6 TRANSITIONAL REGIME

6.1 GENERAL OVERVIEW

In section 0.4 the transitional regime is defined as the scope of Kn number (λ / L) between 0.1 and 10 (see Eq. (0.8)), i.e., the molecular mean free path λ is not too large, nor too small in comparison with the typical flow size L. In such case the collisions between molecules and the collisions of molecules with the surface must be taken into account simultaneously, both the comparatively simple free molecular flow theory and the mature continuum method are not appropriate, one has to solve the Boltzmann equation or to evoke equivalent to it physic-mathematical handling. To solve the integral-differential Boltzmann equation with the collision term and an unknown function having as many as seven arguments is so difficult that many researchers envisaged various methods to solve the problems in transitional regime, some of these methods seemed to carry the implication of roundabout tactics, but could lessen the difficulty and make the problems readily tackled.

The methods of solution of the transitional regime problems can be distinguished into two categories: *the analytic and numerical methods*. The analytic methods without exception start from the Boltzmann equation, but owing to the complexity of this equation they often adopt the small disturbance or linearization assumption (*the linearized Boltzmann equation method*), or make some assumption relative to the form of the distribution function (for example *the moment method*), or make some simplification even of the collision term itself (*the model equation method*), these constitute the contents of the sections 6.2~6.4. These methods of solution despite their belonging to the analytical category seldom attain the analytical solutions, to obtain the final results certain numerical calculations are required. It is noted that except the solutions of the linearized Boltzman equation in the scope of small disturbances these solutions can hardly be called exact solutions. This is especially true for the model equation method, this is a modification of the Boltzmann equation proper and replacement of it by a simplified equation, showing how difficult is the direct solution of the Boltzmann equation. The moment method owing to the arbitrariness and un-uniqueness of the form of the distribution function does not possess either the merit of exact solution.

Two kinds of the numerical methods can be distinguished: the direct numerical solution of the Boltzmann equation and the direct simulation of the flow physics itself, even though the line of demarcation between them becomes not so absolute because the direct simulation method can be proved to be consistent with the Boltzmann equation. Among the methods of direct numerical solution of the Boltzmann equation there is the method (*finite difference method*) which uses specific algorithm (the Monte Carlo method of quadrature) to calculate the collision integral and uses the mature finite different method of the computational fluid dynamics (CFD) to solve the Boltzmann equation, the method (*discrete ordinate* or *discrete velocity method*) which assumes that the velocity space only has finite number of discrete values thus significantly simplifying the calculation of the collision integral, and the method (*the integral method*) that writes the Boltzman equation in the integral from and solves it, they are introduced in sections 6.5~6.7. These methods attempt to base the formulation on the exact Boltzmann equation and have the property of exact solution in the limits of errors (of course, provided the calculation method is correct).

With the development of the electronic computers a kind of methods staring directly from the simulation of physics of the flows appears, including the method of deterministic simulation —*the molecular dynamics* (*MC*) *method* and the probability simulation method which can be distinguished further into the *test particle Monte-Carlo method* and the *direct simulation Monte-Carlo* (*DSMC*) *method* . The direct simulation Monte-Carlo method deserves separate discussion owing to its success in solving rarefied gas flow problems, especially the non-equilibrium flow problems in the transitional regime. The DSMC method possesses the same physical basis and assumptions (the molecular chaos and dilute gas assumption). But DSMC method is different in some aspects from the Boltzmann equation. The latter depends on the assumption of the reverse collisions so could not treat the three body collision problem, but the DSMC method can be applied to complex problems such as with recombination chemical reactions where three-body collisions are involved. In treating the problems of molecular models and molecule-surface interaction when introducing physical models the DSMC method because of its nature of physical simulation can naturally and easily introduce more complicated and more close to reality models. But it is quite difficult to introduce the real and complex models into the mathematical formulation of the Boltzmann equation. For the gas flow cases accompanied by the chemical reactions and radiation the mathematical formulation in the framework of the Boltzmann equation is difficult to accomplish for practical application, but it is easy for the DSMC method to implement the simulation of these flows. Even for flow cases without such processes as chemical reactions and radiation to solve directly the Boltzmann equation is rather difficult and sometimes is limited to simple geometry and sometimes to low speed. Thus, the deep rooted view point, i.e., the view point that a simulation process can be accepted only if it is strictly derived from the Boltzmann equation, seems to be antiquated and non-practical. The DSMC method has been verified experimentally both in the aspect of global flow characteristics and in the aspect of micro-level characteristics such as the velocity distribution function. It is safe to say that the DSMC method is a method that solves successfully various practical flow problems in the transitional flow regime, its meaning and role has been recognized by the scientific community. Owing to the important meaning of the DSMC method in the transitional regime Chapter 7 will be devoted specially to the discussion of this method. And this Chapter will give an overall outline of various methods in the transitional regime including a section 6.8 giving a parallel overview of the direct simulation method.

6.2 LINEARIZED BOLTZMANN EQUATION

It has been stated above that due to the complicated non-linearity of the collision integral of the Boltzmann equation the direct solution of it is very difficult. The existence of the solution of the Boltzmann equation under equilibrium of the gas, the Maxwellian distribution (see section 2.10), allows us to suppose to find the solution of the linearized problem near this solution, this limits the solution to low speed flow problems, i.e., the small disturbance solution about the quiescent gas. For the slowly moving gas flow slightly deviated from the stationary state the difference of its distribution function $f(r,c,t)$ from the Maxwellian distribution is small, and it can be written in the following form

$$f(\boldsymbol{r},c,t)=f_0\left[1+\varphi(\boldsymbol{r},c,t)\right], \tag{6.1}$$

where

$$f_0=n_0\left(\beta/\sqrt{\pi}\right)^3\exp\left(-C^2\right), \tag{6.2}$$

$$\boldsymbol{C}=c\beta\equiv\frac{c}{\sqrt{2\dfrac{k}{m}T_0}}. \tag{6.3}$$

Substituting Eq. (6.1) into the Boltzmann equation (Eq. (2.152) in section 5.2) and retaining only the first order of φ yields

$$\frac{\partial\varphi}{\partial t}+c_i\frac{\partial\varphi}{\partial x_i}=J(\varphi), \tag{6.4}$$

where $J(\varphi)$ is a collision operator linear relative to φ which can be written as

$$J(\varphi)=\int f_{01}\left(\varphi^*+\varphi_1^*-\varphi-\varphi_1\right)cbdbd\varepsilon dc_1\,. \tag{6.5}$$

In obtaining Eq. (6.4) the fact, that $f_0^*f_{01}^*=f_0f_{01}$ and $f(c')$ can be taken out of the integration, has been taken into account.

The linearized Boltzmann equation (6.4) is still a complicated integral-differential equation, but as it is linear, in comparison with the Boltzmann equation it is much simpler. Many authors discussed in detail this equation, see Cercignani [1, 2]. These small disturbance solutions provide with important data having value of reference when they are obtained without the assistance of arbitrary assumptions about the relevant parameters or the modification of the equation, they can serve as merits for other numerical methods and have practical application value in the aspects of gas flow problems in MEMS. Even though the equation is linearized, the available solutions are limited mainly to certain class of relative simple boundary conditions. Sometimes some works are discussing not the linearized Boltzmann equation but the linearized model equation, one should be careful when applying such results.

In the following the equation (6.4) will be written for the case when the space variation occurs only in the y direction and the gas molecules are hard spheres, and the formulation of the boundary conditions for the linearized Bolzmann equation will be discussed for the plane boundary case [3, 4]. When y is the only space coordinate by using the dimensionless molecular velocity $\boldsymbol{C}$ (see Eq. (6.3)) Eq. (6.4) can be written

$$\beta\frac{\partial\varphi}{\partial t}+Cy\frac{\partial\varphi}{\partial y}=J(\varphi). \tag{6.6}$$

For hard sphere molecule it is easy to obtain

$$J(\varphi)=\frac{1}{\sqrt{2}\pi^{5/2}\lambda}\int_0^{2\pi}d\varepsilon\int_0^{\pi}\sin\theta d\theta\int_{-\infty}^{\infty}Ge^{-C_1^2}\{\varphi^*+\varphi_1^*-\varphi-\varphi_1\}d\boldsymbol{C}_1, \tag{6.7}$$

where $G=\beta c_r\equiv c_r/\sqrt{2kT/m}$, the definitions of ε,θ,c_r see Chapter 2, $\varphi^*=\varphi(\boldsymbol{C}^*),\varphi_1^*=\varphi(\boldsymbol{C}_1^*)$; $\boldsymbol{C}^*,\boldsymbol{C}_1^*$ are the velocities after collision of molecules whose velocities before collision are $\boldsymbol{C},\boldsymbol{C}_1$. The relations between $\boldsymbol{C}^*,\boldsymbol{C}_1^*$ and $\boldsymbol{C},\boldsymbol{C}_1$ can be found in Chapter 2 Eq. (2.59)*, Eq. (2.59)**, for example in the direction of x

$$\begin{cases} C_x^*=C_x+(C_{1x}-C_x)\cos^2\dfrac{\chi}{2}+ \\ \qquad\dfrac{1}{2}\left[G^2-(C_{1x}-C_x)^2\right]^{1/2}\sin\chi\cos\varepsilon, \\ C_{1x}^*=C_{1x}-(C_{1x}-C_x)\cos^2\dfrac{\chi}{2}- \\ \qquad\dfrac{1}{2}\left[G^2-(C_{1x}-C_x)^2\right]^{1/2}\sin\chi\cos\varepsilon. \end{cases} \tag{6.8}$$

We discuss the case of the Maxwellian type boundary conditions, i.e., after incidence onto the surface σ portion of the molecules reflects diffusely and the other $(1-\sigma)$ portion reflects specularly. Obviously, when $\sigma\neq 0$, the incident molecules and the reflected molecules have different distribution functions. For the case of a plane surface perpendicular to the y axis the distribution function is non-continuous with respect to the normal to the surface velocity component C_y. Then two distribution functions which are continuous by themselves are to be introduced, they are defined each only in the half velocity space [3, 4]

$$\begin{cases} f = f^{+}(y, \boldsymbol{C}, t), C_y > 0, \\ f = f^{-}(y, \boldsymbol{C}, t), C_y < 0. \end{cases} \tag{6.9}$$

Correspondingly, different disturbance distribution functions φ^{+}, φ^{-} are introduced

$$\begin{cases} f^{+} = f_0\left[1 + \varphi^{+}(y, \boldsymbol{C}, t)\right], C_y > 0, \\ f^{-} = f_0\left[1 + \varphi^{-}(y, \boldsymbol{C}, t)\right], C_y < 0. \end{cases} \tag{6.10}$$

For the case when there is a velocity u_0 of the plane boundary, at plane $y = y_0$ the boundary condition is (denote $S_0 = \beta u_0 \equiv u_0 / \sqrt{2kT/m}$)

$$f^{\pm}(y_0, \boldsymbol{C}, t) = (1 - \sigma) f^{\mp}(y_0, C_x, -C_y, C_z, t) +$$

$$\sigma n_0 \left(\beta / \sqrt{\pi}\right)^3 \exp\left\{-\left[(C_x - S_0)^2 + C_y^2 + C_z^2\right]\right\}$$

Neglecting the second order of S_0, it can be written as

$$f^{\pm}(y_0, \boldsymbol{C}, t) = (1 - \sigma) f^{\mp}(y_0, C_x, -C_y, C_z, t) +$$

$$\sigma n_0 \left(\beta / \sqrt{\pi}\right)^3 \exp\left(-C^2\right)[1 + 2C_x S_0]. \tag{6.11}$$

Substituting Eq. (6.10) into Eq. (6.11) and taking into account Eq. (6.2), one obtains

$$\varphi^{\pm}(y_0, C_x, C_y, C_z, t) = (1 - \sigma)\varphi^{\mp}(y_0, C_x, -C_y, C_z, t) + 2\sigma C_x S_0 . \tag{6.12}$$

The basic equation (6.6) and boundary condition Eq. (6.12) are applicable for cases when the flow varies only in the direction normal to the plane boundary and the boundary conditions are of the Maxwellian type.

