmann constant, and  $T$  the temperature. For an equilibrium flow, the internal variable  $\xi$  accounts for the rotational and vibrational modes, such as  $\xi^2 = \xi_1^2 + \xi_2^2 + \dots + \xi_K^2$ , and the total number of degrees of freedom  $K$  is related to the specific heat ratio  $\gamma$ . In the current paper, we only consider cases, where  $K = 0$  for the monatomic gas and  $K = 2$  for the diatomic gas with two rotational degree of freedom. The relation between mass  $\rho$ , momentum  $\rho\mathbf{U}$ , and energy densities  $\rho E$  with the distribution function  $f$  is

$$(\rho, \rho\mathbf{U}, \rho E)^T = \int \psi_\alpha f d\mathbf{u} d\xi, \quad (2.2)$$

where  $\psi_\alpha$  is the component of the vector of moments  $\psi = (1, \mathbf{u}, \frac{1}{2}(\mathbf{u}^2 + \xi^2))^T$ , and the volume element in the phase space with  $d\mathbf{u} = dudvdw$  and  $d\xi = d\xi_1 d\xi_2 \dots d\xi_K$ . Since mass, momentum and energy are conserved during particle collisions,  $f$  and  $f^{eq}$  satisfy the conservation constraint,

$$\int (f^{eq} - f) \psi_\alpha d\mathbf{u} d\xi = 0, \quad (2.3)$$

at any point in space and time.

The BGK model was originally proposed to describe the essential physics of molecular interactions with  $\tau$  chosen as the molecular collision time. Although the BGK model appears to describe only weak departures from local equilibria, it has long been recognized that such an approximation works well beyond its theoretical limits as long as the relaxation time is known for the physical process. Based on the above BGK model, the Navier-Stokes equations can be derived with the Chapman-Enskog expansion truncated to the 1st-order as,

$$f = f^{eq} + \text{Kn} f_1 = f^{eq} - \tau(\partial f^{eq}/\partial t + \mathbf{u} \cdot \partial f^{eq}/\partial \mathbf{x}). \quad (2.4)$$

For the Burnett and super-Burnett solutions, the above expansion can be naturally extended [25], such as  $f = f^{eq} + \text{Kn} f_1 + \text{Kn}^2 f_2 + \text{Kn}^3 f_3 + \dots$

Based on Eq.(2.4) and the BGK model for the continuum flow limit of the Navier-Stokes equations, the stress and Fourier heat conduction terms can be derived. The Navier-Stokes equations for the monatomic gas in the one-dimensional case can be written as,

$$\begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix}_t + \begin{pmatrix} \rho U \\ \rho U^2 + p \\ (\rho E + p)U \end{pmatrix}_x = \begin{pmatrix} 0 \\ \frac{4}{3}\mu U_x \\ \frac{5}{2}\mu RT_x + \frac{4}{3}\mu U U_x \end{pmatrix}_x,$$

where  $\mu = \tau p$  is the dynamic viscosity coefficient. With the relation  $\lambda = m/2kT$  and  $C_p = 5k/2m$  for a monatomic gas, the heat conduction coefficient in the above equations becomes  $\kappa = 5k\mu/2m$ , and the Prandtl number becomes a fixed value  $\text{Pr} = \mu C_p/\kappa = 1$ . This is a well-known result for the BGK model. One way to modify  $\text{Pr}$  in the kinetic scheme for the above continuum equations will be presented in Section 3. Based on Eq.(2.4), the stress tensor and heat conduction terms can be derived for a diatomic gas

for the translational and rotational modes in equilibrium. In the one dimensional case, the Navier-Stokes equations become

$$\begin{pmatrix} \rho \\ \rho U \\ E \end{pmatrix}_t + \begin{pmatrix} \rho U \\ \rho U^2 + p \\ (E + p)U \end{pmatrix}_x = \begin{pmatrix} 0 \\ \frac{8}{3}\mu U_x \\ \frac{7}{2}R\mu T_x + \frac{8}{5}\mu U U_x \end{pmatrix}_x, \tag{2.5}$$

where the bulk viscosity  $(4/15)\tau p$  to account for the relaxation of the rotational degree of freedom is included in the above formulation [32]. The detail derivation of the above equations can be found in the Appendix. Instead of solving the above Navier-Stokes equations, our numerical procedure implements a finite volume scheme for the viscous flow calculation, constructed directly from the time evolution of the continuum gas distribution function in Eq.(2.4) [33].

### 2.2 Non-equilibrium rotational and translational temperatures model

It is well recognized that the standard form of Navier-Stokes equations with the bulk viscosity given by the Stokes hypothesis, cannot properly describe the non-equilibrium flow. In the general case of non-equilibrium, temperatures for the translational and rotational energy modes will be different. In this subsection, we will discuss implementation of the non-equilibrium rotational relaxation model into the BGK model. The modeling of translational non-equilibrium through the generalization of transport coefficients will be presented in the next subsection.

In general, based on the above-mentioned BGK model, for a diatomic gas we assume two temperatures, one for translational and the other for rotational.

$$f^{eq} = \rho \left(\frac{\lambda_t}{\pi}\right)^{\frac{3}{2}} \left(\frac{\lambda_r}{\pi}\right) e^{-\lambda_t(\mathbf{u}-\mathbf{U})^2 - \lambda_r \xi^2}, \tag{2.6}$$

where  $\rho$  is the density,  $\lambda_t = m/2kT_t$  is related to the translational temperature  $T_t$ , and  $\lambda_r = m/2kT_r$  to the rotational temperature  $T_r$ . The nitrogen molecule has two rotational degrees of freedom  $\xi^2 = \xi_1^2 + \xi_2^2$ . The relation between mass  $\rho$ , momentum  $\rho\mathbf{U}$ , total energy  $\rho E$ , and rotational energy  $\rho E_r$  densities with the distribution function  $f$  is

$$W = (\rho, \rho\mathbf{U}, \rho E, \rho E_r)^T = \int \psi f d\mathbf{u}d\xi,$$

where  $\psi$  has the components

$$\psi = (1, \mathbf{u}, \frac{1}{2}(\mathbf{u}^2 + \xi^2), \frac{1}{2}\xi^2)^T.$$

Only the mass, momentum and total energy are conserved during particle collisions, so  $f$  and  $f^{eq}$  are said to satisfy the condition

$$\int (f^{eq} - f)\psi_\alpha d\mathbf{u}d\xi = \mathbf{S} = (0, 0, 0, s)^T, \quad \alpha = 1, 2, 3, 4. \tag{2.7}$$

From the BGK model, taking the moment of the rotational variables  $\xi^2$ , the source term  $s$  for the rotational energy can be obtained as,  $s = \rho(E_r^{eq} - E_r)/\tau$ . Here  $\tau$  is the relaxation time for rotational energy to reach equilibrium, which will be generalized in section 3 using the Landau-Teller-type model, sometimes referred to as the Jeans equation, to account for the longer relaxation time for the rotational non-equilibrium through the rotational collision number  $Z_R$ . The equilibrium energy  $\rho E_r^{eq}$  in the above equation is determined by  $T_r = T_t = T$ ,

$$\rho E_r^{eq} = \rho/\lambda^{eq} \quad \text{and} \quad \lambda^{eq} = \frac{5}{4} \frac{\rho}{\rho E - \frac{1}{2}\rho U^2}.$$

For a flow with different translational  $T_t$  and rotational  $T_r$  temperatures, the mass, momentum, total energy, and the rotational energy equations in 1D case are obtained as,

$$\begin{pmatrix} \rho \\ \rho U \\ \rho E \\ \rho E_r \end{pmatrix}_t + \begin{pmatrix} \rho U \\ \rho U^2 + p \\ (\rho E + p)U \\ \rho E_r U \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{3\rho}{5\tau} R(T_t - T_r) \end{pmatrix},$$

where  $\rho E = (1/2)\rho(U^2 + 3RT_t + 2RT_r)$  is the total energy,  $\rho E_r = \rho RT_r$  is the rotational energy. The pressure  $p$  is related to the translational temperature using the ideal gas law,  $p = \rho RT_t$ . For  $T_t = T_r$ , the above equations revert to the Euler equations for a diatomic gas.

