Towards fully conservative numerical methods for the nonlinear model Boltzmann equation

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Abstract

A conservative modification of the conventional discrete ordinate method for the nonlinear model Boltzmann equation with Shakhov's collision integral is proposed. The conservation property for arbitrary Knudsen numbers is achieved by satisfing the discrete analogues of conservation laws as well as the boundary conditions exactly, up to machine precision. Additionally, the method ensures the correct approximation of the heat flux.

Key words: kinetic equation, BGK model, Shakhov's model, conservative method.

1 Introduction

Developing numerical methods for the exact and model Boltzmann kinetic equation represents a real challenge for the method's designer. This is due to the nonlinear character and very high dimension of these equations. For small Knudsen numbers an additional difficulty arises: the numerical method must be conservative. Conservative methods for kinetic equations are the methods from which after numerical integration with respect to molecular velocity on the discrete grid the discrete conservation laws for the mass, momentum and energy of the gas follow. Nonconservative methods produce non-physical source terms in the conservation equations of order of $O(\mathrm{Kn}^{-1})$. Therefore, they may not converge to the proper solution as the Knudsen number is decreased unless the velocity grid is substantially refined. Due to the highly nonlinear character of the kinetic equation, both exact and model ones, the conservation property is very difficult to satisfy.

A fully conservative numerical method of discrete ordinates for the exact Boltzmann equation has been developed in [6]. Since the exact and model collision integrals are quite different it is not clear how this method can be applied to the model equation.

In this paper we propose a way of constructing conservative methods for the nonlinear model equation with Shakhov's collision integral [11, 12], which permits computations with arbitrarily small Knudsen numbers on a fixed molecular velocity grid. The conservation property for arbitrary Knudsen numbers is achieved by satisfying the discrete analogues of conservation laws as well as the boundary conditions exactly, up to machine precision. Additionally, the method ensures the correct approximation of the heat flux.

The rest of the paper is organized as follows. In Sections 2 and 3 we review the exact and model Boltzmann equations. A conventional (non-conservative) discrete ordinate method is described in Section 4. The notion of conservative methods is discussed in Section 5. In Sections 6 and 7 we describe the new conservative procedures for evaluation of macroparameters of the gas and boundary values of the velocity distribution function. A numerical example is given in Section 8 and conclusions are drawn in Section 9.

2 The exact kinetic equation

For a monatomic gas the Boltzmann kinetic equation for the velocity distribution function $f(t, \vec{r}, \vec{\xi})$ in non-dimensional form can be written as follows:

$$\frac{\partial f}{\partial t} + \xi_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{1}{\mathrm{Kn}} \int (f' f'_1 - f f_1) g \, d\sigma d\vec{\xi_1} \equiv \frac{1}{\mathrm{Kn}} J(f, \vec{\xi}). \tag{1}$$

Here t is time, $\vec{r} = (x_1, x_2, x_3) = (x, y, z)$ is spatial coordinate, $\vec{\xi} = (\xi_x, \xi_y, \xi_z)$ – molecular velocity, $J(f, \vec{\xi})$ is the Boltzmann collision integral, $d\sigma = bdbd\varepsilon$, $g = |\vec{\xi} - \vec{\xi}_1|$. The parameter Kn is called the Knudsen number.

The macroparameters of the gas, such as number density n, temperature T and vectors of gas velocity u_i and heat flux q_i are computed as the integrals of the distribution function

over the molecular velocity:

$$n = \int f d\vec{\xi}, \quad nu_i = \int \xi_i f d\vec{\xi}, \quad E = \int \xi_i \xi^2 f d\vec{\xi},$$
$$q_i = \frac{1}{2} m \int (\xi_i - u_i)(\vec{\xi} - \vec{u})^2 \, f \, d\vec{\xi}, \quad d\vec{\xi} = d\xi_x d\xi_y d\xi_z, \quad i = 1, 2, 3 \tag{2}$$

