A Unified Gas-kinetic Scheme for Continuum and Rarefied Flows

K. Xu* and J.C. Huang†

*Mathematics Department, Hong Kong University of Science and Technology, Hong Kong
†Department of Merchant Marine, National Taiwan Ocean University, Keelung 20224, Taiwan

Abstract.
With discretized particle velocity space, a multi-scale unified gas-kinetic scheme for entire Knudsen number flows is constructed based on the BGK model. The current scheme couples closely the update of macroscopic conservative variables with the update of microscopic gas distribution function within a time step. In comparison with many existing kinetic schemes for the Boltzmann equation, the current method has no difficulty to get accurate Navier-Stokes (NS) solutions in the continuum flow regime with a time step being much larger than the particle collision time. At the same time, the rarefied flow solution, even in the free molecule limit, can be captured accurately.

Keywords: Unified scheme, Navier-Stokes equations, free molecule flow, gas-kinetic scheme
PACS: 47.10.ad, 47.11.-j, 47.11.St

INTRODUCTION

The development of accurate numerical methods for all flow regimes is challenging. The Boltzmann equation describes the time evolution of the density distribution of a monatomic dilute gas with binary elastic collisions. The fluid dynamic Navier-Stokes (NS), Burnett and Super-Burnett equations can be derived from the Boltzmann equation. The Boltzmann equation is valid from the continuum flow regime to the free molecule flow. So, theoretically a unified kinetic method which is valid in the whole range of Knudsen number can be developed once 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 (DVM) or Discrete Ordinate Method (DOM) of the Boltzmann equation [4, 11, 6, 5]. 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 Navier-Stokes solutions, especially for the high Reynolds number flows, where the intensive particle collisions take place. Under this situation, the requirement of the time step being less than the particle collision time makes these methods prohibitive in the continuum flow application. In order to overcome the above difficulties, we need a correct understanding of the Boltzmann equation. Even though the individual particle movement has distinct transport and collision process, once this process is described by a statistical model, such as the Boltzmann equation, the transport and collision processes are coupled everywhere in space and time. To separate them numerically, such as the operator splitting methods, is inconsistent with the underlying physical model. In the past years, the gas-kinetic BGK-NS scheme for the Navier-Stokes solutions has been well developed [10], and has been successfully applied for the continuum flow simulations from nearly incompressible to hypersonic viscous and heat conducting flows. In the BGK-NS method, the particle velocity space is continuous and is integrated out in the flux evaluations in a finite volume scheme. This is not surprised because in the fluid regime, based on the Chapman-Enskog expansion the gas distribution function for the viscous flow is well-defined. Therefore, the efficiency of the BGK-NS method is similar to the traditional NS flow solver, where the same CFL condition is used for the determination of time step. In this paper we are going to extend the BGK-NS method from the continuum flow to the rarefied regime, which includes the free molecule limit. In order to do that, we have to discretize the particle velocity space as well, because the real gas distribution function in the highly non-equilibrium region can be hardly described by a Maxwellian distribution function and its derivatives. So, the current method can be also considered as a discrete velocity version of the BGK-NS scheme. At the same time, in order to efficiently solve the kinetic scheme, a multi-scale methodology of updating both microscopic and macroscopic flow variables is developed.

UNIFIED GAS-KINETIC SCHEME

The one-dimensional gas-kinetic BGK equation can be written as [2]

$$f_t + u f_x = \frac{g-f}{\tau}, \tag{1}$$

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 ξ. 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,

$$g = \rho(\frac{\lambda}{\pi})^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)},$$

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 $(3-\gamma)/(\gamma-1)$. For example, for a monatomic gas with $\gamma = 5/3$, 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 $\xi^2 = \xi_1^2 + \xi_2^2 + ... + \xi_K^2$. The relation between mass ρ, momentum ρU, and energy ρE densities with the distribution function f is

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

where ψ_α is the component of the vector of moments

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

and $d\Xi = du d\xi_1 d\xi_2 ... d\xi_K$ is the volume element in the phase space with $d\xi = d\xi_1 d\xi_2 ... d\xi_K$. Since mass, momentum, and energy are conserved during particle collisions, f and g satisfy the conservation constraint,

$$\int (g-f)\psi_\alpha d\Xi = 0, \qquad \alpha = 1,2,3, \tag{3}$$

at any point in space and time.