Using the BGK model with the thermodynamic state as in Eq.(2.6) and the Chapman-Enskog expansion up to the 1st order,

$$f = f^{eq} + \text{Kn} f_1 = f^{eq} - \tau(\partial f^{eq}/\partial t + \mathbf{u} \cdot \partial f^{eq}/\partial \mathbf{x}). \quad (2.8)$$

the macroscopic Navier-Stokes continuum equations in 1D case can be derived,

$$\begin{aligned} & \begin{pmatrix} \rho \\ \rho U \\ \rho E \\ \rho E_r \end{pmatrix}_t + \begin{pmatrix} \rho U \\ \rho U^2 + p \\ (\rho E + p)U \\ \rho E_r U \end{pmatrix}_x \\ &= \begin{pmatrix} 0 \\ \frac{3}{4}\tau p U_x - \frac{2}{5}\rho R(T_t - T_r) \\ \frac{4}{3}\tau p U U_x + \tau \rho R T_t (T_r)_x + \frac{5}{2}\tau \rho R T_t (T_t)_x - \frac{2}{5}\rho R U (T_t - T_r) \\ \tau p (T_r)_x + \frac{3}{5}\rho R U (T_t - T_r) \end{pmatrix}_x + \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{3\rho}{5\tau} R(T_t - T_r) \end{pmatrix}. \end{aligned} \quad (2.9)$$

Instead of using the bulk viscosity term as in Eq.(2.5), the relaxation term is obtained in the above equations to model the non-equilibrium process. In the limiting case of small departures from equilibrium, we have

$$T_t - T_r = -\frac{2}{3}\tau T U_x,$$

and the normal bulk viscosity term can be exactly recovered, given by

$$-\frac{2}{5}\rho R(T_t - T_r) = \frac{4}{15}\tau p U_x.$$

As discussed in section 4, the assumption of small departures from equilibrium is not valid inside the shock layer, hence the above governing equations with a relaxation term are more physically meaningful. However, instead of solving the nonlinear system (2.9), the kinetic equation with the distribution function truncated to the Navier-Stokes order (2.8) will be directly used in the numerical scheme for the solution of Eq.(2.9).

From the above relaxation model, we can see that the bulk viscosity is not a physical property of a gas, but rather, an approximation designed to simulate the effect of thermal relaxation when the governing equations are cast in terms of a single temperature. This approximation is based on the assumption that the time scale of the macroscopic gas motion is much larger than the relaxation time for the rotational equilibrium. This is a good approximation only for low Knudsen number flows.

When the characteristic time for rotational relaxation is much longer than that of translational in the shock layer where the characteristic flow time is of the order of particle collision time, the Landau-Teller-Jeans model was used to account for the relaxation of rotational energy [20]. For the translation temperature below 1400K in a nitrogen gas which is of interest here, the use of a single rotational temperature and the Landau-Teller-Jeans model for rotational relaxation is assumed to be adequate in the present study. Then, the source term is defined as

$$\mathbf{S} = \left( 0, 0, 0, \frac{3\rho R}{5Z_R\tau}(T^t - T^r) \right), \quad (2.10)$$

and the value  $Z_R$  for a certain diatomic molecule depends on the temperature [19]. The rotational collision time multiplied by a rotational collision number  $Z_R$  models the relaxation process for the rotational energy to equilibrate with the translational energy. For the nitrogen gas, absorption measurements of ultrasonic sound yielded a value of  $Z_R$  equal to 5.26 [14] and 5.5 [2], while shock wave measurements using the electron-beam fluorescence technique [27] have yielded  $Z_R = 5$  at the room temperature. Determining the value of  $Z_R$  by theoretical and experimental means is an active research area [26] and is beyond the scope of the present work.

### 2.3 Generalization of constitutive relationships for translational non-equilibrium

In the past two decades, the extended hydrodynamics approach for the non-equilibrium flow consisted of the inclusion of higher-order terms resulting in the Burnett or Super-Burnett equations, or regularizing the moment equations. Currently, however, the most successful method to accurately match the experimental data for both monatomic and diatomic gases is the DSMC method. The DSMC method primarily consists of two steps,

i.e., free transport and collision within each computational cell. The determination of the transport coefficients in the DSMC method is based on the particle collision model, which is actually constructed from the well-defined theories developed for continuum flow models. The collision models of the particle cross section and the probability for each collision pair can be used for recovering the dissipative coefficients in the Navier-Stokes limit. For example, the commonly used DSMC's variable hard sphere (VHS) molecular model can be used to recover the first-order Chapman-Enskog expansion with viscosity coefficient  $\mu = \mu_{ref}(T/T_{ref})^\omega$ . This is of the Navier-Stokes order. When DSMC method is extended to highly non-equilibrium flow calculation, besides the intrinsic conservation of mass, momentum, and energy, the relation between the collision model and the viscosity coefficient adjusts itself to correspond to the physical processes occurring in the flow field through the particle transport mechanism, thereby resulting in a shock structure more accurate than that with the Navier-Stokes equations. Therefore, *the capability for the DSMC to simulate rarefied flow is due to the particle transport process, such as the duration between collisions or the control of physical collision time, instead of collision model inside each computational cell.* Traditionally, it is noted that the concepts and measurements of the dissipative coefficients are limited to the continuum flow regime. A generalized mathematical formulation of the stress and heat flux under rarefied flow conditions has not been developed so far. Similarly, when we extend the continuum models to the non-equilibrium flow in the transition and rarefied regimes, we now face the need to figure out the effect of translational non-equilibrium, such as the particle collision time, on the viscosity and heat conduction coefficients in these flow regimes. This generalization could be based on the kinetic equation that is valid for all flow regimes, and further, it is preferable to have a closed solution of the kinetic equation instead of a truncated expansion.

Our present model is based on the existence of the closed solution of the BGK model, which is assumed to be

$$f = f^{eq} - \tau_*(\partial f^{eq}/\partial t + \mathbf{u} \cdot \partial f^{eq}/\partial \mathbf{x}), \quad (2.11)$$

where  $\tau_*$  is the parameter to be determined. The difference between the above solution and the first-order Chapman-Enskog expansion (2.4) and (2.8) is that a generalized collision time  $\tau_*$  is introduced. Substituting the above equation into the BGK model (2.1), we can obtain the relation between the generalized particle collision time  $\tau_*$  and the collision time  $\tau$ , which is well-defined in the continuum flow regime,

$$\tau_* = \frac{\tau(1 - D\tau_*)}{1 + \tau(D^2 f^{eq}/D f^{eq})}, \quad (2.12)$$

where  $D = \partial/\partial t + \mathbf{u} \cdot \partial/\partial \mathbf{x}$ . To the leading order, a simplified local collision time,

$$\tau_* = \frac{\tau}{1 + \tau(D^2 f^{eq}/D f^{eq})}, \quad (2.13)$$

is used in the computation in this paper. Both Eq.(2.12) and (2.13) have been used in a monatomic shock structure calculation and no difference in the simulation results has been found. In the continuum flow regime,  $\tau D^2 f^{eq}/Df^{eq} \sim \text{Kn}$  is expected to be small and  $\tau_*$  reverts back to  $\tau$ , determined from  $\tau = \mu/p$ . The dynamic viscosity coefficient  $\mu$  can be obtained experimentally or theoretically as in Sutherland's law. In order to remove the dependence of the collision time  $\tau_*$  on the individual molecular velocity,  $D^2 f^{eq}/Df^{eq}$  can be evaluated by taking moment  $\phi$ , as  $\int \phi D^2 f^{eq} d\mathbf{u}d\xi / \int \phi Df^{eq} d\mathbf{u}d\xi$  in our numerical examples of shock structure calculations. Since the stress and heat conduction terms are resulting from the moments of the gas distribution function, different from earlier approaches [34], the value of  $\tau_*$  in the viscosity term  $\tau_* p$  and heat conduction coefficient  $\tau_* p C_p / \text{Pr}$  are obtained separately from different moments;  $\phi_1 = (u - U)^2$  for the viscosity coefficient and

$$\phi_2 = (u - U)[(u - U)^2 + \xi^2]$$

for the heat conduction coefficient. Since both  $D^2 f^{eq}$  and  $Df^{eq}$  involve higher spatial and temporal derivatives of an equilibrium gas distribution function, a nonlinear limiter is imposed on the evaluation of  $\tau_*$ ,

$$\tau_* = \frac{\tau}{1 + \max[-0.5, \tau \min((D^2 f^{eq}/Df^{eq}), 0)]}. \tag{2.14}$$