After finding φ the physical macroscopic quantities interesting us are easily obtained, e.g., the macroscopic velocity c_0 and the stress P_{ij}

$$c_{0i} = \frac{1}{n_0}\int c_i f_0 (1+\varphi)\, dc = \beta^{-1} \big/ \pi^{3/2} \int C_i \varphi e^{-C^2} dC \tag{6.13}$$

$$P_{ij} = m\int (c_i - c_{0i})(c_j - c_{0j}) f_0 (1+\varphi) dC = \frac{2n_0 kT}{\pi^{3/2}} \int C_i C_j \varphi\, e^{-C^2} dC \tag{6.14}$$

With the help of the linearized Boltzmann equation Gross and Ziering [3] solved the problem of stress flow between two plates, i.e., the Couette flow problem, Gross and Jackson [4] solved the problem of unsteady flow caused by the instant motion of the plane plate, i.e., the Rayleigh problem. They suggested to express $\varphi^{\pm}$ as

$$\varphi^{\pm} = a_0^{\pm}(y,t) C_x + a_1^{\pm}(y,t) C_x C_y\,. \tag{6.15}$$

Such form of the dependence on the velocity originated from Chapman-Enskog expansion, but as the discontinuous φ relative to C_y is introduced, so $a_0^+ \neq a_0^-, a_1^+ \neq a_1^-$. Substituting the function φ defined in the whole velocity space

$$\varphi = \varphi^+ \left(\frac{1 + signC_y}{2} \right) + \varphi^- \left(\frac{1 - signC_y}{2} \right), \tag{6.16}$$

where

$$signC_y = 1, C_y > 0, signC_y = -1, C_y < 0, \tag{6.17}$$

into the basic equation (6.6), and multiplying both sides of the equation on C_x and $C_x C_y$ and searching the moments separately in the upper half velocity space and the lower half velocity space, the simultaneous equations relative to $a_0^+, a_0^-, a_1^+, a_1^-$ are obtained, the right hand sides are the integral terms including the collision term Eq. (6.7). For the hard sphere molecule the integral terms can be evaluated. The boundary conditions after substitution of Eq. (6.15) can be transformed into the boundary conditions relative to $a_0^+, a_0^-, a_1^+, a_1^-$. So the whole problem can be solved. In searching the solution of the linearized Boltzmann equation the moment method (see section 6.3) has been employed. These were the early attempts of the solution of the transitional regime.

Grad [5] and Cercignani [6] investigated the problem of further transformation of the linearized collision operator $J(\varphi)$, the integration for ε is expressed through zero order Bessel function of the first kind I_0 (Eq. (3.43)), and for the hard sphere model the integration relative to θ can also be accomplished. Thus the linearized Boltzmann equation in the one-dimensional steady case is written as

$$C_y \frac{\partial \varphi}{\partial y} = \frac{1}{\left(\sqrt{\pi}/2\right)\lambda}\left[L_1(\varphi) - L_2(\varphi) - \nu(C)\varphi\right], \tag{6.18}$$

where

$$L_1(\varphi) = \frac{1}{\sqrt{2\pi}} \int \frac{1}{|C - \boldsymbol{\xi}|} \exp\left(-\xi^2\right) + \frac{|C \times \boldsymbol{\xi}|^2}{|C - \boldsymbol{\xi}|^2} \varphi(y, \boldsymbol{\xi})\, d\boldsymbol{\xi}, \tag{6.19}$$

$$L_2(\varphi) = \frac{1}{2\sqrt{2\pi}} \int |C - \boldsymbol{\xi}| \exp\left(-\xi^2\right) \varphi(y, \boldsymbol{\xi})\, d\boldsymbol{\xi}, \tag{6.20}$$

$$\nu(C) = \frac{1}{2\sqrt{2}}\left[\exp\left(-C^2\right) + \left(2C + \frac{1}{C}\right)\int_0^C \exp\left(-t^2\right) dt\right]. \tag{6.21}$$

In the above expressions $\boldsymbol{\xi}$ is the integration variable corresponding to C, $d\boldsymbol{\xi} = d\xi_1 d\xi_2 d\xi_3$, $C \times \boldsymbol{\xi}$ is the vector production of C and $\boldsymbol{\xi}$, the integration domain of L_1 and L_2 is the whole space of the molecular velocity C (or $\boldsymbol{\xi}$).

Sone, Owwada and Aoki et al. developed efficient numerical methods of employing the above linearized Boltzmann equations (6.18)~(6.21) in solving some half space boundary problems – the temperature jump and Knudsen layer problem [7], the problem of evaporation and condensation [8], the problem of shear and thermal creep [9] and some problems of flow between two plates – the Poiseuille flow and thermal transpiration problem [10] and the Couette flow problem [11]. The solutions of these steady boundary value problems are obtained as the stabilized solutions of the initial and boundary-value problems of the unsteady equation obtained from Eq. (6.18) by adding the term $\partial\varphi/\partial t$ to its left hand side. The unsteady problems are solved by the standard implicit finite difference scheme. The key question is the calculation of the collision term. The distribution function (or the reduced distribution function) is expanded by a set of the basis functions in analogue with the basis functions in the finite element method. Thus, the collision integral can be written as the matrix product of the collision integral kernel and the values of distribution function on lattice points. The collision integral kernel is the collision integral of the basis functions at the lattice points and thus can be evaluated universally. As the computation of the collision integral is most time-consuming, the method of computation of the collision integrals of a current problem by using the prepared universal collision integral kernels demonstrates the high efficiency advantage of the method.

6.3 THE MOMENT METHOD

The practice of the so called moment method is not to solve the Boltzmann equation itself but to solve its moment equation. The latter is obtained by multiplying the Boltzmann equation by some molecular quantity Q and integrating over the entire velocity space (i.e., the so called finding moment). For arbitrary form of Q we have obtained the general form of the moment equation (section 2.9, Eq. (2.183))

$$\frac{\partial}{\partial t}\left(n\overline{Q}\right)+\nabla\cdot\left(n\overline{cQ}\right)-nF\cdot\overline{\frac{\partial Q}{\partial c}}=\Delta[Q]. \qquad (6.22)$$

The macroscopic characteristics that interest us are the average values of some microscopic molecular quantities, i.e., the moments of the distribution functions (see the expressions of the macroscopic properties in section 2.2). For example, the density is the zero order moment, the velocity is the first order moment, P_{ij} is the second order moment, p is the contraction of the second moment, Eq. (2.25), q_i is the contraction of the third moment, Eq. (2.27)), etc. Substitution of different quantities Q into Eq. (6.22) yields the system of equations for the macroscopic quantities. In particular, when Q are the collision invariants m, mc and $(1/2)mc^2$, we have $\Delta[Q]=0$, and obtain the conservation equations of the macroscopic quantities. When Q is certain power of c, as there is the term $\overline{cQ}$ on the left hand side of Eq. (6.22), this causes the appearance of a moment of order one order higher than before. When turning to the moment equation in expectation to obtain equation for higher order moment, this term of higher order leads to even higher order moment, and eventually to infinite equations and moments. The moment method assumes that the distribution function can be expressed as function of certain moments (and the molecular velocity c, the space coordinate x and time t), with specific forms of expression through the moments and c, but the variation with the space coordinates is to be determined. The moment equation thus obtained would have higher order of c, but for some flow cases and with some specific treatment, it can be expressed through moments of lower orders, and one attains closed system of equations characterizing the variation in physical space.

In discussing the basic equations of the continuum media (section 5.2 in Chapter 5) we considered the Chapman-Enskog solution of the Boltzmann equation, this is the expansion of the distribution function into the series of terms proportional to the powers of Kn number

$$f=\sum_{r=0}^{\infty}f^{(r)}.$$

$f^{(0)}$ is the Maxwellian distribution, the corresponding zero order moment equation is the Euler equation (5.2) (with $\tau_{ij}=0, q_i=0$), the unknown functions are ρ, u_0 and T. The first order distribution function of this expansion is the Chapman-Enskog distribution function Eq. (5.8), yielding the expression of stress and heat flux in the ordinary fluid mechanics. Substituting them into the corresponding conservation equations or the moment equations, one obtains the continuum Navier-Stokes equations (5.14), (5.15). The second order distribution function of this expansion yields the expressions of the stress τ_{ij} and heat flux q_i, different from the ordinary continuum media mechanics, and gives the Burnett equations. They have been listed in Chapter 2 as the basic equations of the continuum media, but they are applicable to larger scope of Kn, where the Navier-Stokes equations become invalid. For their nature of the expansion into the positive powers of the Kn number, they could not yield good results when Kn is much larger than 0.1, but they can provide results more close to the exact solutions than the ordinary slip flow solutions. How deep they can allow the continuum equations method to penetrate into the transitional regime and to what extent they can provide more exact solution depends on the method of solution and the comparison with experiments and solutions having the merits of verifying standard. The development of effective solution methods for Burnett equations is still an issue needing continuous efforts. The thirteen moment equations of Grad Eq. (5.2), Eq. (5.29) and Eq. (5.30) have ρ, u_0, T, τ_{ij} and q_i as the basic arguments and possess the character of general basic equations, but application of them to the solution of peculiar problems didn't lead to credible results, the possible reason for this has been discussed in section 5.2 of Chapter 5.