Before we introduce discrete ordinate method, let's first discretize the physical space, time, and particle velocity space. The physical space is divided into numerical cells with cell size Δx, and the jth-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 nth-time step. The particle velocity space is discretized by $2N+1$ subcells with cell size Δu, and the center of kth-velocity interval is $u_k = k\Delta u$, and it represents the average velocity u in that interval,

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

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

$$f(x_j, t^n, u_k) = f_{j,k}^n = \frac{1}{\Delta x \Delta u} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{u_k - \frac{1}{2}\Delta u}^{u_k + \frac{1}{2}\Delta u} f(x, t^n, u) dx du, \tag{4}$$

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

The BGK equation (1) can be written as

$$f_t = -u f_x + \frac{g-f}{\tau}. \tag{5}$$

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

$$f_j^{n+1} = f_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} (u \hat{f}_{j-1/2}(t) - u \hat{f}_{j+1/2}(t)) dt + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} \frac{g-f}{\tau} dx dt, \tag{6}$$

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 any 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 equation (6) is

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta x}\int (u_k \hat{f}_{j-1/2,k} - u_k \hat{f}_{j+1/2,k})dt + \frac{1}{\Delta x}\int\int \frac{g-f}{\tau}dxdt, \tag{7}$$

where $f_{j,k}^n$ is the averaged distribution function in the jth-cell $x \in [x_{j-1/2}, x_{j+1/2}]$ at the particle velocity u_k. Instead of using upwinding 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) using the method of characteristics,

$$\begin{aligned} \hat{f}_{j+1/2,k} &= f(x_{j+1/2}, t, u_k, \xi) = \frac{1}{\tau}\int_{t^n}^{t^{n+1}} g(x', t', u_k, \xi) e^{-(t-t')/\tau} dt' \\ &\quad + e^{-(t-t^n)/\tau} f_{0,k}^n (x_{j+1/2} - u_k(t-t^n), t^n, u_k, \xi), \end{aligned} \tag{8}$$

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., $f_{0,k}^n = f_0^n(x, t^n, u_k, \xi)$. In the above equation, $f_{0,k}^n$, is known at the beginning of each time step t^n. With the implementation of BGK-NS techniques for the integration of equilibrium distribution function, the distribution in Eq.(8) at the discretized particle velocity u_k can be expressed as

$$\hat{f}_{j+1/2,k}(0,t) = \tilde{g}_{j+1/2,k} + \tilde{f}_{j+1/2,k}, \tag{9}$$

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 initial condition f_0. The collision time τ in the above distribution function is determined by $\tau = \mu(T_0)/p_0$, where T_0 is the temperature and p_0 is the pressure, and both of them can be evaluated from W_0 at the cell interface. The above time-accurate gas distribution function can be used in Eq.(7) for the fluxes at a cell interface.

In order to discretize the collision term in Eq.(7) efficiently and accurately, a multiscale unified formulation is the following. Let's first take moment ψ on Eq.(7). Due to the vanishing of the particle collision term for the conservative variables, we have

$$\begin{aligned} W_j^{n+1} &= W_j^n + \frac{1}{\Delta x}\int\int_{t^n}^{t^{n+1}} u(\tilde{g}_{j-1/2} - \tilde{g}_{j+1/2})\psi dt du \\ &\quad + \frac{1}{\Delta x}\sum_k \int_{t^n}^{t^{n+1}} u_k(\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k})\psi dt, \end{aligned} \tag{10}$$

where $\tilde{g}_{j+1/2}$ has the same expression as $\tilde{g}_{j+1/2,k}$, but is interested in a continuous particle velocity space $u_k = u$. The integration of the equilibrium part $\tilde{g}$ can be evaluated exactly and the integration of the non-equilibrium part $\tilde{f}$ can be done using the quadrature. For the update of the conservative variables, the difference between the above formulation and the BGK-NS scheme is that the discrete sum is used for the integration of the initial distribution function f_0 in particle velocity space. For a highly non-equilibrium flow, the real distribution function f_0 can be a complicated function, and a discretization of particle velocity space has to be used. For the original BGK-NS scheme targeting on the NS solutions [10], the initial gas distribution function f_0 can be reconstructed from the distribution of macroscopic variables according to the Chapman-Enskog expansion. Therefore, the specific form of initial condition f_0 can be mathematically reconstructed. In the continuum flow limit, due to the sufficient number of particle collisions and with the condition of time step being much larger than the particle collision time, the contribution of the integration of the equilibrium state $\tilde{g}_{j+1/2}$ will be dominant in the final solution of the distribution function $\hat{f}_{j+1/2,k}$. The $\tilde{g}_{j+1/2}$ itself gives a corresponding NS distribution function, and the contribution from initial term $\tilde{f}_{j+1/2,k}$ vanishes. As a result, the updated discrete form of the distribution function $f_{j,k}^{n+1}$ will present a Chapman-Enskog NS distribution function. Therefore, in the continuum flow regime, the BGK-NS scheme with continuous particle velocity space and the current unified method with discretized particle velocity space will become the same scheme. In the continuum flow regime, for the NS solutions the update of the conservative variables through the above equation (10) is enough, because the gas distribution function $f_{j,k}^{n+1}$ can be reconstructed from the updated conservative variables. Therefore, for the continuum flow only, like the BGK-NS scheme [10], we don't need to update the gas distribution function.