There are two ways to understand the function of the above limiter. Firstly, since there are several terms involved in  $D^2 f^{eq}/Df^{eq}$ , the numerical evaluation of the ratio will be sensitive to the numerical error and large fluctuations will be generated, especially close to the upstream and downstream region, where both 1st and 2nd derivatives both tend to vanish. Secondly, the linear relation between stress and strain and Fourier is physically correct for the small distortion of fluid element or temperature gradients. As the strain and temperature gradients become large, the linear relationship will need to be adjusted dynamically. The dynamic limiter not only guarantees the positivity of the particle collision time, but also imposes  $\tau_* \geq \tau$  everywhere. This generalization and the use of the dynamical limiter is important to pass the test of Elliott [11] that the physical stress ( $\sim \tau_*$ ) inside the shock layer should be larger than the stress ( $\sim \tau$ ) defined in the Navier-Stokes equation. Since the Navier-Stokes relations are not globally valid even in the weakest of shock waves [11], the above limited particle collision time presents a novel methodology to develop nonlinear constitutive relations. One of the reasons for the success of modern shock capturing scheme for the discontinuous solutions is the introduction of the nonlinear limiter on the spatial gradients. Analogously, we introduce a dynamic limiter here for the stress and Fourier terms. The above generalization of the viscosity and heat conduction coefficients to the rarefied regime is through kinetic equation and its solution is supplied to the macroscopic flow evolution equations. Numerically, for the shock structure calculations in this paper, the limiters will take place occasionally close to the upstream and downstream regions. Most time, the limiter is not in action in the interesting non-equilibrium part of the flow. Philosophically, this is a good example for the multi-scale methodology, which has been studied extensively recently [10].

### 3 Finite volume gas-kinetic method

The continuum model developed in the previous section is solved based on the gas-kinetic BGK scheme [33]. It is a conservative finite volume method, and the numerical fluxes at cell interfaces are evaluated based on the time-dependent gas distribution function,

$$f = f^{eq} - \tau_* (\partial f^{eq} / \partial t + \mathbf{u} \cdot \partial f^{eq} / \partial \mathbf{x}) + t \frac{\partial f^{eq}}{\partial t}. \quad (3.1)$$

The relation between  $\tau_*$  and  $\tau$  is given in Eq.(2.13), where  $\tau = \mu/p$  and  $\mu$  is given by the Sutherland's law.

In 1D case, for a diatomic gas the equilibrium state  $f^{eq}$  with translational and rotational temperature is

$$f^{eq} = \rho \left(\frac{\lambda_t}{\pi}\right)^{3/2} \left(\frac{\lambda_r}{\pi}\right) \exp(-\lambda_t(\mathbf{u} - \mathbf{U})^2 - \lambda_r \xi^2). \quad (3.2)$$

The expansion  $\partial f^{eq} / \partial x$  can be expressed as

$$\frac{\partial f^{eq}}{\partial x} = (a_1 + a_2 \mathbf{u} + a_3 \mathbf{u}^2 + a_4 \xi^2) f^{eq} = a f^{eq}.$$

Here, all the coefficients can be explicitly determined by relating the microscopic and macroscopic variables at the cell interface, i.e.,  $W = \int \psi f^{eq} d\mathbf{u} d\xi$  and  $\partial \mathbf{W} / \partial x = \int \psi a f^{eq} d\mathbf{u} d\xi$ , where  $\mathbf{W} = (\rho, \rho U, \rho E, \rho E_r)^T$  are the macroscopic flow variables. The temporal variation of  $\partial f^{eq} / \partial t$  can be expanded similarly as a spatial expansion and the corresponding coefficients can be obtained from the compatibility condition for the Chapman-Enskog expansion, i.e.,

$$\int \psi (\partial f^{eq} / \partial t + \mathbf{u} \cdot \partial f^{eq} / \partial \mathbf{x}) d\Xi = 0.$$

The numerical method developed for Eq.(2.9) is a finite volume method,

$$\mathbf{W}_j^{n+1} = \mathbf{W}_j^n + \frac{1}{\Delta x} \int_0^{\Delta t} (\mathbf{F}_{j-1/2}(t) - \mathbf{F}_{j+1/2}(t)) dt + \mathbf{S}_j^n \Delta t, \quad (3.3)$$

where  $\mathbf{W}_j^n$  is the cell averaged mass, momentum, total energy, and rotational energy, and  $\mathbf{F}_{j+1/2}$  are the corresponding fluxes at a cell interface, evaluated using the solution (3.1),

$$F = \int \mathbf{u} \psi f d\mathbf{u} d\xi.$$

Note that  $\Delta t$  is the time step  $\Delta t = t^{n+1} - t^n$ , and  $\mathbf{S}_j^n$  is the source term for the rotational energy, given in Eq.(2.10). For a monatomic gas, a similar scheme based on the distribution function without the rotational degrees of freedom can be constructed as well. In this case, the source term in Eq.(2.10) is zero. For a diatomic gas, the main difference between the current non-equilibrium kinetic method, the so-called extended NS solver, and the

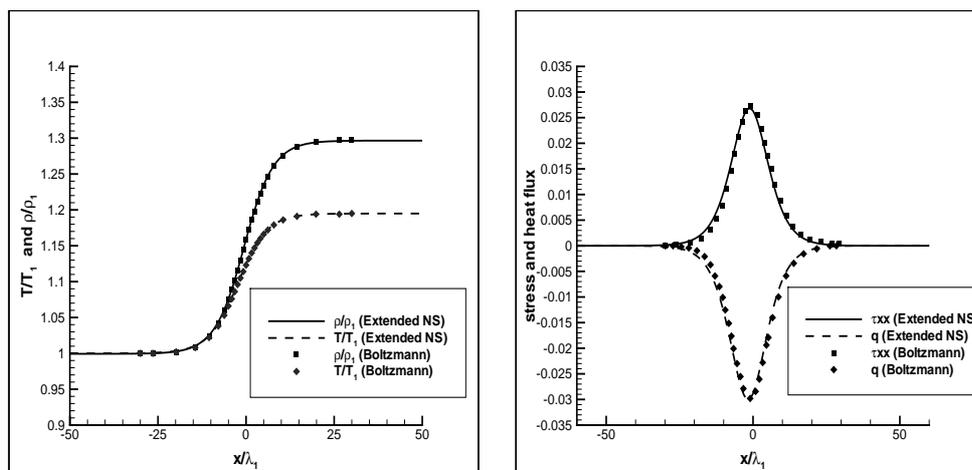


Figure 1:  $M = 1.2$  argon shock structure for hard sphere gas. Boltzmann solution [24] vs. extended continuum model.

equilibrium BGK-NS method in [33] is that two temperatures  $T_t$  and  $T_r$  are used with a generalized particle collision time  $\tau_*$  in the current non-equilibrium kinetic method.

In order to simulate the flow with a realistic Prandtl number, a modification of the heat flux in the energy transport, such as that used in [33], is also implemented in the present study.

## 4 Non-equilibrium shock structure

One of the simplest and most fundamental 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. Firstly, the shock wave represents a flow condition that is far from thermodynamic equilibrium, and secondly shock wave phenomena is unique in that it allows one to separate the continuum 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.

To illustrate the performance of the generalized continuum formulation, henceforth known as the extended NS method, we present some results in the shock structures from the continuum cases to highly non-equilibrium cases. Besides the mass density and temperature distributions, the stress and heat flux will also be presented in some cases. The solutions based on the new formulation are compared for both monatomic and diatomic gases, where applicable, with the exact solution of the Boltzmann equation [24], DSMC results [6], and experimental measurements [1,27].

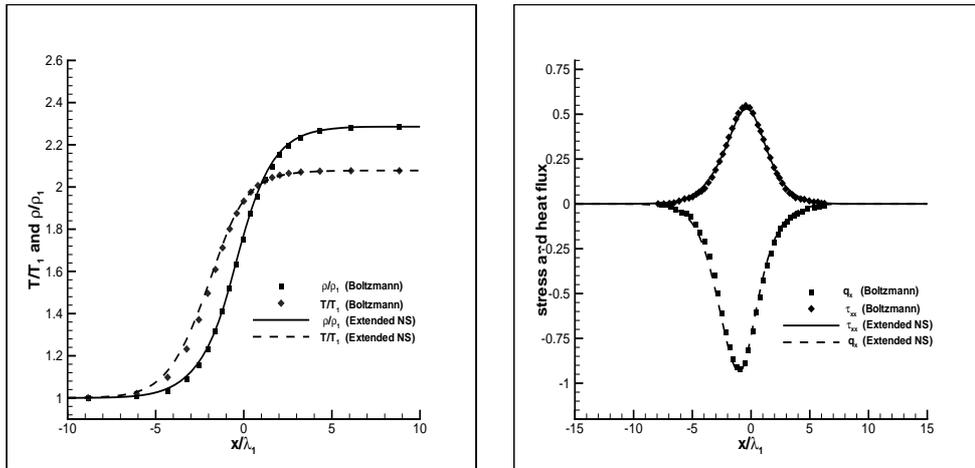


Figure 2:  $M = 2.0$  argon shock structure for hard sphere gas. Boltzmann solution [24] vs. extended continuum model.