The collision integral has the fundamental property of conserving mass, momentum and energy of colliding molecules, which is expressed by the following equations:

$$\int \varphi(\vec{\xi}) J(f, \vec{\xi}) d\vec{\xi} = 0, \quad \varphi(\vec{\xi}) = 1, \ \vec{\xi}, \ \xi^2. \tag{3}$$

The quantities 1, $\vec{\xi}$, ξ^2 are called collision invariants. Multiplying the kinetic equation by these invariants and integrating with respect to $\vec{\xi}$ we obtain conservation equations [12]

$$\left.\begin{aligned} \frac{\partial}{\partial t} n + \frac{\partial}{\partial x_\alpha} n u_\alpha = 0, \\ \frac{\partial}{\partial t} n u_i + \frac{\partial}{\partial x_\alpha} (n u_i u_\alpha + P_{i\alpha}) = 0, \\ \frac{\partial}{\partial t} (n u^2 + 3p) + \frac{\partial}{\partial x_\alpha} (n u^2 u_\alpha + 3 p u_\alpha + 2 u_\beta P_{\alpha\beta} + 2 q_\alpha) = 0, \end{aligned}\right\} \tag{4}$$

where $i = 1, 2, 3$. In the limit of small Knudsen numbers the application of Chapman-Enskog procedure to (4) produces the compressible Navier-Stokes equations.

The kinetic equation must be supplied with initial and boundary conditions. The initial condition for the kinetic equation is set as:

$$f(0, \vec{r}, \vec{\xi}) = f_0(\vec{r}, \vec{\xi}) \tag{5}$$

where quite often $f_0(\vec{r}, \vec{\xi})$ is chosen to be a locally Maxwellian function of the initial distribution of macroparameters:

$$f_0(\vec{\xi}) = \frac{n_0(\vec{r})}{(\pi T_0(\vec{r}))^{3/2}} \exp\left(- \frac{(\vec{\xi} - \vec{u}_0(x))^2}{T_0(x)} \right). \tag{6}$$

The boundary conditions of diffusive reflection of molecules from rigid bodies are defined as follows. Let $\vec{n}$ be a normal unit vector of the body, and $\vec{\xi}_n = (\vec{\xi}, \vec{n})$ be the component of molecular velocity normal to the body. Then the distribution function of reflected molecules $f_w(\vec{\xi})$ is

$$f_w = \frac{n_w}{(\pi T_w)^{3/2}} \exp\left(- \frac{\xi^2}{T_w} \right), \quad \xi_n > 0, \quad \int\limits_{\xi_n < 0} \xi_n f d\vec{\xi} + \int\limits_{\xi_n > 0} \xi_n f_w d\vec{\xi} = 0, \tag{7}$$

where n_w and T_w are density and temperature of reflected molecules. The second equation in (7) expresses the condition that there is no mass flux through a rigid body and defines n_w. The temperature of reflected molecules T_w can be defined in two ways. In the

case of the cold body the temperature is given and equal to the body temperature T_s. Alternatively, for a heat-insulated body T_w is found from the condition that the energy flux through the surface of the body be equal to zero:

$$\int\limits_{\xi_n<0} \xi_n \xi^2 f d\vec{\xi} + \int\limits_{\xi_n>0} \xi_n \xi^2 f_w d\vec{\xi} = 0. \tag{8}$$

More precisely, n_w and T_w are computed as the solution of system (7),(8):

$$T_w = \frac{\int\limits_{\xi_n<0} \xi_n \xi^2 f d\vec{\xi}}{2\int\limits_{\xi_n<0} \xi_n f d\vec{\xi}}, \quad n_w = 2\sqrt{2\pi}\,(T_w)^{-1/2} \int\limits_{\xi_n<0} \xi_n f d\vec{\xi}. \tag{9}$$

3 The nonlinear model kinetic equation

Although considerable progress has been made in developing accurate methods for the exact Boltzmann equation [1, 2, 6, 10] it is still very costly and difficult to solve on modern computers. This is mostly because of the five-dimensional collision integral which must be computed at each point of the space mesh. Moreover, even for spatially one-dimensional problems all three components of $\vec{\xi}$ must be preserved resulting in excessive memory requirements.