Except those above mentioned methods leading to basic equations possessing general meaning, individual moment methods have been developed for different problems and boundary geometries. Aiming at the physical feathers of different problems the expressions of the distribution functions are proposed and useful solutions have been obtained.

Among this kind of the moment methods the early and the most famous one is certainly the method of *binomial distribution function* developed by Mott-Smith for dealing with the *problem of shock wave structure* [12]. The distribution function f in the shock wave transition zone is expressed as the combination of the upstream and downstream uniform distribution functions

$$f = a_1(x)f_1 + a_2(x)f_2 \equiv N_1(x)F_1(c) + N_2(x)F_2(c), \tag{6.23}$$

where

$$F_1(c) = \frac{f_1}{n_1} = \left(\beta_1/\sqrt{\pi}\right)^3 \exp\left\{-\beta_1^2\left[\left(u-u_{01}\right)^2 + v^2 + w^2\right]\right\}, \tag{6.24}$$

$$F_2(c) = \frac{f_2}{n_2} = \left(\beta_2/\sqrt{\pi}\right)^3 \exp\left\{-\beta_2^2\left[\left(u-u_{02}\right)^2 + v^2 + w^2\right]\right\}, \tag{6.25}$$

in which f_1, f_2 are the upstream and downstream equilibrium distribution functions (see Eq. (2.196)), n_1, n_2 are the upstream and downstream uniform number densities, u_{01}, u_{02} are the upstream and downstream uniform velocities, $a_1(x) \equiv N_1(x)/n_1$ and $a_2(x) \equiv N_2(x)/n_2$ represent the proportions the two known upstream and downstream distribution functions occupy at different positions of x. Obviously

$$N_1 = n_1,\quad N_2 = 0,\ \text{when}\quad x \to -\infty$$
$$N_1 = 0,\quad N_2 = n_2,\ \text{when}\quad x \to \infty .$$

The mass, momentum and energy across the shock wave are conserved

$$m\int uf_1 dc = m\int uf_2 dc,\quad \text{i.e.}\quad \rho_1 u_{01} = \rho_2 u_{02} = j, \tag{6.26}$$

$$m\int u^2 f_1 dc = m\int u^2 f_2 dc,\quad \text{i.e.}\quad ju_{01} + kn_1T_1 = ju_{02} + kn_2T_2, \tag{6.27}$$

and

$$\frac{m}{2}\int uc^2 f_1 dc = \frac{m}{2}\int uc^2 f_2 dc,$$

i.e.

$$j\left(\frac{u_{01}^2}{2} + \frac{5}{2}\frac{k}{m}T_1\right) = j\left(\frac{u_{02}^2}{2} + \frac{5}{2}\frac{k}{m}T_2\right). \tag{6.28}$$

These are the well known Rankine-Hugonio relations. To find the distribution function, the mass conservation is applied to some upstream point and some point inside the shock wave to yield

$$m\int uf_1 dc = m\int ufdc ,$$

i.e.,

$$n_1 u_{01} = nu_0 . \tag{6.29}$$

From Eq. (6.23) and the definition of density (see Eq. (2.5)) one has

$$\int fdc = n(x) = N_1(x) + N_2(x) . \tag{6.30}$$

And according to Eq. (6.23) and the definition of the macroscopic velocity (see Eq. (2.8))

$$nu_0 \int ufdc = N_1(x)u_{01} + N_2(x)u_{02} . \tag{6.31}$$

Thus from Eq. (6.29) one has

$$u_{01} N_1(x) + u_{02} N_2(x) = n_1 u_{01} . \tag{6.32}$$

To determine three unknown functions $n(x), N_1(x), N_2(x)$, except Eq. (6.30) and Eq. (6.32) one extra moment equation must be employed. Take $Q = u^2$, for the one-dimensional steady problem under discussion, this equation is

$$\frac{d}{dx}\left(n\overline{u^3}\right) = \Delta\left[u^2\right] . \tag{6.33}$$

Discuss at first the right hand side of this equation with the purpose to express it through the unknown functions n, N_1, N_2. The expression $\Delta[u^2]$ is a collision term, this integral has been evaluated for Maxwellian molecules and VHS molecules with $\xi = 1/2$ (see Eq. (2.175) and Eq. (2.175)')

$$\Delta\left[u^2\right] = \frac{p}{m}\frac{\tau_{xx}}{\mu} .$$

For both these molecular models one has $\mu = CT$ (see Eq. (2.93) and Eq. (2.96)'), and with the employment of the expression of their mean free path Eq. (2.217)', the viscosity μ can be written

$$\mu = \frac{\rho_1 \lambda_1}{2}\left(\frac{2\pi k}{mT_1}\right)^{1/2} T ,$$

thus, one has

$$\Delta\left[u^2\right] = \frac{\left(2kT_1/\pi m\right)^{1/2}}{n_1\lambda_1}\frac{n}{m}\tau_{xx} . \tag{6.34}$$

According to the definition of τ_{xx} (Eq. (2.24) and Eq. (2.25)), one has

$$\tau_{xx} = mn\left(\frac{\overline{c'^2}}{3} - \overline{u'^2}\right) = mn\left(\frac{\overline{u'^2} + \overline{v'^2} + \overline{w'^2}}{3} - \overline{u'^2}\right) = \frac{2}{3}mn\left(\overline{v'^2} - \overline{u'^2}\right). \tag{6.35}$$

When writing the last expression, the equality $\overline{v'^2} = \overline{w'^2}$ has been used, for the problem is symmetric with the x axis. Obviously, $\overline{u'^2}$ can be written

$$\overline{u'^2} = \overline{\left(u - u_0\right)^2} = \overline{u^2} - 2\overline{uu_0} + \overline{u_0^2} = \overline{u^2} - u_0^2 .$$

According to the definition

$$n\overline{u^2} = \int u^2 f dc = N_1 \int u^2 F_1 dc + N_2 \int u^2 F_2 dc ,$$

where the first term is

$$N_1 \int u^2 F_1 dc = N_1 \frac{\beta_1^3}{\pi^{3/2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left[u_{01} + \left(u - u_{01}\right)\right]^2 \times$$

$$\exp\left\{-\beta_1^2\left[\left(u - u_{01}\right)^2 + v^2 + w^2\right]\right\} du dv dw =$$

$$N_1 \frac{\beta_1^3}{\pi^{3/2}}\left[u_{01}^2\left(\frac{\pi^{1/2}}{\beta_1}\right)^3 + 2u_{01}\cdot O + \frac{1}{2\beta_1^2}\left(\frac{\pi^{1/2}}{\beta_1}\right)^3\right] =$$

$$N_1\left(u_{01}^2 + \frac{1}{2\beta_1^2}\right) = N_1\left(u_{01}^2 + RT_1\right).$$

Analogously, the second term is

$$N_2\int u^2F_2dc = N_2\left(u_{02}^2 + RT_2\right).$$

And $n\overline{v'^2}$ can be written as

$$n\overline{v'^2} = N_1\int v'^2F_1dc + N_2\int v'^2F_2dc = N_1RT_1 + N_2RT_2.$$

Substituting the expressions of $\overline{u'^2}$ and $\overline{v'}$ into Eq. (6.35), one obtains

$$\tau_{xx} = \frac{2}{3}m\left(nu_0^2 - N_1u_{01}^2 - N_2u_{02}^2\right).$$

Substitution of Eq. (6.30) and Eq. (6.31) enable the above equation to be written as

$$\frac{n}{m}\tau_{xx} = \frac{2}{3}\left[\left(N_1u_{01} + N_2u_{02}\right)^2 - N_1\left(N_1 + N_2\right)u_{01}^2 - N_2\left(N_1 + N_2\right)u_{02}^2\right] =$$

$$-\frac{2}{3}N_1N_2\left(u_{01} - u_{02}\right)^2 = -\frac{2}{3}N_1\left(n_1 - N_1\right)\frac{u_{01}}{u_{02}}\left(u_{01} - u_{02}\right)^2. \qquad (6.36)$$

In writing the last equality Eq.(6.32) has been employed.

Now discuss the left hand side term of Eq. (6.33). Similarly with the evaluation of $n\overline{u^2}$, according to the definition

$$n\overline{u^3} = N_1\int_{-\infty}^{\infty} u^3F_1dc + N_2\int_{-\infty}^{\infty} u^3F_2dc =$$

$$N_1u_{01}\left(u_{01}^2 + 3RT_1\right) + N_2u_{02}\left(u_{02}^2 + 3RT_2\right) =$$

$$N_1u_{01}\left(u_{01}^2 + 3RT_1 - u_{02}^2 - 3RT_2\right) + n_1u_{01}\left(u_{02}^2 + 3RT_2\right).$$

With the help of Eq. (6.28) the expression ($\left(u_{01}^2 + 3RT_1 - u_{02}^2 - 3RT_2\right)$) can be written as $(2/5)(u_{01}^2 - u_{02}^2)$, and the latter is independent of x, so one has

$$\frac{d\left(n\overline{u^3}\right)}{dx} = \frac{2}{5}u_{01}\left(u_{01}^2 - u_{02}^2\right)\frac{dN_1}{dx}. \qquad (6.37)$$

Substituting Eq. (6.36) (through Eq. (6.34)) and Eq. (6.37) into the moment equation (6.33) yields the equation relative to $N_1(x)/n_1$

$$\frac{d(N_1/n_1)}{d(x/\lambda_1)} = -\alpha(N_1/n_1)\left(1 - \frac{N_1}{n_1}\right), \tag{6.38}$$

where

$$\alpha = \frac{5}{3\pi^{1/2}} \frac{(2kT_1/m)^{1/2}}{u_{02}} \frac{u_{01} - u_{02}}{u_{01} + u_{02}}. \tag{6.39}$$

The solution of Eq. (6.38) is

$$\frac{N_1}{n_1} = \frac{1}{1 + \exp[\alpha(x/\lambda_1)]}. \tag{6.40}$$

Substituting this expression of $N_1(x)$ and that of $N_2(x)$ (obtained from Eq. (6.32)) into Eq. (6.23), one obtains the distribution function of the entire shock wave transition zone. The density across the shock transition zone (with the employment of Eq. (6.30) and Eq. (6.32)) is

$$n(x) = N_1(x) + N_2(x) = N_1 + (n_1 - N_1)\frac{u_{01}}{u_{02}} = N_1\left(1 - \frac{n_2}{n_1}\right) + n_2,$$

i.e.,

$$\frac{n}{n_1} = \frac{n_2}{n_1}\left(1 - \frac{N_1}{n_1}\right) + \frac{N_1}{n_1}.$$

Substituting Eq. (6.40) into it yields

$$\frac{n}{n_1} = \frac{1 + \frac{n_2}{n_1}\exp(\alpha x/\lambda_1)}{1 + \exp(\alpha x/\lambda_1)}. \tag{6.41}$$

The post and pre shock density ratio n_2/n_1 can be expressed through the *Ma* number in front of the shock (see for example [13]), e.g., for monatomic molecules the specific heat ratio $\gamma = 5/3$, one has

$$\frac{n}{n_1} = \frac{1 + \frac{4Ma^2}{3 + Ma^2}\exp(\alpha x/\lambda_1)}{1 + \exp(\alpha x/\lambda_1)}. \tag{6.42}$$

The solution of Mott-Smith is extended by Muckenfus [14] to other inverse power law molecular models. When the power is chosen by fitting the viscosity law, the Mott-Smith method under relatively strong *Ma* number can predict fairly well the shock structure. The result of the method is dependent on the choice of u^2 as the object of averaging in the moment method [15]. Despande and Narasimha [16] pointed out that the employment of u^3 should be better than the employment of u^2. However, the main problem of the Mott-Smith method is it could not provide the correct description of the distribution function (see section 7.1).