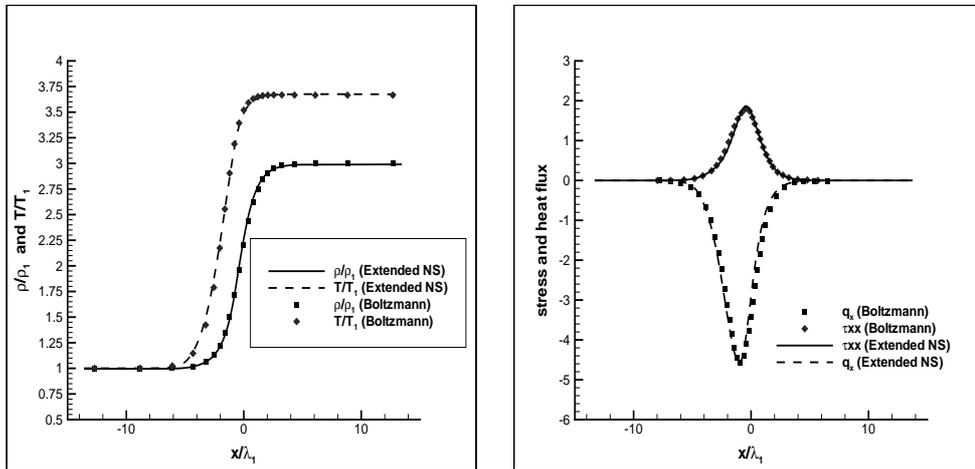


Figure 3:  $M = 3.0$  argon shock structure for hard sphere gas. Boltzmann solution [24] vs. extended continuum model.

### 4.1 Shock structure in monatomic gas

First we present test cases on the shock structure for a monatomic gas with the nonequilibrium limited to the translational energy mode. Comparisons of our results are made with DSMC solutions and the theoretical solution of the full Boltzmann equation obtained by Ohwada for the hard sphere molecules up to Mach number 3 [24]. For the hard sphere molecules, the viscosity coefficient  $\tau \sim \mu \sim T^{0.5}$ , where the 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. Figs. 1-3 show the density, temperature, stress and heat flux of an argon shock structure for Mach numbers 1.2, 2.0, and 3. Comparisons of the current extended continuum model

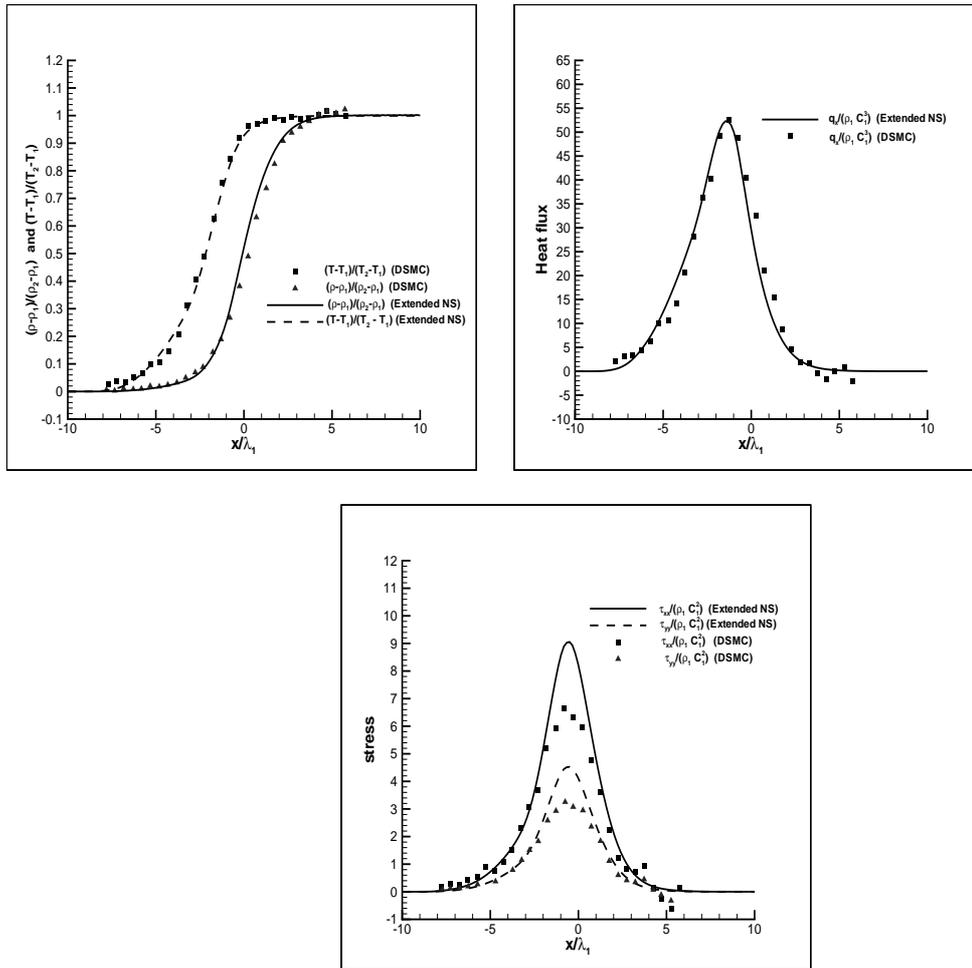


Figure 4:  $M = 8$  argon shock structure for  $\mu \sim T^{0.68}$  gas. DSMC solution [6] vs. extended continuum model.

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 extended continuum method have good agreement. It is noteworthy that the predicted stress from the discretized particle velocity Boltzmann solver of Beylich [5] (not shown in the figures) does not have as good of a match with the Boltzmann solution. At Mach number 1.2, where the local Knudsen numbers are less than 0.02, as expected, the standard Navier-Stokes equations suffice.

For the Mach 8 argon shock structure, Bird's [6] DSMC method using an inverse 11<sup>th</sup> power repulsive potential,  $\mu \sim T^{0.68}$ , gave a good agreement with the experimental profile of Schmidt [28]. Fig. 4 shows the solution of temperature, density, heat flux, and stresses from the current extended continuum model compared with Bird's DSMC solutions. For this Mach 8 case, the shock thickness and the separation distance between the density and

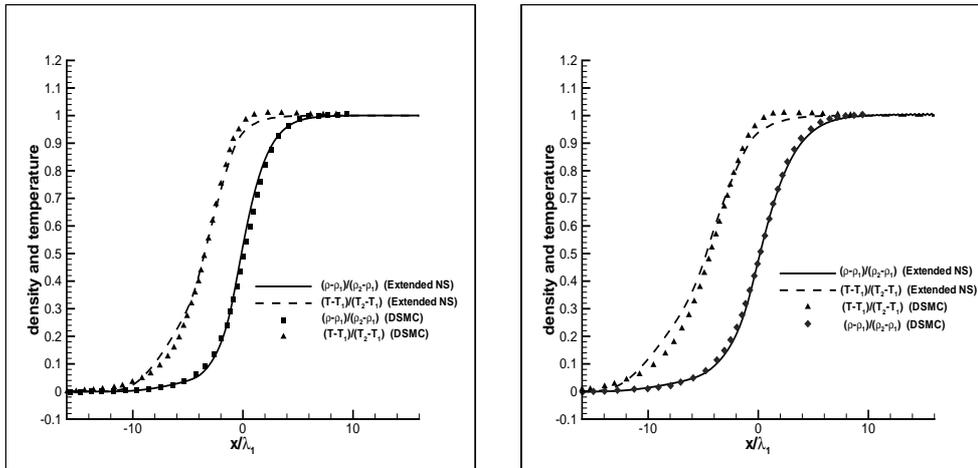


Figure 5:  $M = 8$  argon shock structure for  $\mu \sim T^{0.75}$  and  $\sim T^{0.81}$  gas. DSMC solution [7] vs. extended continuum model.