There are two main alternatives to solving the exact kinetic equation. The first is the Monte-Carlo methods [3, 4]. The version due to Bird is probably the most commonly used tool for simulating rarefied flows. The second alternative is to develop model kinetic equations for pseudo-Maxwellian molecules by replacing the exact five-dimensional collision integral by a model collision integral. Probably the first such model is the so-called BGK (or Krook) model [5]. A more accurate model, which is a generalization of the BGK model, is due to Shakhov [11, 12] and is written as follows:

$$\frac{\partial f}{\partial t} + \xi_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{1}{\mathrm{Kn}} \nu (f^+ - f) \equiv \frac{1}{\mathrm{Kn}} Q(f, \vec{\xi}),$$

$$\nu = \frac{8}{5\sqrt{\pi}} \frac{nT}{\mu}, \quad f^+ = f_m \left(1 + \frac{4}{5}(1-\mathrm{Pr}) S_\alpha c_\alpha (c^2 - 5/2)\right), \tag{10}$$

$$f_m = \frac{n}{(\pi T)^{3/2}} \exp(-c^2), \quad S_i = \frac{1}{n} \int c_i c^2 f \, d\vec{\xi}, \quad c^2 = c_\alpha c_\alpha, \quad c_i = \frac{\xi_i - u_i}{\sqrt{T}}.$$

Here f_m is the locally Maxwellian function, Pr is Prandtl number ($\mathrm{Pr} = 2/3$ for a monatomic gas). We assume summation over repeated greek indexes. The BGK model can be formally obtained from the Shakhov model by setting $\mathrm{Pr} = 1$.

The model collision integral $Q(f, \vec{\xi})$ contains unknown parameters n, $\vec{u}$, T, $\vec{q}$. These parameters are determined by the condition that the model kinetic equation should approximate the exact Boltzmann kinetic equation in terms of momentum equations, that

is few first momentum equations should coincide for the model and exact kinetic equations. Since the differential parts of the equations are the same, this is equivalent to the condition that first few moments of the model and exact collision integrals coincide.

For the Shakhov model we have the following eight conditions to determine the unknowns:

$$\int \varphi(\vec{\xi}) J(f,\vec{\xi}) d\vec{\xi} = \int \varphi(\vec{\xi}) Q(f,\vec{\xi}) d\vec{\xi}, \quad \varphi(\vec{\xi}) = 1, \quad \vec{\xi}, \quad \xi^2, \quad \vec{\xi}\xi^2. \tag{11}$$

We note that the first five equations in (11) coincide with (4). Integrating with respect to $\vec{\xi}$ and taking into account that for pseudo-Maxwellian molecules [12]

$$\int \vec{\xi}\xi^2 J(f,\vec{\xi}) d\vec{\xi} = -\frac{4}{3}\nu\vec{q} \tag{12}$$

we obtain the conventional expressions (2). Therefore, the unknown parameters in the model collision integral are in fact macroparameters of the gas.

The last three equations in (11) ensure that application of the Chapman-Enskog procedure to the model equation yields correct values of viscosity and heat conductivity coefficients for small Knudsen numbers Kn. This property constitutes a major advantage of the Shakhov's model over the BGK model for which the wrong Prandtl number is obtained.

4 Discrete ordinate method

A standard approach to solve the model kinetic equation with given boundary and initial conditions is the so-called discrete ordinate method. In this method the exact integration with respect to molecular velocity $\vec{\xi}$ over all velocity space is replaced by an approximate numerical integration over a finite domain using a discrete set of points in $\vec{\xi}$ space. Let $\vec{\xi}_{klm}$ be a node in (ξ_x, ξ_y, ξ_z) grid, $f_{klm} = f(t,\vec{r},\vec{\xi}_{klm})$, $f^+_{klm} = f^+(t,\vec{r},\vec{\xi}_{klm})$. Then the kinetic equation (1) is replaced by a system of equations for f_{klm}:

$$\frac{\partial f_{klm}}{\partial t} + (\xi_{klm})_\alpha \frac{\partial f_{klm}}{\partial x_\alpha} = Q_{klm}, \quad Q_{klm} = \frac{1}{\mathrm{Kn}}\nu(f^+_{klm} - f_{klm}). \tag{13}$$