The moment methods are mostly applied to steady one-dimensional problems, for example the heat transfer problem between two plates [17] and the problem of evaporation of the plane condensed phase [18], and others. Gross and others employed also the moment method in solving the Couette flow [3] and Rayleigh problem [4] staring from the linearised Boltzmann equation. For the two-dimensional and axi-symmetric flows it is difficult to construct distribution function suitable for the flow field.

6.4 MODEL EQUATIOINS

The Boltzmann equation (Eq. (2.152))

$$\frac{\partial f}{\partial t}+\boldsymbol{c}\cdot\frac{\partial f}{\partial \boldsymbol{r}}+\boldsymbol{F}\cdot\frac{\partial f}{\partial \boldsymbol{c}}=\left(\frac{\partial f}{\partial t}\right)_c \equiv \int_{-\infty}^{\infty}\int_{0}^{4\pi}\left(f^* f_1^* - f f_1\right) c_r \sigma d\Omega d\boldsymbol{c}_1 \tag{6.43}$$

causes so tremendous difficulties to the mathematical solution for the complexity of the right hand side collision term, that many researchers proposed the employment of simplified collision term or collision model to replace it. The most famous model equation was put forward by Bhatnagar, Gross and Krook [19] and is called the *BGK equation* (also was called Krook equation). This equation has the following form

$$\frac{\partial f}{\partial t}+\boldsymbol{c}\cdot\frac{\partial f}{\partial \boldsymbol{r}}+\boldsymbol{F}\cdot\frac{\partial f}{\partial \boldsymbol{c}}=\nu\left(f_e - f\right), \tag{6.44}$$

where $f_e = f_e(c_0, T)$ is the local equilibrium distribution or Maxwellian distribution and is the function of the density ρ, the flow velocity c_0 and the temperature T, and they are obtained by integration of f (see Eq. (2.5), Eq. (2.8) and Eq. (2.31))

$$f_e = \frac{n}{\left(2\pi \frac{k}{m} T\right)^{3/2}} \exp\left[-\frac{(c_i - c_{0i})^2}{2\frac{k}{m}T}\right], \tag{6.45}$$

$$n = \int f dc, \tag{6.46}$$

$$c_{0i} = \frac{1}{n} \int c_i f dc, \tag{6.47}$$

$$T = \frac{1}{3\frac{k}{m} n} \int (c_i - c_{0i})^2 f dc. \tag{6.48}$$

So the equation (6.44) is still a non-linear integral-differential equation, ν is the collision frequency, it is proportional to the density and is related to the temperature but is not dependent on the molecular velocity. Welander [20] almost simultaneously independently proposed the same model equation, so this equation sometimes is also called Boltzmann-Krook-Welander equation (for short *BKW equation*).

It is evident that BGK equation gives the correct solution $f = f_0$ at equilibrium. It also provides the correct collision-less and free molecular solution, for here the collision term is irrelevant. Employing the Chapman-Enskog method to the BGK equation yields the conservation equations having the form of Navier-Stoke equations (for detail see Vincenti and Kruger [21]), unfortunately, the transport coefficients thus obtained, i.e. the viscosity and the heat conductivity, do not possess the correct values.

The collision integral of the Boltzmann equation is the sum of two terms : one term involves $-f(c)f(c_1)$, meaning the depletion of the molecules of class c

caused by collisions, the other involves $f\left(c^{*}\right)f\left(c_{1}^{*}\right)$, meaning the increase of the number of molecules of this class caused by collisions.

In the model equation (6.44) the term $-\nu f$ is used to replace the collision term in the Boltzmann equation causing the depletion of the c molecules. This can have some explanation for a peculiar but not realistic molecular model, i.e., the Maxwallian molecules. The function $f(c)$ in the second term at the right hand side of Eq. (6.43) is independent of c_1, and can be taken out of the symbol of integration, and the remaining expression

$$\int_{-\infty}^{\infty}\int_{0}^{4\pi} f_1 c_r \sigma d\Omega dc_1 \tag{6.49}$$

in general is dependent on c, for $c_r = c - c_1$, but in the specific case of Maxwell molecules it is independent of c, and is the collision frequency ν [1]. So this term of the BGK equation gained some kind of proof for the Maxwell molecules.

Replacement of the first term on the right hand side of the Boltzmann equation (6.43) by νf_e does not have such a kind of proof. We only can understand it as an assumption, i.e., the number of molecules scattered out of the c class in collisions is assumed to be equal to the number of molecules scattered out of the c class by the molecules in local equilibrium with a collision frequency independent of the molecular velocity.

Employing the Chapman-Enskog method to the BGK equation yields the conservation equations in the form of Navier-Stoke equations with the transport coefficients ([21], p.384, Eq. (3.13))

$$\mu_{BGK} = \frac{nkT}{\nu}, \tag{6.50}$$

$$K_{BGK} = \frac{5}{2}\left(\frac{k}{m}\right)\frac{nkT}{\nu}. \tag{6.51}$$

---

[1] The expression of the collision frequency ν is Eq. (2.206), when $\sigma_T c_r$ is independent of c_r, it can be written as the product of Eq. (6.49) and $\frac{1}{n}\int_{-\infty}^{\infty} f dc = 1$.

At the same time for the Boltzmann equation Chapman-Enskog method yields the following values of μ and K ([22], p.226, p.247)

$$\mu = 0.499 \rho \bar{c} \lambda , \tag{6.52}$$

$$K = \frac{15}{4} \frac{k}{m} \left(0.499 \rho \bar{c} \lambda \right) . \tag{6.53}$$

For ensuring a reasonable expression for μ one can adopt an expedient measure, i.e., instead of $\nu = \bar{c} / \lambda$ the following expression is used for the collision frequency

$$\nu = \left(\pi / 3.992 \right) \left(\bar{c} / \lambda \right) . \tag{6.54}$$

Thus the viscosity coefficient obtained from the BGK equation would have the correct expression equal to Eq. (6.52). This is beneficial for solving the flow problem with momentum exchange as the dominant effect, for it can lead to correct reference parameters. But for flow problems with dominant energy exchanges to ensure a reasonable expression for K the following expression for the collision frequency should be adopted

$$\nu = \left(\pi / 5.988 \right) \left(\bar{c} / \lambda \right) . \tag{6.55}$$

Thus the conductivity coefficient K_{BGK} (Eq. (6.51)) obtained from the BGK equation would have the correct expression Eq. (6.53). Unfortunately, it is impossible to ensure μ and K to have the correct expressions simultaneously. From Eq. (6.50) and Eq. (6.51) it is seen, that for the BGK model the Prandtl number $Pr_{BGK} = c_p \mu_{BGK} / K_{BGK} = 1$ does not have the correct value of 2/3. This is already an indication of the limitation of this expedient measure, it is powerless in solving problems involving momentum and energy exchanges of equal importance.

The BGK model equation is widely used in the transitional regime for its simplicity. For problems of small disturbance deviated not far from the equilibrium, the shortcoming of the approximation of the BGK equation becomes not so remarkable. For the Maxwellian molecules it has been proved that the linear form of the BGK equation is the first term of a model-series approximating the Boltzmann equation with arbitrary accuracy. There is a number of small disturbance problems with practical meaning that are solved using the BGK model but not the Boltzmann equation. Some methods of statistical models for constructing the collision term has been put forward which can provide with correct Prandtl number (see e.g. [24]). For the system of Boltzmann equations of multi-component gas the right hand sides involve the self-collision operator for molecules of one component and cross-collision operators for molecules from various components. For the self-collision operator the BGK model is applicable, for the cross-collision operators Boley and Yip [25] put forward the theory of obtaining the model equation basing on the eigenfunction theory and obtained the system of model equations for multi-component gas. There have been many works devoted to the research and the application of the model equations on solving small disturbance problems of simple geometry.

The BGK equation after all is an approximation using a simplified term to replace the exact term basing on solid physical reality. Its applicability scope must be tested and verified by the experiments or exact computations. The DSMC method has stood the strict test of the experiment (see next Chapter) and has the merit of verified solution to test various approximation models. We simulated the problem of the gas flow caused by the sudden wall temperature change and the Rayleigh problem using the DSMC method with the employment of Maxwellian molecular model [26, 27] and compared the results with the exact numerical results of solution of the BGK equation [28]. Fig.6.1 shows this comparison. From this figure it is seen that near equilibrium (in 1~2 collision times) the BGK equation yields correct results (in agreement with the DSMC result), but when far from equilibrium (after 5 or more collision times from the starting of the flow) the BGK model equation is inexact (deviated from the correct DSMC simulation result).

The idea of the BGK equation considering the transition of a gas from its present state to equilibrium as a simple relaxation process is applied to the solution of the Euler equation and the Navier-Stokes equations. In section 5.2 we have seen that the zero order approximation of the Chapman-Enskog expansion in the solution of the Boltzmann equation gives the Euler equation, the first order approximation gives the Navier-Stokes equations. Employment of the Chapman-Enskog

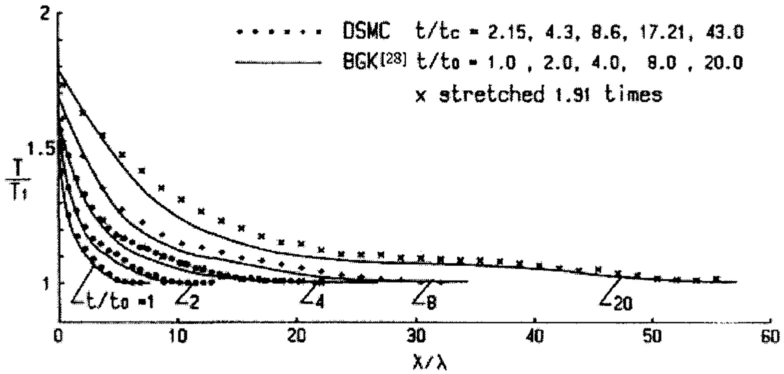

Fig. 6.1 Transients of temperature in the sudden temperature change problem. Comparison of DSMC simulation [26] and BGK calculation [28]. In BGK the expedience of modifying collision frequency is made

method to the BGK equation yields the same result. This leads Xu et al. to put forward the *gas kinetic scheme* for solving the fluid mechanics equations [29].