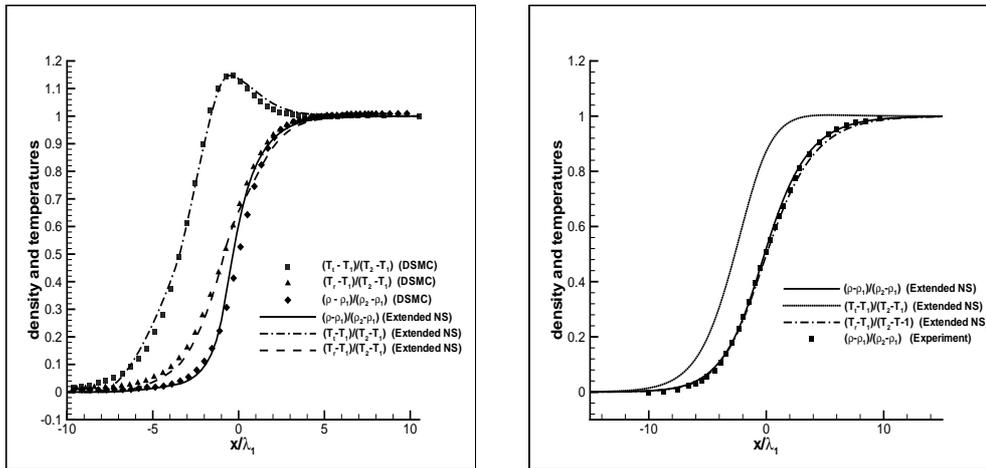


Figure 6:  $M = 11$  nitrogen shock structure. DSMC solution vs. extended continuum model.

Figure 7:  $M = 1.53$  nitrogen shock structure. Experiment measurements [1] vs. extended continuum model.

temperature profiles by the current model compare well with those of DSMC's. The peak values of the stress profile by the DSMC method are lower than the current Extended NS solutions. The reason for this needs further investigation. For the same case, the direct BGK solver with discretized particle velocity space [18] (not shown in the figures) predicts a wider separation ( $\sim 4\lambda_1$ ) between the density and temperature.

Fig. 5 shows the shock structures for other viscosity coefficients of  $\mu \sim T^{0.75}$  and  $T^{0.81}$ , where the solution by the current continuum model and that of DSMC [7] have good agreement as well. For the  $\mu \sim T^{0.81}$  case, the current calculation gives the separation

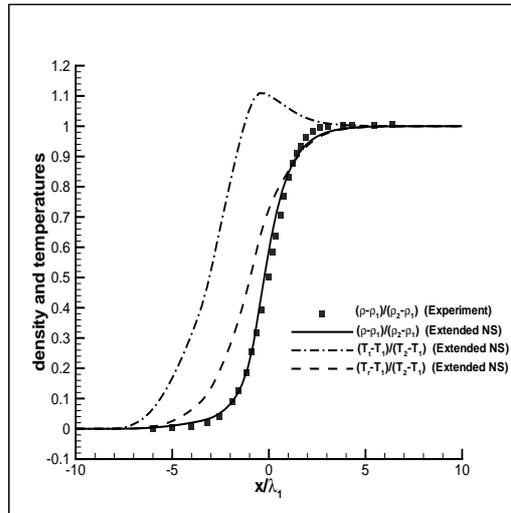


Figure 8:  $M = 6.1$  nitrogen shock structure. Experiment measurements [1] vs. extended continuum model.

between the density and temperature of about  $4.5\lambda_1$ , whereas the discrete velocity BGK model in [22] (not shown in the figures) has the separation around  $2.7\lambda_1$ ; there is deviation in the temperature profiles as well. In the current approach,  $\tau_*$  is from different moments ( $\phi$ ) in the viscous and heat conduction fluxes. In an earlier work [34], the same  $\phi$  was used. It is noted that although the earlier work captures the density and temperature profiles accurately inside the shock layer, the separation distance between the density and temperature is smaller than the current one.

#### 4.2 Shock structure in diatomic gas

The proper value of  $\tau_*$  can accurately capture the translational non-equilibrium, so one can obtain the density and temperature profiles inside a shock layer. For diatomic gases, besides the translational relaxation, the rotational relaxation is included as well. The relaxation time between the rotational and translation energy exchange is determined by the rotational collision number  $Z_R$ . For the nitrogen shock wave, the DSMC method is known to provide accurate separation distance between the translational and rotational temperature profiles. With the same parameters as used in the DSMC computation [1] and using the Sutherland’s law for viscosity, the shock structure for nitrogen gas at Mach number 11 was simulated by the current method and the results are shown in Fig. 6. The current extended NS continuum model reproduced the DSMC solution very accurately.

Figs. 7 and 8 show comparisons of present computations (using  $Z_R = 3.5$ ) and experimental data [1] for nitrogen gas at Mach numbers 1.53 and 6.1. Fig. 9 shows the shock profiles at higher Mach numbers 7 and 12.9 [27]. Since the incoming gas in the experiment had a temperature as low as 15K, a small value of  $Z_R = 1.5$  is used in the

current computations. The measured rotational temperature and density are predicted by the continuum model very well. As realized by many authors [31], Fig. 9 is a tough test case even for the DSMC method. The results from the preceding test cases show that the current continuum model can be used for a non-equilibrium shock wave simulation if a gas kinetic theory can be used to properly generalize the viscosity and heat conduction coefficients.

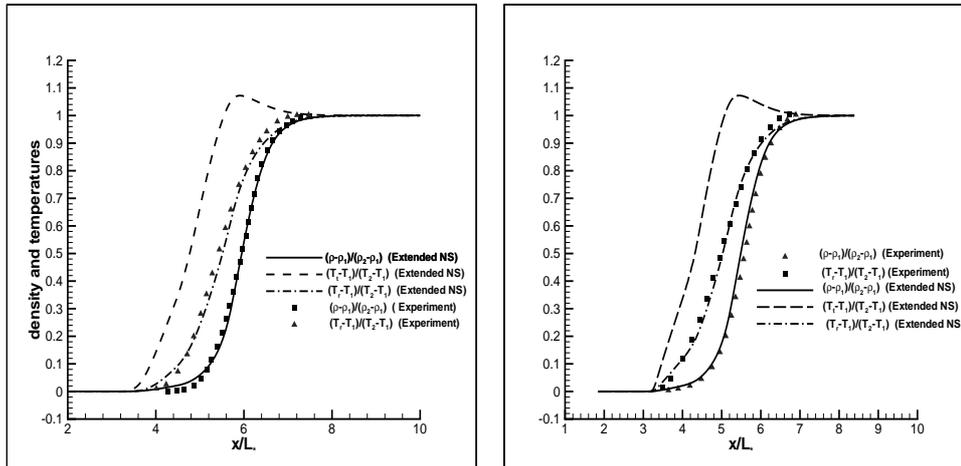


Figure 9:  $M = 7$  and  $12.9$  nitrogen shock structure. Experiment measurement [27] vs. extended continuum model.

## 5 Conclusion

In this paper, a continuum gas-kinetic formulation for the translational and rotational non-equilibrium flow is constructed. Based on the generalized constitutive relationships through the modification of particle collision time, the kinetic formulation truncated up to the Navier-Stokes order has been used in the shock structure computations. The new formulation is applied to both monatomic and diatomic shock structure calculations, i.e., argon and nitrogen gases, from a low Mach number 1.2 up to a strong shock wave with  $M = 12.5$ . The extensive tests using the current continuum formulation and the comparisons with DSMC solutions, Boltzmann solutions, and experimental measurements provide confidence that besides the DSMC method, the kinetic method provides another effective tool for the study of flow motion in the rarefied flow regime. The study shows that it can be possible to use a continuum model, particularly in the near-continuum flow regime, where the DSMC method can be very expensive. Theoretically, the DSMC method is an operator splitting steps of free particle transport and collision. It requires that the numerical time step is smaller than the particle collision time, which cannot be tolerated in the continuum regime, especially for high Reynolds number flow. However, the current method can accurately and efficiently simulate the continuum flow at  $\text{Kn} \ll 1$  as well.

The future of this method depends on its successful applications in multidimensional flow problems.

### Acknowledgments

The work described in this paper was substantially supported by grants from the Research Grants Council of the Hong Kong Special Administrative region, China (Project No. HKUST6102/04E, 621005), and by U.S. Air Force Office of Scientific Research contracts monitored by F. Fahroo and J. Schmisser.