For the given value $\vec{\xi}_{klm}$ each of equations (13) can be solved using any modern advection scheme. For example, a semi-discrete scheme can be written as

$$\frac{\partial f_{klm}}{\partial t} = -\vec{\xi}_{klm} D_h(f_{klm}) + Q_{klm}, \tag{14}$$

where D_h is a conservative numerical approximation to the gradient operator:

$$\begin{aligned}
[D_h(f_{klm})]_{i_x,i_y,i_z} = \quad & \xi_x \frac{(f_{kml})_{i_x+1/2,i_y,i_z} - (f_{kml})_{i_x-1/2,i_y,i_z}}{\Delta x} + \\
& \xi_y \frac{(f_{kml})_{i_x,i_y+1/2,i_z} - (f_{kml})_{i_x,i_y-1/2,i_z}}{\Delta y} + \\
& \xi_z \frac{(f_{kml})_{i_x,i_y,i_z+1/2} - (f_{kml})_{i_x,i_y,i_z-1/2}}{\Delta z}
\end{aligned} \tag{15}$$

Here i_x, i_y and i_z are spatial indexes. Usually, a high order monotone method, such as a TVD method [14] or WENO method [9] is used to compute D_h. Time discretization in (14) can be carried out either in a time splitting manner or by means of a Runge-Kutta method.

Conventionally, macroparameters are evaluated as discrete sums:

$$\begin{gathered} n = \sum_{klm} A_{klm} f_{klm}, \quad n\vec{u} = \sum_{klm} A_{klm} \vec{\xi}_{klm} f_{klm}, \quad E = \sum_{klm} A_{klm} (\xi_{klm})^2 f_{klm}, \\ \vec{q} = \sum_{klm} A_{klm} (\vec{\xi}_{klm} - \vec{u})(\vec{\xi}_{klm} - \vec{u})^2 f_{klm}, \end{gathered} \tag{16}$$

and so on. Here A_{klm} are weights of the integration rule.

The boundary conditions are treated in a similar way. The numerical integration yields

$$T_w = \frac{1}{2} \frac{\sum\limits_{klm, \xi_n<0} (\xi_n)_{klm} \xi_{klm}^2 f_{klm} C_{klm}}{\sum\limits_{klm, \xi_n<0} \xi_n f d\vec{\xi}}, \quad n_w = 2\sqrt{2\pi} \, (T_w)^{-1/2} \sum_{klm, \xi_n<0} (\xi_n)_{klm} f_{klm} C_{klm}), \tag{17}$$

where C_{klm} are weights of the integration rule at the boundary.

Usually, a high order integration rules, such as Simpson or Gauss rules, are employed in the molecular velocity space.

The outlined framework of the discrete ordinate method has been used quite often recently, e.g. [15, 13], with good results.

5 The conservation property

Now we come to a very important property of numerical methods – the conservation property. Following [1, 2] we call the numerical method conservative if two conditions are satisfied. Firstly, the summation of (14) with weights 1, $\vec{\xi}_{klm}$, ξ_{klm}^2 using the given integration rule of the method produces the discrete analogues of conservation laws (4). Secondly, discrete analogs of (7), (8) hold.