For the two-dimensional flows the BGK equation in the x direction can be written as

$$\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}=\frac{g-f}{\tau}, \tag{6.56}$$

where for convenience the symbol is changed into g to denote the equilibrium state the distribution function f approaches, τ is the reciprocal of the collision frequency ν or the collision time of the particles. The equilibrium Maxwell distribution, when the thermal motion in the third dimension is considered as the internal energy, can be written as

$$g=n\left(\frac{\beta^2}{\pi}\right)^{\frac{N+2}{2}}\exp\left[-\beta^2\left((u-u_0)^2+(v-v_0)^2+\xi^2\right)\right],$$

where ξ is the variable of internal degree of freedom and includes the internal energy of the gas and the thermal motion in the z direction. The total number of freedom of ξ is $N=(5-3\gamma)/(\gamma-1)+1$, $(5-3\gamma)/(\gamma-1)$ is the number of freedom of the internal energy (see Eq. (4.40)).

The BGK kinetic scheme starts from the solution of the BGK equation (6.56) at $x_{j+1/2}$ of the grid boundary surface

$$f\left(x_{j+\frac{1}{2}},t,u,v,\xi\right)=\frac{1}{\tau}\int_0^t g\left(x',t',u,v,\xi\right)e^{-(t-t')/\tau}dt'+e^{-t/\tau}f_0\left(x_{j+\frac{1}{2}}-ut\right), \tag{6.57}$$

where $x'=x_{j=1/2}-u(t-t')$ is the trajectory of the motion of the particle, and f_0 is the initial distribution function at the star of every time step ($t=0$). For obtaining f the unknown functions g and f_0 in Eq. (6.57) should be determined. For the sake of simplifying the notation in the following $x_{j+1/2}=0$ is used to represent the position of $x_{j+1/2}$.

In the early BGK scheme f_0 is supposed to be

$$f_0=\begin{cases} g^l\left(1+a^l x\right), x\leq 0 \\ g^r\left(1+a^r x\right), x\geq 0 \end{cases}. \tag{6.58}$$

g^l and g^r are the Maxwell distributions on the left hand side and the right hand side of the cell boundary. The slopes a^l and a^r are obtained from the space derivatives of the Maxwell distribution, the latter has the unique relation of correspondence with the slopes of the conservation variables. The basic assumption here is, even when there is discontinuity on the cell boundary, the gas on both sides of the discontinuity is assumed to be in equilibrium states. Such an assumption is suitable for the case when the cell size Δx is large in comparison with the thickness of the shock or the case of Euler equation. For the case when Δx is small and the shock structure can be distinguished, i.e., when deal with the Navier-Stokes equations, the initial distribution f_0 should present the deviation from the equilibrium Maxwell distribution and describe the interior structure of the shock transition zone. So in the recent gas kinetic BGK scheme method aiming at the application on equation solution the initial distribution function f_0 is assumed to be

$$f_0=\begin{cases} g^l\left[1+a^l x-\tau\left(a^l u+A^l\right)\right], x\leq 0 \\ g^r\left[1+a^r x-\tau\left(a^r u+A^r\right)\right], x\geq 0 \end{cases}. \tag{6.59}$$

The additional terms $-\tau(a^l u + A^l)g^l$, $-\tau(a^r u + A^r)g^r$ are the deviations of the non-equilibrium state obtained from the Chapman-Enskog expansion of the BGK equation from the Maxwell distribution.

The equilibrium state g to which the initial distribution f_0 approaches in the recent version [30] is supposed to have two slopes at the two sides of the cell boundary and have time derivative

$$g = g_0\left[1 + \left(1 - H(x)\right)\overline{a^l}x + H(x)\overline{a^r}x + \overline{A}t\right], \tag{6.60}$$

where $H(x)$ is the Heaviside function defined as

$$H(x) = \begin{cases} 0, x < 0 \\ 1, x \geq 0 \end{cases},$$

and g_0 is the local Maxwell distribution at $x = 0$.

It is noted, f_0 is discontinuous at the boundary surface $x = 0$, on each side of the boundary it is the non-equilibrium distribution function in local cell, g is continuous at $x = 0$, but has different slopes at $x < 0$ and at $x > 0$. $a^l, a^r, A^l, A^r, \overline{a^l}, \overline{a^r}$ and $\overline{A}$ characterize the deviations from the equilibrium Maxwell state in space and time. Their determination see reference [30].

Substituting thus obtained f_0 and g into Eq. (6.57) yields the distribution function $f(x_{j+1/2}, t\, \mu, v, \xi)$ of the gas at the cell boundary. The fluxes of the mass, momentum and energy across the cell boundary can be obtained by searching the moments relative to f. The technical details in the application of the gas kinetic BGK scheme can not be explained here thoroughly (see [29, 30]). Here only confine to noting that as the distribution function is introduced in the method, at the wall the reflection model of the molecule surface interaction can be applied to obtain the changes of the mass, momentum and energy of the molecules on the boundary (suitable for the entire transitional regime). This under small Kn number corresponds to the introduction of the slip boundary condition. Besides, after ensuring the correct viscosity coefficient μ through the modification of the computation result of the heat flux the method can guarantee also the correct conductivity coefficient K, so the correct Pr number is assured.

The method has been applied to the Couette flow with temperature gradient, the shock wave structure, the two-dimensional Mach=3 step flow, the interaction of the laminar boundary layer with shock wave etc. (see reference [30]. As the efficiency of the gas kinetic scheme is higher than that of the DSMC method, validation of the accuracy of the scheme by the DSMC or experimental results in its applications to the near continuum and transitional regime is an interesting issue having practical meaning.

Li and Zhang attempted to find a *gas kinetic unified algorithm* to solve the transitional flow bridging the free molecular flow to the continuum flow [31]. The starting point is that the basic equation of the kinetic theory is replaced by the model equation, the latter adopted the so called S-model equation [32] developed by Shakhov from the BGK model. The authors introduced the discrete velocity method, adapted the Gause-Hermite method of quadrature, applied and developed the method of quadrature of Hua and Wang approximating multiple integral by single sums, and employed the equally spaced three-point composite Newton-Cotes quadrature formula, and implemented the solution of the model equation successfully. The method was applied to one-dimensional shock-tube problems, the flows past two-dimensional circular cylinder, and the three-dimensional flows around sphere and spacecraft with various Knudsen numbers. In the case where the experimental data are available (the drags of the cylinder and sphere) the agreement with experiment is fairly good. It is desirable to have more exact quantitative comparison. The transplantation of the method to the solution of the Boltzmann equation is of value.

6.5 THE FINITE DIFFERENCE METHOD

The most natural numerical method in solving the Boltzmann equation is analogous to the finite difference method in the computational fluid dynamics(CFD). The velocity distribution function is the unique dependent variable, but in general (three-dimensional and unsteady flow) it is a function of seven independent arguments, and it is a difficult task to solve it by the finite difference method. If allocate in each dimension 100 cells, then for the 3-D unsteady flow 10^{14} cells is required, and in addition the velocity space is infinite. The upper bound of the finite velocity should be chosen reasonably to make the problem manageable. This leads to even larger difficulty to the hypersonic flow, for in this case there are some molecules having velocity much larger than that of most molecules, although they constitute only a small portion of all the molecules, but have strong influence on the whole macroscopic motion.

Except the above difficulty the peculiar trouble in solving the Boltzmann equation by CFD method is of course in the computation of the collision term. The computation of the collision integral requires for each phase point the summation over all points of the other velocity space, requires finding the contribution of the reverse collision for each collision and each term should be summed over all impact parameters of the collision. So the methods of the solution of the Boltzmann equation are mainly embodied in the treatment of the computation of the collision integral.

Nordsieck and Hicks [33] and Yen et al. [34] suggested a method of Monte-Carlo quadrature of the collision term of the Boltzmann equation. Replacement of the direct numerical quadrature by this Monte-Carlo quadrature reduced the computation time by a factor of 10^{-4}. The infinite velocity space was firstly replaced by the finite velocity domain R, which was taken large enough to involve all except 0.1% molecules. The Monte-Carlo quadrature is to replace the integration over the domain R by the product of the mean of the values of the under-integral expression at N randomly chosen points and the volume of R. The error of this replacement is proportional to $N^{-1/2}$. The under-integral expression is the function of 8 arguments, i.e., c^*, c and two impact parameters. For the fluid dynamics terms on the left hand side of the equation the ordinary finite difference method was employed. Here the usual problems of dependence on the grid and the computational stability would be encountered. Nordsieck et al. by using this method solved some one-dimensional problems including the structure of shock wave problem etc., satisfactory results were obtained

Tcheremissine, Aristov and others developed the algorithm to use the finite difference method for solving the Boltzmann equation (for relatively recent references see [36] and works cited there). In the computation of the collision integral the Monte-Carlo quadrature method is still used, but some improvements are introduced. The symmetry of the binary collision is utilized to remarkably reduce the arithmetic amount and a special projection technique is introduced for the calculation of the collision integral to ensure the conservation of mass, momentum and energy. These accelerated the solution process and enable to use the method to solve some unsteady, 2-D and 3-D problems.