### Appendix: Connection between BGK, Navier Stokes and Euler equations for equilibrium polyatomic gases

The derivation of the Navier-Stokes equations from the Boltzmann equation can be found in Kogan [17], Chapman and Cowling [9], and from the Bhatnagar-Gross-Krook equation in Vincenti and Kruger [30] for the case of perfect monotonic gases. Here we reconsider the derivation of the Navier-Stokes and Euler equations from the BGK equation, i.e.,  $f_t + u_i f_{x_i} = (g - f)/\tau$  with equilibrium state  $g$ , right from the outset for polyatomic gases.

To derive the Navier-Stokes equations, let  $\tau = \epsilon \hat{\tau}$  where  $\epsilon$  is a small dimensionless quantity, and suppose that  $g$  has a Taylor series expansion about some point  $x_i, t$ . Since  $\tau$  depends on the local thermodynamic variables, and since these depend on the moments of  $g$ , we may assume that  $\tau$  and consequently  $\hat{\tau}$  can be expanded about the point  $x_i, t$ . Now consider the formal solution of the BGK equation for  $f$ , supposing that  $g$  is known, and suppose that  $t \gg \tau$ ; i.e. that the initial condition were imposed many relaxation times ago. We can then ignore the initial value of  $f$ , and, with negligible error, the difference between  $t' = 0$  and  $t' = -\infty$  in the integral solution of the BGK model. It can be shown from the integral solution that the Taylor series expansion of  $\tau$  and  $g$  about  $x_i, t$  may be written as power series in  $\epsilon$ , and therefore  $f$  has an expansion in powers of  $\epsilon$ . We can find the terms in this expansion from the formal solution for  $f$ , or, more easily, by putting

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \dots$$

and  $\tau = \epsilon \hat{\tau}$  into the BGK equation directly. Let

$$D_{\mathbf{u}} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i},$$

and write the BGK equation as  $\epsilon \hat{\tau} D_{\mathbf{u}} f + f - g = 0$ . An expansion of this equation in powers of  $\epsilon$  yields

$$f = g - \epsilon \hat{\tau} D_{\mathbf{u}} g + \epsilon^2 \hat{\tau} D_{\mathbf{u}} (\hat{\tau} D_{\mathbf{u}} g) + \dots,$$

and the compatibility condition, after dividing by  $\epsilon \hat{\tau}$ , gives

$$\int \psi_{\alpha} D_{\mathbf{u}} g d\Xi = \epsilon \int \psi_{\alpha} D_{\mathbf{u}} (\hat{\tau} D_{\mathbf{u}} g) d\Xi + \mathcal{O}(\epsilon^2). \tag{A.1}$$

We define  $\mathcal{L}_\alpha$  to be the integral on the left side of this equation, and  $\mathcal{R}_\alpha$  to be the integral on the right, so that Eq.(A.1) can be written as

$$\mathcal{L}_\alpha = \epsilon \mathcal{R}_\alpha + \mathcal{O}(\epsilon^2). \tag{A.2}$$

We show that these equations give the Euler equations if we drop the term of  $\mathcal{O}(\epsilon)$ , and the Navier-Stokes equations if we drop terms of  $\mathcal{O}(\epsilon^2)$ . To simplify the notation, let

$$\langle \psi_\alpha(\dots) \rangle \equiv \int \psi_\alpha(\dots) g d\Xi,$$

and consider

$$\begin{aligned} \mathcal{L}_\alpha &\equiv \int \psi_\alpha D_{\mathbf{u}} g d\Xi = \int \psi_\alpha (g_{,t} + u_l g_{,l}) d\Xi \\ &= \langle \psi_\alpha \rangle_{,t} + \langle \psi_\alpha u_l \rangle_{,l}, \end{aligned}$$

since  $\psi_\alpha$  is independent of  $x_i$  and  $t$ . Now Eq.(A.2) shows that

$$\langle \psi_\alpha \rangle_{,t} + \langle \psi_\alpha u_l \rangle_{,l} = \mathcal{O}(\epsilon) \tag{A.3}$$

for all  $\alpha$ , and therefore, in reducing  $\mathcal{R}_\alpha$  on the right side of Eq.(A.2), which is already  $\mathcal{O}(\epsilon)$ , we can drop  $\mathcal{O}(\epsilon)$  quantities and their derivatives. Put differently, we first reduce the  $\mathcal{L}_\alpha$  to find that  $\mathcal{L}_\alpha = 0$  ( $\alpha = 1, \dots, 5$ ) is identical to the Euler equations; then we use the fact that  $\mathcal{L}_\alpha$  is  $\mathcal{O}(\epsilon)$  to simplify  $\mathcal{R}_\alpha$  — the result is the Navier-Stokes equations.

The expression for  $\mathcal{R}_\alpha$  contains time derivatives which must be eliminated. We have, from the definition of  $\mathcal{R}_\alpha$ ,

$$\begin{aligned} \mathcal{R}_\alpha &= \hat{\tau} [\langle \psi_\alpha \rangle_{,tt} + 2 \langle \psi_\alpha u_k \rangle_{,tk} + \langle \psi_\alpha u_k u_l \rangle_{,lk}] \\ &\quad + \hat{\tau}_{,t} [\langle \psi_\alpha \rangle_{,t} + \langle \psi_\alpha u_l \rangle_{,l}] + \hat{\tau}_{,k} [\langle \psi_\alpha u_k \rangle_{,t} + \langle \psi_\alpha u_k u_l \rangle_{,l}]. \end{aligned} \tag{A.4}$$

According to Eq.(A.3) the coefficient of  $\hat{\tau}_{,t}$  in this expression is  $\mathcal{O}(\epsilon)$ , and can therefore be neglected. As for the first term, consider

$$\begin{aligned} &\frac{\partial}{\partial t} [\langle \psi_\alpha \rangle_{,t} + \langle \psi_\alpha u_k \rangle_{,k}] \\ &= \langle \psi_\alpha \rangle_{,tt} + \langle \psi_\alpha u_k \rangle_{,kt} = \mathcal{L}_{\alpha,t} = \mathcal{O}(\epsilon). \end{aligned}$$

Then the first term in Eq.(A.4) is

$$\hat{\tau} \frac{\partial}{\partial x_k} [\langle \psi_\alpha u_k \rangle_{,t} + \langle \psi_\alpha u_k u_l \rangle_{,l}] + \mathcal{O}(\epsilon),$$

which can be combined with the third term to give

$$\mathcal{R}_\alpha = \frac{\partial}{\partial x_k} \{ \hat{\tau} [\langle \psi_\alpha u_k \rangle_{,t} + \langle \psi_\alpha u_k u_l \rangle_{,l}] \} + \mathcal{O}(\epsilon).$$

This eliminates the second time derivatives from  $\mathcal{R}_\alpha$ ; the first time derivatives will be removed by using  $\mathcal{L}_\alpha \simeq 0$ .

The Euler equations follow from putting  $\mathcal{L}_\alpha = 0$ . To see this, consider

$$\mathcal{L}_1 = \langle \psi_1 \rangle_{,t} + \langle \psi_1 u_k \rangle_{,k} = \rho_{,t} + (\rho U_k)_{,k},$$

since  $\psi_1 = 1$ ;  $\mathcal{L}_1 = \mathcal{O}(\epsilon)$  is the continuity equation if we neglect  $\mathcal{O}(\epsilon)$ . For  $\alpha = 2, 3, 4$ , it is convenient to define  $\mathcal{L}_i$  and  $\mathcal{R}_i$  such that  $i = \alpha - 1$  and to let  $w_i = u_i - U_i$ . Then

$$\mathcal{L}_i = \langle u_i \rangle_{,t} + \langle u_i u_k \rangle_{,k} = (\rho U_i)_{,t} + [\rho U_i U_k + \langle w_i w_k \rangle]_{,k},$$

since all moments of  $g$  odd in  $w_l$  vanish. The pressure tensor is defined by

$$p_{ik} = \langle w_i w_k \rangle \equiv p \delta_{ik}.$$

(The diagonal form of  $p_{ik}$  is obvious from the fact that  $g$  can be written as a function of  $w_k^2$ ). Then

$$\mathcal{L}_i = (\rho U_i)_{,t} + (\rho U_i U_k + p \delta_{ik})_{,k}, \tag{A.5}$$

and  $\mathcal{L}_i = 0$  is the Euler equation for the conservation of momentum. For the energy equation we have

$$\mathcal{L}_5 = \frac{1}{2} \langle u_n^2 + \xi^2 \rangle_{,t} + \frac{1}{2} \langle u_l (u_n^2 + \xi^2) \rangle_{,l}$$

or

$$\mathcal{L}_5 = \left( \frac{1}{2} \rho U_n^2 + \frac{K+3}{2} p \right)_{,t} + \left( \frac{1}{2} \rho U_k U_n^2 + \frac{K+5}{2} p U_k \right)_{,k}.$$

Setting  $\mathcal{L}_5 = 0$  gives the energy equation in the absence of dissipation.