When a conservative advection scheme is used in (14) the first condition essentially means that 1, $\vec{\xi}_{klm}$ and ξ_{klm}^2 are collision invariants of the discrete collision integral Q_{klm}:

$$\sum_{klm} \frac{1}{\mathrm{Kn}} \nu A_{klm} \varphi_{klm} Q_{klm} = 0 \quad \text{for} \quad \varphi = 1, \quad \vec{\xi}_{klm}, \quad \xi_{klm}^2. \tag{18}$$

The second condition leads to the following equations:

$$\begin{aligned} \sum_{klm,\, \xi_n>0} (\xi_n)_{klm} (f_w)_{klm} C_{klm} + \sum_{klm,\, \xi_n<0} (\xi_n)_{klm} f_{klm} C_{klm} &= 0, \\ \sum_{klm,\, \xi_n>0} (\xi_n)_{klm} \xi_{klm}^2 (f_w)_{klm} C_{klm} + \sum_{klm,\, \xi_n<0} (\xi_n)_{klm} \xi_{klm}^2 f_{klm} C_{klm} &= 0. \end{aligned} \tag{19}$$

Conservative methods do not produce non-physical sources of mass, momentum and energy and therefore in the limit of small Knudsen numbers (continuous flow regime) the

kinetic solution approaches the solution of Navier-Stokes equations away from boundaries. Basically, such methods mimic the conservation property of the collision integral (3) on any discrete molecular velocity grid. On the contrary, as will be shown below, for non-conservative methods very fine meshes in $\vec{\xi}$ space are needed to keep the conservation error small when the Knudsen number decreases.

In addition to the conservation property, given the locally Maxwellian distribution f_0, one would also like the numerical integration with respect to $\vec{\xi}$ to reproduce the initial values of macroparameters, namely $n_0(x)$, $\vec{u}_0(x)$, $T_0(x)$, $\vec{q}_0(x) = 0$. This is sometimes called *compatibility with the initial distribution of macroparameters* [2].

It is obvious that a conventional discrete ordinate method, given by (14), (16), (17) is not conservative and is not compatible with the initial data. The numerical integration of (14) with respect to $\vec{\xi}$ leads to conservation equations with the vector of numerical source terms given by

$$\vec{\delta} = \frac{1}{\mathrm{Kn}}\nu \sum_{klm} \begin{pmatrix} 1 \\ \xi_x \\ \xi_y \\ \xi_z \\ \xi^2 \end{pmatrix}_{klm} (f^+_{klm} - f_{klm}) A_{klm}, \tag{20}$$

or

$$\vec{\delta} = \frac{1}{\mathrm{Kn}}\nu \left[\sum_{klm} \begin{pmatrix} 1 \\ \xi_x \\ \xi_y \\ \xi_z \\ \xi^2 \end{pmatrix}_{klm} f^+_{klm} A_{klm} - \int \begin{pmatrix} 1 \\ \xi_x \\ \xi_y \\ \xi_z \\ \xi^2 \end{pmatrix} f^+ \, d\vec{\xi} \right]. \tag{21}$$

Essentially, the conservation error arises from the fact that expressions (16),(17) can be regarded as produced by performing exact integration for f^+ and f_w and numerical integration for f in (2), (7), (8). Assuming that A_{klm} gives an r^{th} order integration rule and $\Delta\xi$ is the cell size in $\vec{\xi}$ mesh, the expression for $\vec{\Delta}$ can be written as

$$|\vec{\delta}| \approx \frac{1}{\mathrm{Kn}} \mathrm{const}\ \nu \, (\Delta\xi)^r \, . \tag{22}$$

From (22) it is obvious that $\vec{\delta} \to \infty$ as $\mathrm{Kn} \to 0$ unless the velocity grid is refined. In the case of small Knudsen numbers $\vec{\delta}$ can be very large. In practical calculations one cannot afford a fine mesh for $\vec{\xi}$ due to excessive memory requirements. As a result, computing flows with $\mathrm{Kn} \leq 10^{-2}$ becomes difficult.

Given the distribution function f the macroparameters are computed with an error, proportional to $(\Delta\xi)^r$. This explains why the numerical method is not compatible with the initial data. Although the error is small, due to the present of the large numerical source term of order of $\frac{1}{\mathrm{Kn}} (\Delta\xi)^r$, it grows rapidly with time.

A similar conservation error occurs at the boundary; however, it does not depend directly on the Knudsen number.