6.6 DISCRETE ORDINATE METHOD

In section 2.11 of Chapter 2 on the example of Couette flow we studied in detail the 8 velocity gas model introduced by Broadwell [37], in which the velocities of molecules can assume only 8 magnitudes $c_1, c_2, \cdots, c_8$ (see Fig.2.9). Such an approach of using finite number of discrete velocities to replace the entire velocity space is called the *discrete ordinate or discrete velocity method*. In an 8 velocity gas the number density of the molecules having a certain velocity can be counted, and corresponding to 8 velocities there are 8 number densities $n_1, n_2, \cdots, n_8$. The velocity distribution function of the gas now is degenerated into the set of 8 number densities. For the molecules of class 1 Boltzmann equation is degenerated into (see Eq. (2.141))

$$\frac{\partial n_1}{\partial t} - q\frac{\partial n_1}{\partial x} + q\frac{\partial n_1}{\partial y} = 2\theta\left(n_2 n_3 - n_1 n_4\right)/n . \tag{6.61}$$

Analogously, the equations for molecules of classes 2, 3, and 4 can be written

$$\frac{\partial n_2}{\partial t} + q\frac{\partial n_2}{\partial x} + q\frac{\partial n_2}{\partial y} = 2\theta\left(n_1 n_4 - n_2 n_3\right)/n , \tag{6.62}$$

$$\frac{\partial n_3}{\partial t} - q\frac{\partial n_3}{\partial x} - q\frac{\partial n_3}{\partial y} = 2\theta\left(n_1 n_4 - n_2 n_3\right)/n , \tag{6.63}$$

$$\frac{\partial n_4}{\partial t} + q\frac{\partial n_4}{\partial x} - q\frac{\partial n_4}{\partial y} = 2\theta\left(n_2 n_3 - n_1 n_4\right)/n , \tag{6.64}$$

where q is the magnitude of the projection of velocity on the rectangular coordinate system, θ is a magnitude proportional to the collision frequency and equals to $0.7v$ (see Eq. (2.142)), n is the number density of the gas, for the case of low speed to be discussed here $n = const$. In deriving the above equations two-dimensional flow is assumed: the flow characteristics are not dependent on z, hence the symmetry condition holds

$$n_1 = n_5, \quad n_2 = n_6, \quad n_3 = n_7, \quad n_4 = n_8 . \tag{6.65}$$

Now we continue to examine with the help of the 8 velocity gas the problem of *shear flow between two plates* or *the Couette flow*, i.e., two plates separated by a distance d moving in the x, z plane in opposite directions, the velocity in the y direction is 0:

$$V = \sum_{i=1}^{8} v_i n_i / n = 0 .$$

Thus one has

$$n_1/n + n_5/n + n_2/n + n_6/n = n_3/n + n_7/n + n_4/n + n_8/n = \frac{1}{2} .$$

From the symmetry condition Eq. (6.65) we have

$$n_1/n + n_2/n = n_3/n + n_4/n = \frac{1}{4} . \tag{6.66}$$

This condition makes the equations (6.62) and (6.64) out of the system (6.61)~(6.64) superfluous, and Eq. (6.61) and Eq. (6.63) can be written as

$$\frac{\partial n_1}{\partial t} + q\frac{\partial n_1}{\partial y} = \frac{\theta}{2}\left(-n_1 + n_3\right), \tag{6.67}$$

$$\frac{\partial n_3}{\partial t} - q\frac{\partial n_3}{\partial y} = -\frac{\theta}{2}\left(-n_1 + n_3\right). \tag{6.68}$$

For the steady flow $\partial/\partial t = 0$, by introducing the dimensionless quantities

$$\eta = y/d, \quad \alpha = \theta d/2q ,$$

the equations (6.67) and (6.68) can be written as

$$\frac{dn_1}{d\eta} = \alpha\left(-n_1 + n_3\right), \tag{6.69}$$

$$\frac{dn_3}{d\eta} = \alpha\left(-n_1 + n_3\right). \tag{6.70}$$

The boundary conditions for the Couette flow problem are

$$U\Big|_{\eta=\frac{1}{2}} = -\frac{1}{2}U_w, U\Big|_{\eta=-\frac{1}{2}} = \frac{1}{2}U_w .$$

The mean velocity in the x direction leaving the upper plate at $\eta = 1/2$ and the mean velocity in the x direction leaving the lower plate at $\eta = -1/2$ are

$$\begin{aligned}
&q^2\left[-n_3\left(\frac{1}{2}\right)+n_4\left(\frac{1}{2}\right)\right]\Big/q\left[n_3\left(\frac{1}{2}\right)+n_4\left(\frac{1}{2}\right)\right] = -\frac{1}{2}U_W ,\\
&q^2\left[-n_1\left(-\frac{1}{2}\right)+n_2\left(-\frac{1}{2}\right)\right]\Big/q\left[n_1\left(-\frac{1}{2}\right)+n_2\left(-\frac{1}{2}\right)\right] = \frac{1}{2}U_W ,\\
&n_1\left(-\frac{1}{2}\right)\Big/n = \frac{1}{8}\left(1 - U_W/2q\right),\\
&n_3\left(-\frac{1}{2}\right)\Big/n = \frac{1}{8}\left(1 - U_W/2q\right).
\end{aligned} \tag{6.71}$$

The solution of equations (6.69) and (6.70) satisfying Eq. (6.71) is

$$n_1/n = \frac{1}{8}\left[\frac{\alpha}{(\alpha+1)}\frac{U_W}{q}\eta + 1 - \frac{1}{2(\alpha+1)}\frac{U_W}{q}\right], \tag{6.72}$$

$$n_3/n = \frac{1}{8}\left[\frac{\alpha}{(\alpha+1)}\frac{U_W}{q}\eta + 1 + \frac{1}{2(\alpha+1)}\frac{U_W}{q}\right]. \tag{6.73}$$

The velocity of the fluid in the direction of x is obtained from the above density solution

$$U = \sum_i u_i\left(n_i/n\right) = 2q\left[-n_1/n + n_2/n + n_3/n - n_4/n\right] = -\frac{\alpha}{(\alpha+1)}U_{W\eta} . \tag{6.74}$$

The shear stress is

$$\tau_{yx} = \rho \sum_i u_i v_i (n_i/n) = 2\rho q^2 [-n_1 + n_2 + n_3 - n_4]/n =$$

$$4\rho q^2 (-n_1 + n_3)/n = \frac{1}{2(\alpha+1)} \rho q U_W . \tag{6.75}$$

Expressing τ_{ij} as $\mu(\partial U/\partial y)$, from Eq. (6.74) the expression of μ can be obtained

$$\mu = \rho q d/2\alpha = \rho q^2 \theta .$$

Substituting $\theta = 0.70\bar{c}/\lambda$ and $q = \bar{c}/\sqrt{3}$ yields

$$\mu = 0.48 \rho \bar{c} \lambda . \tag{6.76}$$

Although this value is quite close to the viscosity expression Eq. (2.222) of the Chapman-Enskog approximation for the hard sphere model, but if examine the value of τ_{ij} in the entire transitional regime (when $Kn = \lambda / d$ is between 0.01 and 100) then the result of the discrete ordinate method of the 8 velocity approximation is not so good. This is undoubtedly the result of adopting a too simple discrete velocity model to replace the continuous velocity space.

Broadwell in [37] investigated also the Rayleigh problem using the 8 velocity model. He also tested the 6 velocity model (6 velocities with equal speed value and pointed into the positive and negative directions of the x,y,z axes) applying it to the study of shock wave structure [38]. Gatignol utilized the coplanar 6 velocity model [39] (pointed into the apexes of a right hexagon) to investigate the shock wave structure and the Couette flow, and with help of the coplanar 4 velocity model [40] discussed the boundary conditions and the H theorem in the discrete velocity model. Cabannes [41] introduced the 14 velocity model (combined from the Broadwell 8 velocity and 6 velocity models) and investigated the Couette flow problem. A result of universal meaning is that when 4 velocities in the flow plane is eliminated from the 14 velocities the result on the contrary is improved. The reason for this is that the molecules moving along the direction of the surface do not collide with the surface, are isolated from the surface, the existence of such parasitic molecules causes the errors at the wall. Gatignol [42] and Cabannes [43] introduced in general form the discrete velocity model, utilizing the set of $c_1, c_2, \cdots, c_p$ to replace the entire velocity space and n_i to represent the number density in time t at position $\boldsymbol{r}$ having velocity c_i, and write the discrete Boltzmann equation (compare Eqs. (6.61)~(6.64))

$$\frac{\partial n_i}{\partial t} + c_i \cdot \frac{\partial}{\partial \boldsymbol{r}} n_i = \sum_{j=1}^{p} \sum_{(k,l)} A_{ij}^{kl} \left(n_k n_l - n_i n_j \right), \quad i = 1, 2, \cdots, p, \tag{6.77}$$

where A_{ij}^{kl} is the transition probability

$$A_{ij}^{kl} = \sigma_T c_{rij} p_{ij}^{kl}, \tag{6.78}$$

no summation convention is implied in Eq. (6.78)

$$\sum_{k,l} p_{ij}^{kl} = 1, \text{ valid for any } i,\ j. \tag{6.79}$$

p_{ij}^{kl} is the probability the pair of molecules with velocities c_i, c_j before collision changes into pair of molecules with velocities c_k, c_l after collision. An often used model is the one in which the ends of the velocity vectors are the uniformly distributed grid points in the phase space [44, 45]. Fig 6.2 shows a peculiar example of such model in planar case with the values of velocity components equal to semi-integers

$$\begin{cases} u = \left(n + \dfrac{1}{2} \right) \Delta v, -5 \le n \le 4, \\ v = \left(n + \dfrac{1}{2} \right) \Delta v, -5 \le n \le 4, \\ \Delta v / \sqrt{2kT/m} = 0.667. \end{cases} \tag{6.80}$$

The semi-integer points are chosen because the molecules with velocities parallel with the body surface would cause errors near the wall as indicated in reference

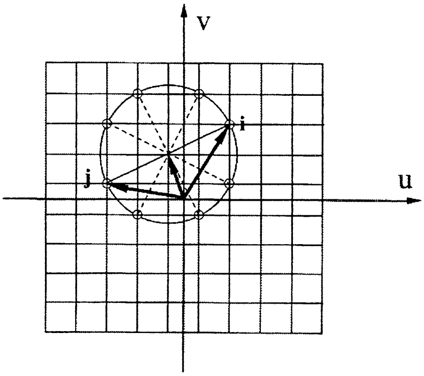

Fig. 6.2 The model with the ends of the velocity vectors as uniformly distributed grid points is shown in planar case. In the figure are shown $c_i(1.5,2.5)$ and its certain collision partner $c_j(-2.5,0.5)$ and the possible velocity pairs c_k, c_l after collision (shown by small circles, altogether 4 of them)

[41]. For such a model Eq. (6.77) is written for each $c_i(u,v)$ (in Fig 6.2 the case $c_i = (1.5\,\Delta x, 2.5\Delta x)$ is shown). The partner c_j of molecule c_i goes through the whole p velocity set (in the present example $p = 10\times 10$, the figure shows the case of $c_j = (-2.5\Delta x, 0.5\Delta x)$). The conservation of momentum and energy yields the invariance of the value of the relative velocity ($|c_i - c_j|$, in the present example $= \sqrt{20}\Delta v$) and the invariance of the velocity of the mass center. So all the after collision velocity pairs lay on the circle with center at the end of the velocity vector of the mass center and diameter of the value of the relative velocity. In the figure the velocity pairs from set $c_1, c_2, \cdots, c_p$ satisfying such condition are shown by the small circles connected by dashed lines (there are 4 pairs in the present example). For hard sphere model the appearance of all after collision pairs are of equal probability. The probability p_{ij}^{kl} in Eq. (6.77) is easily calculated

$$p_{ij}^{kl} = 1/N_{ij}\text{, valid for any } k,\ l, \tag{6.81}$$

where $N_{i,j}$ is the number of all possible c_k, c_l pairs after collision resulted from the pre -collision c_i, c_j pairs. According to the discussion about the reverse collision in Chapter 2, the collision $(c_k, c_l \to c_i, c_j)$ is the reverse collision of $(c_i, c_j \to c_k, c_l)$. So we have $p_{ij}^{kl} = p_{kl}^{ij} = p_{lk}^{ji}$, this result has been employed in writing Eq. (6.77).