In the highly non-equilibrium flow regime, Equation (10) for the update of conservative variables is still correct. For example, in the collisionless limit, the non-equilibrium part $\tilde{f}_{j-1/2,k}$ and $\tilde{f}_{j+1/2,k}$ will take dominant effect, and the contribution from the equilibrium part vanishes. Therefore, the unified scheme has the correct collision-less limit as well.

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 Eq.(7) the unified kinetic scheme for the update of gas distribution function becomes

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

where 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

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

where no iteration is needed for the update of the above solution. 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 update of macroscopic flow variables in Eq.(10).

The unified scheme is a multiscale hybrid method with both macroscopic and microscopic variable updates. The traditional hybrid approach is based on a geometrical one [9]. In different flow regions, different governing equations are solved. At the same time, different patches are connected through buffer zone. However, instead of solving different governing equations as most hybrid schemes do, we couple them in the way of evaluating the flux function across the cell interface. In the continuum flow regime, the intensive particle collision will drive the system close to equilibrium state. Therefore, the part based on the integration of equilibrium state $\tilde{g}_{j+1/2,k}$ in Eq.(9) at the cell interface will automatically take a dominant role. It can be shown that in smooth flow region $\tilde{g}_{j+1/2,k}$ gives precisely the NS gas distribution function. Since there is one-to-one correspondence between macroscopic flow variables and the equilibrium distribution, the integration of the equilibrium part can be also fairly considered as the macroscopic composition part of the scheme. In the free molecule limit with inadequate particle collisions, the integral solution at the cell interface will automatically present a purely upwinding scheme, where the particle transport from $\tilde{f}_{j+1/2,k}$ will be the main part. Therefore, the scheme captures the flow physics in the collisionless limit as well. This unified approach can be considered as a dynamic hybrid method instead of geometrical one. The reason for most other approaches to use a geometrical way is due to the fact that their flux functions across a cell interface are solely based on the kinetic upwinding discretization, i.e., the so-called $\tilde{f}_{j+1/2,k}$ term in Eq.(9). As we know, the kinetic upwinding is only correct in the collisionless or highly non-equilibrium regime. Therefore, in the traditional hybrid scheme, the computational domain has to be divided into equilibrium and non-equilibrium flow regions. Physically this kind of geometrical division is artificial and there should have no region where both approaches are applicable, because the above two approaches have significant dynamic differences in their flux evaluation. In the unified method, a single computation domain is used and the dynamic differences in the particle behavior is obtained by solving the full approximate Boltzmann equation, which is valid all the way from the continuum to rarefied flows. Certainly, in order to save computational time we may also develop a hybrid method which uses the current unified scheme as a non-equilibrium flow solver and adopts the BGK-NS method as a continuum flow solver. In the continuum flow regime, this kind of hybrid scheme is actually a scheme which is different from the unified method only by simply replacing the discretized particle distribution function f_0 of Eq.(8) by a distribution function f_0 of the Chapman-Enskog NS-type with a continuous particle velocity space [10]. In the continuum flow regime, only conservative flow variables are concerned. The flux evaluation for the conservative variables update in Eq.(10) is simply a discretized version of the BGK-NS method for the NS equations. Therfore, in this flow regime, we can use a time step which is much larger than the particle collision time, i.e., $\Delta t >> \tau$. In other words, in the continuum limit, the integral solution from the

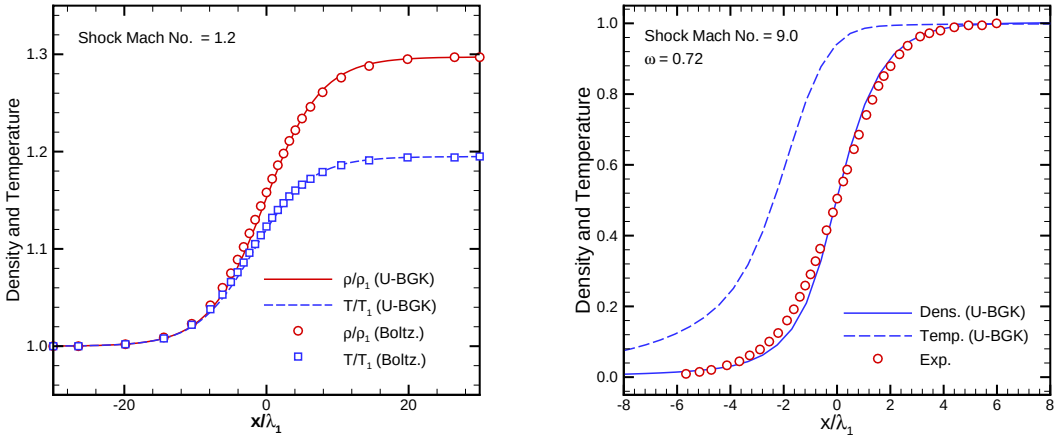

FIGURE 1. Argon shock structure at Mach number2 1.2 (left) and 9 (right). The solutions are compared with Boltzmann solution [8] and experimental measurement [1].