We proceed to eliminate the time derivatives from  $\mathcal{R}_\alpha$  using the fact that  $\mathcal{L}_\alpha = \mathcal{O}(\epsilon)$ . For  $\alpha = 1$ , we have

$$\mathcal{R}_1 = \{ \hat{\tau} [ \langle u_k \rangle_{,t} + \langle u_k u_l \rangle_{,l} ] \}_{,k}.$$

The quantity in square brackets is  $\mathcal{L}_k$ , which implies that  $\mathcal{R}_1 = \mathcal{O}(\epsilon)$ , and  $\mathcal{L}_1 = \epsilon \mathcal{R}_1 = \mathcal{O}(\epsilon^2)$ . Hence, to the order we have retained,  $\mathcal{R}_1 = 0$  and  $\mathcal{L}_1 = 0$ , or

$$\rho_{,t} + (\rho U_k)_{,k} = 0, \tag{A.6}$$

which is the continuity equation. We can use the continuity equation to simplify the momentum equations and the energy equation. Multiplying the continuity equation by  $U_i$  and subtracting the result from  $\mathcal{L}_i$  gives, according to Eq.(A.5),

$$\mathcal{L}_i = \rho U_{i,t} + \rho U_k U_{i,k} + p_{,i} + \mathcal{O}(\epsilon^2). \tag{A.7}$$

For  $\mathcal{L}_5$ , we group the terms as follows:

$$\begin{aligned} \mathcal{L}_5 &= \frac{1}{2} U_n^2 [\rho_{,t} + (\rho U_k)_{,k}] + \rho U_n U_{n,t} + \rho U_k U_n U_{n,k} + U_k p_{,k} \\ &+ \frac{K+3}{2} [p_{,t} + U_k p_{,k}] + \frac{K+5}{2} p U_{k,k}. \end{aligned}$$

The first term is  $\frac{1}{2}U_n^2\mathcal{L}_1$  which is  $\mathcal{O}(\epsilon^2)$ , and the next three are  $U_n\mathcal{L}_n$ , and are therefore  $\mathcal{O}(\epsilon)$ . Then

$$\mathcal{L}_5 = \frac{K+3}{2}[p_{,t} + U_k p_{,k}] + \frac{K+5}{2}pU_{k,k} + U_n\mathcal{L}_n. \tag{A.8}$$

We can drop the last term in the reduction of  $\mathcal{R}_\alpha$ , but the term  $U_n\mathcal{L}_n$  must be retained in the reduction of  $\mathcal{L}_5$  when we finally write  $\mathcal{L}_5 = \epsilon\mathcal{R}_5$  in detail. For the right sides of the momentum equations, consider  $\mathcal{R}_j = (\hat{\tau}F_{jk})_{,k}$ , where

$$F_{jk} \equiv \langle u_j u_k \rangle_{,t} + \langle u_j u_k u_l \rangle_{,l}$$

or

$$F_{jk} = U_j[(\rho U_k)_{,t} + (\rho U_k U_l + p\delta_{kl})_{,l}] + \rho U_k U_{j,t} + (\rho U_k U_l + p\delta_{kl})U_{j,l} + (p\delta_{jk})_{,t} + (U_l p\delta_{jk} + U_k p\delta_{jl})_{,l},$$

using the fact that all moments odd in  $w_k$  vanish. The term in square brackets multiplying  $U_j$  is  $\mathcal{L}_k$ , *i.e.* it is  $\mathcal{O}(\epsilon)$ , and can therefore be ignored. Then, after gathering terms with coefficients  $U_k$  and  $p$ , we have

$$F_{jk} = U_k[\rho U_{j,t} + \rho U_l U_{j,l} + p_{,j}] + p[U_{k,j} + U_{j,k} + U_{l,l}\delta_{jk}] + \delta_{jk}[p_{,t} + U_l p_{,l}].$$

The coefficient of  $U_k$  is  $\mathcal{L}_j$ , according to Eq.(A.7), and can therefore be neglected. To eliminate  $p_{,t}$  from the last term we use the Eq.(A.8) for  $\mathcal{L}_5$ ; this gives

$$p_{,t} + U_k p_{,k} = -\frac{K+5}{K+3}pU_{k,k} + \mathcal{O}(\epsilon).$$

Finally, we decompose the tensor  $U_{k,j}$  into its dilation and shear parts in the usual way, which gives

$$F_{jk} = p \left[ U_{k,j} + U_{j,k} - \frac{2}{3}U_{l,l}\delta_{jk} \right] + \frac{2}{3} \left( \frac{K}{K+3} \right) pU_{l,l}\delta_{jk}. \tag{A.9}$$

The last term is due to bulk viscosity; it vanishes, as it should, for  $K = 0$ , since the physical mechanism for bulk viscosity involves energy sharing between translational and internal degrees of freedom of the molecules, and  $K = 0$  corresponds to a monatomic ( $\gamma = \frac{5}{3}$ ) gas.

For  $\alpha = 5$ , we write

$$\mathcal{R}_5 = (\hat{\tau}N_k)_{,k}, \tag{A.10}$$

where

$$N_k \equiv \langle u_k \frac{(u_n^2 + \xi^2)}{2} \rangle_{,t} + \langle u_k u_l \frac{(u_n^2 + \xi^2)}{2} \rangle_{,l}.$$

This can be written as  $N_k = N_k^{(1)} + N_k^{(2)}$ , where

$$N_k^{(1)} = \left[ U_k \frac{\langle u_n^2 + \xi^2 \rangle}{2} \right]_{,t} + \left[ U_k \langle u_l \frac{(u_n^2 + \xi^2)}{2} \rangle \right]_{,l},$$

$$N_k^{(2)} = \langle w_k \frac{u_n^2 + \xi^2}{2} \rangle_{,t} + \langle w_k u_l \frac{(u_n^2 + \xi^2)}{2} \rangle_{,l}$$

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

$$N_k^{(1)} = U_k \left[ \frac{\langle u_n^2 + \xi^2 \rangle_{,t}}{2} + \frac{\langle u_l(u_n^2 + \xi^2) \rangle_{,l}}{2} \right] + \left[ \frac{1}{2}\rho U_n^2 + \frac{K+3}{2}p \right] U_{k,t} + \frac{1}{2}\rho U_l \left[ U_n^2 + \frac{(K+5)p}{\rho} \right] U_{k,l}.$$

The coefficient of  $U_k$  in the equation above is  $\mathcal{L}_5$ , and can therefore be neglected, and the remaining terms can be rewritten as

$$\left[ \frac{1}{2}\rho U_n^2 + \frac{K+3}{2}p \right] [U_{k,t} + U_l U_{k,l}] + p U_l U_{k,l},$$

or, using the fact that  $\mathcal{L}_k = \mathcal{O}(\epsilon)$ , as

$$N_k^{(1)} = - \left[ \frac{1}{2}U_n^2 + \frac{K+3}{2}\frac{p}{\rho} \right] p_{,k} + p U_l U_{k,l}.$$

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

$$N_k^{(2)} = \langle U_n w_n w_k \rangle_{,t} + \langle U_l U_n w_n w_k \rangle_{,l} + \frac{1}{2}\langle U_n^2 w_k w_l \rangle_{,l} + \frac{1}{2}\langle w_k w_l (w_n^2 + \xi^2) \rangle_{,l},$$

or

$$N_k^{(2)} = (p U_k)_{,t} + (p U_k U_l)_{,l} + \frac{1}{2}(U_n^2 p)_{,k} + \frac{K+5}{2} \left( \frac{p^2}{\rho} \right)_{,k}.$$

This result can be rewritten as

$$N_k^{(2)} = p[U_{k,t} + U_l U_{k,l} + U_k U_{l,l} + U_l U_{l,k}] + U_k(p_{,t} + U_l p_{,l}) + \frac{1}{2}U_l^2 p_{,k} + \frac{K+5}{2} \left( \frac{p^2}{\rho} \right)_{,k},$$

and the time derivatives can be removed by using  $\mathcal{L}_k = \mathcal{O}(\epsilon)$ , and  $\mathcal{L}_5 = \mathcal{O}(\epsilon)$ , neglecting  $\mathcal{O}(\epsilon)$ , since we are evaluating  $\mathcal{R}_5$ . Finally,  $N_k^{(1)} + N_k^{(2)}$  can be combined to yield (after some algebra)

$$N_k = \frac{K+5}{2}p \left( \frac{p}{\rho} \right)_{,k} + p \left[ -\frac{2}{K+3}U_k U_{l,l} + U_l(U_{k,l} + U_{l,k}) \right]. \tag{A.11}$$

All time derivatives have now been removed from  $\mathcal{R}_\alpha$  (for all  $\alpha$ ). The remaining steps in the derivation of the Navier-Stokes equations may be summarized briefly as follows:

- 1). Drop  $\mathcal{O}(\epsilon^2)$  in Eq.(A.2).