The above expounding of the discrete velocity model and the discrete Boltzamnn equation is only a kind of physical heuristic elucidation, the relationship of them with the Boltzmann equation still requires strict mathematical proof. In 1994 Bobylev et al. [46] proved that the uniform grid discrete velocity model [44, 45, 47] converges to the Botzmann equation and gave an estimate of the error of the quadrature by the discrete velocity method. This is an important development of the discrete velocity method. From the heuristic explanation of the method for the planar case where the ends of the velocity-vector pairs are situated on a circle and at the same time are on the nodal points of a integer grid, it is understandable why this mathematical proof is closely relevant to a congruence problem in number theory related with the presentation of a integer number by the sum of three squires. An assertion in number theory states: any number t which is not congruent to 7 relative to 8 ($t \neq 7(\text{mod}8)$) can be represented as the sum of three squires $t = p^2 + q^2 + r^2$, and the number of ways of presentation grows sufficiently fast with t.

Gatignol [48] discussed the boundary condition problem of the discrete velocity model in detail. Despite the above progresses on the whole the problems solved by the discrete velocity method are mainly of simple geometry and molecular models.

6.7 INTEGRAL METHODS

The Boltzmann equation (2.152) can be written in the following form

$$\frac{df}{dt} = J_1(t, r, c) - fJ_2(t, r, c), \tag{6.82}$$

where

$$J_1 = \int_{-\infty}^{\infty} \int_{0}^{4\pi} f^* f_1^* \, \varsigma\sigma \, d\Omega dc_1 , \tag{6.83}$$

$$J_2 = \int_{-\infty}^{\infty}\int_{0}^{4\pi} f_1 c_r \sigma d\Omega dc_1 . \tag{6.84}$$

The differentiation is carried along a certain molecular trajectory. Equation (6.82) can be considered as a ordinary differential equation relative to f

$$\frac{df}{dt} + fJ_2(t,f) = J_1(t,f) . \tag{6.85}$$

Suppose the f in J_1 and J_2 of Eq. (6.85) is known, the formal solution of the first order linear ordinary differential equation can be written

$$f(t,\boldsymbol{r},\boldsymbol{c}) = f\left(t_0,\boldsymbol{r} - \boldsymbol{c}(t - t_0),\boldsymbol{c}\right)\times$$

$$\exp\left\{-\int_{t_0}^{t} J_2\left(s,\boldsymbol{r} - \boldsymbol{c}(t-s),\boldsymbol{c}\right)ds\right\} + \int_{t_0}^{t} J_1\left(\tau,\boldsymbol{r} - \boldsymbol{c}(t-\tau),\boldsymbol{c}\right)\times$$

$$\exp\left\{-\int_{\tau}^{t} J_2\left(s,\boldsymbol{r} - \boldsymbol{c}(t-s),\boldsymbol{c}\right)ds\right\}d\tau . \tag{6.86}$$

The right hand side of Eq. (6.86) includes unknown function f and is a integral equation relative to f . This is the Boltzmann equation in the integral form.

Vallander [49] presented the direct physical derivation of the integral equation (6.86) without citing on the Boltzmann equation, he initiated the method of solving the rarefied gas dynamics problems basing on the integral form of the basic equation, i.e., the integral method [50]. The most convenient approach of searching solution of the integral equation is of course the method of iteration. The iteration method of the integral equation is utilized to prove the existence theorem of the solution of the Boltzmann equation.

6.8 DIRECT SIMULATION METHODS

These are the methods different from those of numerical solution of the Boltzmann equation but based directly on the simulation of the physics of the flow.

They were born with the appearance of the electronic computers and are fully developed with the enhancement of the speed and the capacity of the computers. Direct simulation methods distinguish *deterministic simulation methods* and *probabilistic simulation methods*. Both categories of methods trace the motion of enormous number of molecules, their encounter with the boundaries, the collisions between themselves, the exchange of internal energies during the collisions and chemical reactions, etc. The simulation should ensure that the processes traced in the computer are able to reproduce the processes in the real flows. In the computer a time (clock) is introduced synchronously with the physical time in the flows. The positions, velocities and the internal energies of the molecules are recorded, they change due to the motion of the molecules, their interaction with the wall surfaces and the collisions between themselves. Obviously such simulation calculation is an unsteady process. The steady process is obtained as the stabilized state of the unsteady process.

The deterministic direct simulation method is the most early suggested physical simulation method put forward by Alder and Wainwright [51] in 1957, and is called the *molecular dynamics (MD) method*. In this method the probabilistic method is employed only when distribute the initial position and velocities, and when compute the molecular motion, the interaction of molecules with the boundaries and their collisions between themselves, the deterministic method is used without exception. For example, when judge the occurrence of a certain collision, the overlap of the collision cross sections of two mo lecules at the same time is considered and the impact parameters of the collision are provided by the mutual configuration of the molecules, and the velocities after the collision are determined. Such a simulation method aims at the full reproduction of the physical processes, so the size of the molecules, the number density of the molecules and the flow geometry are to be simulated. Thus the number of simulated molecules in a certain simulation region should keep entirely identical with actual situation of the physical flow.

Such a requirement is more apt to be implemented for dense gas than for dilute gas. This point can be explained through the consideration of the number of molecules in a cube with side of one mean free path

$$N_\lambda = n\lambda^3. \tag{6.87}$$

As λ is inversely proportional to the number density n of the molecules, so N_λ is inversely proportional to n^2, with the help of Eq. (2.220) N_λ can be written

$$N_\lambda \equiv n\lambda^3 = \frac{1}{2\sqrt{2}\left(\pi d^2\right)^3 n^2}.$$

If introduce the number density $n_0 = 2.687\times10^{25} m^{-3}$ under the standard state ($p_0 = 0.101325MPa,\ \ T_0 = 273K$), the above equation can be written

$$N_\lambda = \frac{1}{2\sqrt{2}\left(\pi d^2\right)^3 n_0^2}\left(\frac{n_0}{n}\right)^2.$$

For certain definite molecule d is fixed, the expression before $(n_0/n)^2$ is a constant, if take a typical value $d = 4\times10^{-10}m$ (the VHS model gives $d = 4.17\times10^{-10}m$ for nitrogen and $d = 4.07\times10^{-10}m$ for oxygen at $273K$), the required number of molecules is written

$$N_\lambda = 3856\left(\frac{n_0}{n}\right)^2. \tag{6.88}$$

Thus, if study a certain problem involving N_2, O_2 or gas of alike size under standard density using the MD method, around 3856 molecules should be allocated in a cube of mean free path, which will be difficult for a three-dimensional problem with a space scope of many mean free paths. But if study the same problem under a density 100 times higher than the standard state, only less than half (0.39) a molecule is needed to be allocated in a volume of λ^3, or in a cube of side of 10λ allocate around 386 molecules. This is already a relatively easy task. Thus, the molecular dynamics method is particularly suited for the simulation of dense gas or liquid but not for simulating the dilute gas. At the same time the Boltzmann equation is appropriate for the dilute gas where binary collision prevails but not for the dense gas where some modifications are needed, e.g., the Enskog put forward the Enskog equation to take into account the influence of the dense gas. The MD method supplement an additional computational means at the particle level in the domain of dense gas and at the same time is a deterministic method, so it is readily accepted by people working in this field.

The *direct simulation Monte-Carlo (DSMC)* method was put forward by G. A. Bird and was first applied to the simulation of the relaxation in the uniform gas [52] and the shock wave structure [53] problems, and then was developed to the application in simulating two-dimensional, three-dimensional and problems with complex geometry, including cases of flows with complex physic-chemical processes (see the monograph of Bird published in 1976 [54] and the new extended edition 1994 [55]). The DSMC method as the MD method traces in the computer the motion, the collisions and the change of internal energies etc. of enormous number molecules, but its specific feature is the employment of the probability processes. Not only the allocation of the initial positions and states of the molecules, but also the judgment of the occurrence and the outcomes of the collisions (including the change of the velocities and the internal energies of molecules), are determined by the test (generation and transformation) of random functions. This is just the origination of the name of Monte-Carlo method[2]. The DSMC method traces the binary collisions in gas, and we see in the discussion at beginning of section 2.3 that the binary collisions are prevailing over the three-body collisions only for dilute gas. So the prerequisite of the probabilistic simulation of collisions is the assumption of the dilute gas. This is entirely different from the MD method suitable for simulation of dense gas. And it is not like the deterministic MD method in which the equality of the number of simulated molecules in the simulation region and the number of molecules in the actual flow is required, but relatively few simulation molecules are used to represent the enormous number of real molecules. This is another difference between the DSMC method and the MD

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[2] Monte-Carlo – a city in Monaco dukedom, the world famous gambling city. The Monte-Carlo method is so called because the implementation of its process depends on the generation and transformation of the uniform random number as the outcome in the turntable gambling depends on where the arrow stops. Von Neumann and Ulam put forward this method when studying the reactor in 1949. The method is also called method of statistical test.

method. In the early stage of the method the product of the number density and the collision cross section is kept identical for the simulated molecules and in the real flow (so the mean free path similarity is gained) to ensure the similarity law of *Kn* number. This led to very huge molecular size but did not have any essential influence on the simulation. The present approach is to fix the number of actual molecules a simulated molecule represents and take this into account when calculate the collision number and the macroscopic quantities. The key point of the DSMC method is also in the decoupling of the molecular motion and collision in a time stepΔt. Each molecule moves a distance according to its velocity and Δt (taking into account the interaction with the boundary and the motion after reflection) and then calculate the representative collisions corresponding to this time interval Δt.The foundation of algorithm of choosing the representative collisions to ensure the identity of the motion and collisions in the simulation and in the real flow is the kinetic theory of gases. In fact the assumption of molecular chaos and dilute gas is the prerequisite for both the Boltzmann equation and the DSMC method. And Bird proved that following the procedures of the DSMC method the Boltzmann equation can be derived [56]. Wagner et al. proved that the DSMC method converges to the Boltzmann equation [57, 58].