Conservation of the method can be restored by using some kind of a correction procedure at each time step. Such procedures were developed in [2, 8]. Although good results were obtained for $\mathrm{Kn} = 10^{-2}$ the correction procedure appears to be artificial and it is not clear how well it will work for long time evolution problems for many time steps. For the exact Boltzmann equation a fully conservative method was proposed in [6]; however, it has not yet been applied to the model equation.

In the next section we present a new and very simple procedure for making the numerical method conservative.

6 Restoring conservation away from the boundary

For the Shakhov model the macroparameters of the gas can be defined not as integrals (2) but rather as solutions of approximation equations (11). As was seen in the previous section, the source of conservation errors is the fact that exact integration is applied to f^+, whereas numerical integration is used for the distribution function f producing expressions (16). The error would not occur if instead of using (16) we used equations (11) themselves in the discrete form.

More precisely, we require that the following discrete analogues of (11) hold for each t, $\vec{r}$:

$$\begin{aligned}
\sum_{klm} A_{klm}\,(f^+_{klm} - f_{klm}) &= 0, \\
\sum_{klm} A_{klm}\,(\xi_i)_{klm}\,(f^+ - f)_{klm} &= 0, \qquad i = 1,2,3 \\
\sum_{klm} A_{klm}\,\xi^2_{klm}\,(f^+ - f)_{klm} &= 0, \\
\sum_{klm} A_{klm}\,(\xi_i)_{klm}\,\xi^2_{klm}\,(f^+ - f)_{klm} &= -\frac{4}{3} q_i, \qquad i = 1,2,3
\end{aligned} \tag{23}$$

Eqs. (23) represent a nonlinear system of eight equations for eight unknowns n, $\vec{u}$, T, $\vec{q}$. Note that first five equations are exactly conditions (18) for the method to be conservative away from the boundary. Morever, the last three equations ensure the correct transition to the continuous flow regime as $\mathrm{Kn} \to 0$. For the BGK model, the model collision integral $Q(f, \vec{\xi})$ does not contain the values of $\vec{q}$ and thus it is enough to use only the first five equations in (23).

We use the Newton iteration method to solve system (23). Let n be an iteration number. The Newton iterations are then written as

$$K(W^{n+1} - W^n) = B, \tag{24}$$

where W is the vector of unknown macroparameters and B is the vector of errors:

$$W = \begin{pmatrix} n \\ u \\ v \\ w \\ T \\ q_x \\ q_y \\ q_z \end{pmatrix}, \qquad B = -\begin{pmatrix} \sum\limits_{klm} A_{klm}(f^+ - f)_{klm} \\ \sum\limits_{klm} A_{klm}[\xi_x(f^+ - f)]_{klm} \\ \sum\limits_{klm} A_{klm}[\xi_y(f^+ - f)]_{klm} \\ \sum\limits_{klm} A_{klm}[\xi_z(f^+ - f)]_{klm} \\ \sum\limits_{klm} A_{klm}[\xi^2(f^+ - f)]_{klm} \\ \sum\limits_{klm} A_{klm}[\xi_x\xi^2(f^+ - f)]_{klm} + \frac{4}{3}q_x \\ \sum\limits_{klm} A_{klm}[\xi_y\xi^2(f^+ - f)]_{klm} + \frac{4}{3}q_y \\ \sum\limits_{klm} A_{klm}[\xi_z\xi^2(f^+ - f)]_{klm} + \frac{4}{3}q_z \end{pmatrix} \tag{25}$$

K is the Jacobian matrix:

$$K = K_1 + K_2, \qquad K_2 = \mathrm{diag}\left(0,\, 0,\, 0,\, 0,\, 0,\, \frac{4}{3},\, \frac{4}{3},\, \frac{4}{3}\right), \tag{26}$$