- 2). Combine  $\epsilon$  and  $\hat{\tau}$  to recover  $\tau = \epsilon\hat{\tau}$ .
- 3). Define the stress tensor

$$\sigma'_{jk} = \eta \left[ U_{j,k} + U_{k,j} - \frac{2}{3} U_{l,l} \delta_{jk} \right] + \varsigma U_{l,l} \delta_{jk},$$

where

$$\eta = \tau p, \quad \varsigma = \frac{2}{3} \frac{K}{K+3} \tau p$$

are the dynamic viscosity and second viscosity coefficients respectively.

- 4). From Eq.(A.7) for  $\mathcal{L}_j$  and Eq.(A.9) for  $F_{jk}$ , it follows that  $\mathcal{L}_j = \epsilon\mathcal{R}_j$  may now be written as

$$\rho U_{j,t} + \rho U_k U_{j,k} + p_{,j} = \sigma'_{jk,k},$$

which is the Navier-Stokes equation.

- 5.) The energy equation follows from  $\mathcal{L}_5 = \epsilon\mathcal{R}_5$  by using Eq.(A.8), (A.7) and (A.6) to write  $\mathcal{L}_5$  in detail, and using Eq.(A.10) and (A.11) for  $\mathcal{R}_5$ . The result is

$$\frac{K+3}{2} (p_{,t} + U_k p_{,k}) - \frac{K+5}{2} p (\rho_{,t} + U_k \rho_{,k}) = (\kappa T_{,k})_{,k} + (U_l \sigma'_{lk})_{,k},$$

where

$$\kappa = \frac{K+5}{2} \frac{k}{m} \tau p$$

is the thermal conductivity,  $k$  is the Boltzmann constant,  $m$  is the mass of a molecule and  $T$  is the temperature. The equations can be written in terms of  $\gamma$  instead of  $K$  by using  $K = (5 - 3\gamma)/(\gamma - 1)$  for 3-dimensional gas flow.

## References

- [1] H. Alsmeyer, Density profiles in argon and nitrogen shock waves measured by the absorption of an electron beam, *J. Fluid Mech.*, 74 (1976), p. 497.
- [2] W. H. Andersen and D. F. Horning, The structure of shock fronts in various gases, *Mol. Phys.*, 2 (1959), p. 49.
- [3] V. V. Aristov, *Direct Methods for Solving the Boltzmann Equation and Study of Nonequilibrium Flows*, Kluwer Academic Publisher, 2001.
- [4] R. Balakrishnan, R. K. Agarwal and K. Y. Yun, BGK-Burnett equations for flows in the continuum-transition regime, *J. Thermophys. Heat Tr.*, 13 (1999), 397–410.
- [5] A. E. Beylich, Solving the kinetic equation for all Knudsen numbers, *Phys. Fluids*, 12(2) (2000), 444–465.
- [6] G. A. Bird, Aspects of the structure of strong shock waves, *Phys. Fluids*, 13 (1970), 1172–1177.
- [7] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford Science Publications, 1994.
- [8] A. V. Bobylev, The Chapman-Enskog and Grad methods for solving the Boltzmann equation, *Sov. Phys. Dokl.*, 27 (1982), p. 29.

- [9] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-uniform Gases*, Cambridge University Press, 1990.
- [10] W. N. E and B. Engquist, Multiscale modeling and computation, *Notices AMS*, 50(9) (2003), 1062–1070, 2003.
- [11] J. P. Elliott, On the validity of the Navier-Stokes relation in a shock wave, *Can. J. Phys.*, 53 (1975), 583–586.
- [12] M. Gad-el Hak, The fluid mechanics of microdevices, *J. Fluids Eng.*, 121 (1999), p. 5.
- [13] H. Grad, On the kinetic theory of rarefied gases, *Commun. Pure Appl. Math.*, 2 (1949), 331–407.
- [14] M. Greenspan, Rotational relaxation in nitrogen, oxygen, and air, *J. Acoust. Soc. Am.*, 31 (1959), 155–160.
- [15] M. S. Ivanov and S. F. Gimelshein, Computational hypersonic rarefied flows, *Annu. Rev. Fluid Mech.*, 30 (1998), 469–505.
- [16] S. Jin, L. Pareschi and M. Slemrod, A relaxation scheme for solving the Boltzmann equation based on the Chapman-Enskog expansion, *Acta Math. Appl. Sin. (Eng. Ser.)*, 18 (2002), p. 37.
- [17] M. N. Kogan, *Rarefied Gas Dynamics*, Plenum Press, New York, 1969.
- [18] Z. H. Li and H. X. Zhang, Numerical investigation from rarefied flow to continuum by solving the Boltzmann model equation, *Int. J. Numer. Meth. Fluids*, 42 (2003), 361–382.
- [19] J. A. Lordi and R. E. Mates, Rotational relaxation in nonpolar diatomic gases, *Phys. Fluids*, 13 (1970), 291–308.
- [20] F. E. III Lumpkin, Development and Evaluation of Continuum Models for Translational-rotational Nonequilibrium, Ph.D. Thesis, Stanford University, 1990.
- [21] M. Torrilhon and H. Struchtrup, Regularized 13-moment-equations: Shock structure calculations and comparison to Burnett models, *J. Fluid Mech.*, 513 (2004), 171–198.
- [22] L. Mieussens, Discrete velocity model and implicit scheme for the BGK equation of rarefied gas dynamics, *Math. Mod. Meth. Appl. Sci.*, 10 (2002), 1121–1149.
- [23] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics*, Springer Tracts in Natural Philosophy, vol 37, Springer Verlag, 1998.
- [24] T. Ohwada, Structure of normal shock waves: Direct numerical analysis of the Boltzmann equation for hard-sphere molecules, *Phys. Fluids A*, 5 (1993), 217–234.
- [25] T. Ohwada and K. Xu, The kinetic scheme for the full-Burnett equations, *J. Comput. Phys.*, 201 (2004), 315–332.
- [26] C. Park, Rotational relaxation of N<sub>2</sub> behind a strong shock wave, *AIAA 2002-3218*, 2002.
- [27] F. Robben and L. Talbot, Experimental study of the rotational distribution function of nitrogen in a shock wave, *Phys. Fluids*, 9 (1966), 653–662.
- [28] B. Schmidt, Electron beam density measurements of rotational temperatures in a low density wind tunnel, *J. Fluid Mech.*, 39 (1969), p. 361.
- [29] H. Struchtrup and M. Torrilhon, Regularization of Grad's 13 moment equations: Derivation and linear analysis, *Phys. Fluids*, 15 (2003), 2668–2680.
- [30] W. G. Vincenti and C. H. Jr. Kruger, *Introduction to Physical Gas Dynamics*, John Wiley & Sons, INC., 1965.
- [31] I. J. Wysong and D. C. Wadsworth, Assessment of direct simulation Monte Carlo phenomenological rotational relaxation models, *Phys. Fluids*, 10 (1998), 2983–2994.
- [32] K. Xu, Gas-kinetic schemes for unsteady compressible flow simulations, Technical Report 1998-03, von Karman Institute for Fluid Dynamics, Belgium, March 1998, <http://www.math.ust.hk/~makxu>.

- [33] K. Xu, A gas-kinetic BGK scheme for the Navier-Stokes equations and its connection with artificial dissipation and Godunov method, *J. Comput. Phys.*, 171 (2001), 289–335.
- [34] K. Xu, Regularization of the Chapman-Enskog expansion and its description of shock structure, *Phys. Fluids*, 14 (2002), L17.
- [35] X. Zhong, R. W. MacCormack and D. R. Chapman, Stabilization of the Burnett equations and application to hypersonic flows, *AIAA J.*, 31 (1993), 1036–1043.