The *test molecule Monte-Carlo method* put forward by Haviland and Levin [59] was one of the probabilistic simulation methods developed the earliest. The Monte-Carlo method developed by Kogan in the book [60] is also a test molecule method. This kind of method requires the initial estimate of the distribution function over the grid of the flow field and the allocation of the so called target molecules. Then the trajectories of numerous so called test molecules are calculated, their collisions with the target molecules are considered and the new distribution of the target molecules is established basing on the trajectories of the test molecules. Iterate such processes until convergence is reached. This method was limited to the one dimensional steady flow owing to the necessity of starting the iteration from the supposed known initial distribution and the proportionality of the computation time to the number of trajectories of the test molecules.

Nanbu developed a version of DSMC method directly derived from the Boltzmann equation [61], the main feature of it is that only one of the two molecules involved in each collision changes its velocity, this is consistent with the fact that the dependent variable of the Boltzmann equation is the single molecule distribution function. Thus, the momentum and energy conservation in each collision is not satisfied. However, the Boltzmann equation does not require such conservation but requires the overall conservation of the physical space quantities, the momentum and the energy, and this is satisfied in the simulation. The problem is: when the molecular momentum and energy is not exactly conserved but is only conserved in the average sense, the random walk is brought about, that is, the deviation from the mean value grows with the squire root of time. This must be taken into account when dealing with small disturbance or low speed problems. Babovsky gave the strict proof of the convergence of the method of Nanbu to the Boltzmann equation [62].

REFERENCES

1. Cercignani C (1969) Mathematical Methods in Kinetic Theory. Plenum Press
2. Cercignani C (1975, 1987) Theory and Application of the Boltzmann Equation, Scottish Academic; The Boltzmann equation and Its Applications, Springer
3. Gross EP and Ziering S(1958) Kinetic theory of linear shear flow. Phys. of Fluids, 1: 213-224
4. Gross EP and Jackson EA. (1958) kinetic theory of the impulsive motion of an infinite plate. Phys of Fluids, 1: 318
5. Grad H (1963) Asymptotic theory of the Boltzmann equation. In: JA Laurmann edited Rarefied Gas Dynamics, Academic, 1:26-59
6. Cercignani C (1975, 1987) See [2] Chapter 4, sec 5
7. Sone Y, Ohwada T and Aoki K (1989) Temperature jump and Knudsen layer in a rarefied gas over a plane wall. Phys. of Fluids, A1: 363-370
8. Sone Y, Ohwada T and Aoki K (1989) Evaporation and condensations of plane condensed phase. Phys. of Fluids, A1: 1398-1405
9. Ohwada T, Sone Y and Aoki K (1989) Numerical analysis of the shear and thermal creep flows of a rarefied gas over a plane wall. Phys. of Fluids A1: 1588-1599
10. Ohwada T, Sone Y and Aoki K (1989) Numerical analysis of the Poiseuille and thermal transpiration flows of a rarefied gas between two parallel plates. Phys. of Fluids A1: 2042-2049

11.Sone Y, Takata S and Ohwada T (1990) Numerical analysis of the plane Couette flow of a rarefied gas. Eur J Mech., B/Fluids, 9: 273-288

12.Mott-Smith HM (1951) The solution of the Boltzmann equation for a shock wave. Phys. Re.v, 82:855-892

13.Shapiro AH. (1953) Compressible Fluid Flow. Ronald Press, 1: 118

14.Muckenfuss C (1962) Some aspects of shock structure according to the bimodal model. Phys. of Fluids, 5: 1325

15.Rode DL, Tanenbaum BS (1962) Mott-Smith shock thickness using the v_x^p method, Phys. of Fluids, 10: 1352

16.Deshpande SM and Narasimha R (1969) The Boltzmann collision integrals for a combination of Maxwellians. J Fluid Mech., 36: 545

17.Liu CY and Lees L (1961) Kinetic theory description of plane compressible Couette flow. In: L Talbot edited Rarefied Gas Dynamics, Academic Press, NY, 391

18.Ostmo S, Ytrehus T (1995) Strong evaporation in a dusty polyatomic gas. In: J Harvey and G Lord edited Rarefied Gas Dynamics 19, 1: 291

19.Bhatnagar P L, Gross E P and Krook M. (1954) A model for collision processes in gases. I, Phys. Rev., 94: 511-525

20.Welander P (1954) On the temperature jump in a rarefied gas. Ark Fys, 7: 507-553

21.Vincenti WG and Kruger CH Jr (1965) Introduction to Physical Gas Dynamics. John Wiley & Sons

22.Chapman S, Cowling TG (1970) The Mathematical Theory of Non-uniform Gases, 3rd ed., Cambridge Univ. Press

23.Gross EP and Jackson EA (1959) Kinetic models and the linearized Boltzmann equation. Phys. of Fluids, 2: 432-441

24.Holway LH Jr (1966) New statistical models for kinetic theory: methods of construction. Phys. of Fluids, 9: 1658

25.Boley CD and Yip S (1972) Modeling theory of the linearized collision operator for a gas mixture. Phys. of Fluids, 18: 1424-1433

26.Shen C, Xu XY, Hu ZH and Wu WQ (1994) Transient motion of rarefied gas caused by heat addition simulated by DSMC method. In: BD Shizgal and DP Weaver edited Rarefied Gas Dynamics, Progress in Astronautics and Aeronautics, 159: 234-242

27.Shen C, Yi Z (2000) Direct numerical test of the BGK model equation by the DSMC method. Acta Mechanica Sinica, 16: 133

28.Aoki K, Sone Y, Nishino K, Sugimoto H (1991) Numerical analysis of motion of rarefied gas caused by sudden change of wall temperature. In: AE Beylich edited Rarefied Gas Dynamics, VCH, 222-231

29.Xu K (1993) Numerical Hydrodynamics from Gas Kinetic Theory. Ph D thesis, Columbia University

30.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

31.Li ZH and Zhang HX, (2003) Study on gas kinetic unified algorithm for flows from rarefied transition to continuum. Acta Aerodynamica Sinica, 21: 255-266 (in Chinese)

32.Shakhov EM (1985) Kinetic model equations and numerical results. In: H Oguch edited Rarefied Gas Dynamics, Univ. of Tokyo Press, 1:137-148

33.Nordsieck A, Hicks BL (1967) Monte Carlo evaluation of the Boltzmann collision integral. In: C L Brundin edited Rarefied Gas Dynamics, Academic Press, 675-710

34.Yen SM. (1970) Monte Carlo solutions of nonlinear Boltzmann equations for problems of heat transfer in rarefied gases. International J of Heat Mass Transfer, 14: 1865-69

35.Hicks BL, Yen SM and Reiley BJ (1972) The internal structure of shock waves. J Fluid Mech., 53:85-112

36.Tcheremissine FG (1999) Solution of the Boltzmann equation for arbitrary molecular potentials. In: R Brun et al. edited Rarefied Gas Dynamics, 2: 165-172

37.Broadwell JE (1964) Study of rarefied flow by the discrete velocity method. J Fluid Mech., 19: 404-414

38.Broadwell JE (1964) Shock structure in a simple discrete velocity gas. Phys. of Fluids, 7: 1243

39.Gatignol R (1975) Kinetic theory for a discrete velocity gas and application to the shock structure. Phys. of Fluids 18: 153

40.Gatignol R (1977) Kinetic theory boundary conditions for discrete velocity gases. Phys. of Fluids, 20: 2022

41.Cabannes H (1976) Couette flow for a gas with a discrete velocity distribution. J Fluid Mech., 76: 273

42.Gatignol R (1975) Theorie Cinetique des Gas a Repartition Discrete de Vitesses. Lecture Notes in Physics, Springer, Berlin, 36

43.Cabannes H (1980) The Discrete Boltzmann Equation, Lecture Notes, Univ. of California, Berkeley

44.Goldstein D, Sturtevent B and Broadwell JE (1989) Investigation of the motion of discrete velocity gases. In Progress in Astro-Aeronautics, 118: 100

45.Inamuro T, Sturtevent B (1990) Numerical study of discrete velocity gases. Phys. of Fluids, A2: 2196

46.Bobylev AV, Palczewski A and Schneider J (1995) Discretization of the Boltzmann equation and discrete velocity models. In: J Harvey and G Lord edited Rarefied Gas Dynamics 19, Oxford Univ. Press, Oxford, 2: 857

47.Rogier F and Schneider J (1994) A direct method for solving the Boltzmann equation. Transport Theory and Statist. Physics, 23: 313

48.Gatignol R. (1997) Boundary conditions in discrete kinetic theory-application to the problem of evaporation and condensation, In: C Shen edited Rarefied Gas Dynamics 20, Peking Univ. Press, 253-262

49.Vallander SV (1960) Doklady Akad Nauk SSSR, 131 (1) (in Russian)

50.Aerodynamics of Rarefied Gases, collected works, (1963-) edited by SV Vallander, Leningrad Univ. Press, vol.1-vol.10 (in Russian)

51.Alder BJ and Wainwright TE (1957) Studies in molecular dynamics. Journal of Chem. Physics, 27: 1208-1209

52.Bird GA (1963) Approach to translational equilibrium in a rigid sphere gas. Phys. of Fluids, 6: 1518-1519

53.Bird GA (1965) Shock wave structure in a rigid sphere gas. In: J H de Lesuw edited Rarefied Gas Dynamics, 1: 216-222, Ac. Press

54.Bird GA (1976) Molecular Gas Dynamics, Clarendon Press

55.Bird GA (1994) Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Clarendon Press, Oxford

56.Bird GA (1970) Direct simulation of the Boltzmann equation. Phys. of Fluids, 13: 2676-2681

57.Wagner W (1992) A convergence proof for Bird's direct simulation Monte Carlo method for the Boltzmann equation. J Stat Phys, 66: 1011

58.Pulvirenti M, Wagner W and Zavelani MB (1994) Convergence of particle schemes for the Boltzmann equation. Euro J Mech., B7: 339

59.Haviland JK and Lavin ML (1962) Applications of the Monte Carlo method to heat transfer in a rarefied gas. Phys. of Fluids, 5: 1399-1405

60.Kogan MN (1969) Rarefied Gas Dynamics. Plenum Press

61.Nanbu K (1980) Direct simulation scheme derived from the Boltzmann equation. I Multi-component gases, J Phys Soc Japan, 45: 2042-2049

62.Babovsky H (1989) A convergence proof for Nanbu's Boltzmann simulation scheme. Euro J Mech. B: Fluids, 8 (1): 41-45