equilibrium state is dominant, and the updating of the macroscopic flow variables follow the NS solutions. Also, due to the update of both macroscopic and microscopic variables, an implicit discretization of particle collision term can be achieved, and the time step for the unified scheme is much increased, especially in the continuum flow regime. Most importantly, due to the update of macroscopic variables, the heat flux can be modified and the Prandtl number of the scheme can be adjusted to any number[10] without modifying the BGK model itself.

NUMERICAL EXPERIMENTS

The unified scheme has been tested from free molecule flow to the Navier-Stokes solutions. In this section, we only present the shock structure tests from the low Mach number (continuum flow) to high Mach number (highly non-equilibrium flow). First we present test cases on the shock structure for argon gas at $M = 1.2$ with $Pr = 2/3$. Ohwada solved the full Boltzmann equation for this case [8]. For the hard sphere molecules, the viscosity coefficient $\mu \sim T^{0.5}$ and $Pr = 2/3$, where the x-coordinate is normalized by $\sqrt{\pi}\lambda_1/2$ and λ_1 is the mean free path of the gas molecules at the upstream condition. Figure 1 shows the density, temperature of a shock structure. Comparisons of the results from the unified scheme are made with the solutions of the Boltzmann equation. The results from the direct Boltzmann solver and the current solutions have good agreement. At Mach number 1.2, where the local Knudsen numbers are less than 0.02, as expected, the standard Navier-Stokes equations suffice. The current solution also indicates that the unified scheme can capture accurately the NS solutions. Next we calculate Mach 9 argon shock structure from the unified scheme. Figure 1 also shows the shock structures for viscosity coefficient $\mu \sim T^{0.72}$ and $Pr = 2/3$ case. Both solution from the unified scheme and experimental data are presented. Figure 2 presents the reciprocal of shock thickness vs. Mach numbers. The solutions from the unified scheme, DSMC [3], experimental measurements [1], and Burnett solution [7], are presented. Shock structure calculation is one of the most difficult test cases for the validation of non-equilibrium flow solvers. The above simulation results validate the unified approach presented in this paper.

CONCLUSION

In this paper, we present a unified kinetic approach for flows in the entire Knudsen number. The validity of the approach is based on its fully coupled representation of particle movement, i.e., transport and collision. Different from many other approaches, the critical step is that the integral solution of the kinetic model is used in the flux evaluation across the cell interface. The integral solution gives an accurate representation in both continuum and free molecule flows. The current scheme can be considered as a dynamic hybrid method, where the different flow behavior is obtained through the different limits of the integral solution of a single kinetic equation, instead of solving different governing

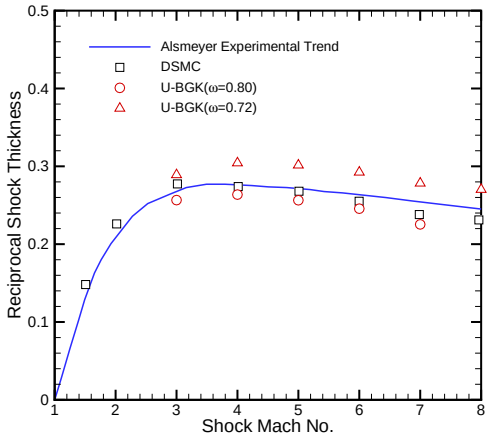

FIGURE 2. Reciprocal shock thickness vs. Mach number. The results include unified method, DSMC [3], experimental measurements [1], and Burnett solutions [7].

equations in different flow regimes. The weakness for the most existing kinetic methods is that a purely upwinding technique is used in the flux evaluation for the transport term uf_x, which is equivalent to solving the collision-less Boltzmann equation and its solution is only a partial solution of the full integral solution used in the unified scheme. Theoretically, the Boltzmann equation is a statistical model with a continuous particle transport and collision process at any point in space and time. So, there is no reason to believe that these particles which transport across the cell interface will not suffer particle collision during its movement toward the cell interface. Therefore, an "exact" integral solution of the full kinetic equation has to be used and it is the key for the success of the unified scheme. Due to its multi-scale nature of the unified scheme, through the update of macroscopic flow variables the heat flux of the scheme can be modified as well according to correct Prandtl number.

The current research was supported by Hong Kong Research Grant Council 621709, National Natural Science Foundation of China (Project No. 10928205), and National Science Council of Taiwan through grant no. NSC 96-2221-E-019-067-MY2.

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