$$K_1 = \sum_{klm} A_{klm} \begin{pmatrix} \frac{\partial f^+}{\partial n} & \frac{\partial f^+}{\partial u} & \frac{\partial f^+}{\partial v} & \frac{\partial f^+}{\partial w} & \frac{\partial f^+}{\partial T} & \frac{\partial f^+}{\partial q_x} & \frac{\partial f^+}{\partial q_y} & \frac{\partial f^+}{\partial q_z} \\ \xi_x\frac{\partial f^+}{\partial n} & \xi_x\frac{\partial f^+}{\partial u} & \xi_x\frac{\partial f^+}{\partial v} & \xi_x\frac{\partial f^+}{\partial w} & \xi_x\frac{\partial f^+}{\partial T} & \xi_x\frac{\partial f^+}{\partial q_x} & \xi_x\frac{\partial f^+}{\partial q_y} & \xi_x\frac{\partial f^+}{\partial q_z} \\ \xi_y\frac{\partial f^+}{\partial n} & \xi_y\frac{\partial f^+}{\partial u} & \xi_y\frac{\partial f^+}{\partial v} & \xi_y\frac{\partial f^+}{\partial w} & \xi_y\frac{\partial f^+}{\partial T} & \xi_y\frac{\partial f^+}{\partial q_x} & \xi_y\frac{\partial f^+}{\partial q_y} & \xi_y\frac{\partial f^+}{\partial q_z} \\ \xi_z\frac{\partial f^+}{\partial n} & \xi_z\frac{\partial f^+}{\partial u} & \xi_z\frac{\partial f^+}{\partial v} & \xi_z\frac{\partial f^+}{\partial w} & \xi_z\frac{\partial f^+}{\partial T} & \xi_z\frac{\partial f^+}{\partial q_x} & \xi_z\frac{\partial f^+}{\partial q_y} & \xi_z\frac{\partial f^+}{\partial q_z} \\ \xi^2\frac{\partial f^+}{\partial n} & \xi^2\frac{\partial f^+}{\partial u} & \xi^2\frac{\partial f^+}{\partial v} & \xi^2\frac{\partial f^+}{\partial w} & \xi^2\frac{\partial f^+}{\partial T} & \xi^2\frac{\partial f^+}{\partial q_x} & \xi^2\frac{\partial f^+}{\partial q_y} & \xi^2\frac{\partial f^+}{\partial q_z} \\ \xi_x\xi^2\frac{\partial f^+}{\partial n} & \xi_x\xi^2\frac{\partial f^+}{\partial u} & \xi_x\xi^2\frac{\partial f^+}{\partial v} & \xi_x\xi^2\frac{\partial f^+}{\partial w} & \xi_x\xi^2\frac{\partial f^+}{\partial T} & \xi_x\xi^2\frac{\partial f^+}{\partial q_x} & \xi_x\xi^2\frac{\partial f^+}{\partial q_y} & \xi_x\xi^2\frac{\partial f^+}{\partial q_z} \\ \xi_y\xi^2\frac{\partial f^+}{\partial n} & \xi_y\xi^2\frac{\partial f^+}{\partial u} & \xi_y\xi^2\frac{\partial f^+}{\partial v} & \xi_y\xi^2\frac{\partial f^+}{\partial w} & \xi_y\xi^2\frac{\partial f^+}{\partial T} & \xi_y\xi^2\frac{\partial f^+}{\partial q_x} & \xi_y\xi^2\frac{\partial f^+}{\partial q_y} & \xi_y\xi^2\frac{\partial f^+}{\partial q_z} \\ \xi_z\xi^2\frac{\partial f^+}{\partial n} & \xi_z\xi^2\frac{\partial f^+}{\partial u} & \xi_z\xi^2\frac{\partial f^+}{\partial v} & \xi_z\xi^2\frac{\partial f^+}{\partial w} & \xi_z\xi^2\frac{\partial f^+}{\partial T} & \xi_z\xi^2\frac{\partial f^+}{\partial q_x} & \xi_z\xi^2\frac{\partial f^+}{\partial q_y} & \xi_z\xi^2\frac{\partial f^+}{\partial q_z} \end{pmatrix}_{klm}$$

The iteration process requires an initial guess. This is provided by the conventional expressions (16). Usually, it is enough to do two or three iterations since the Newton process converges very quickly.

For the BGK model $f^+ = f_m$ and the derivatives of f^+ have a very simple form:

$$\frac{\partial f^+}{\partial n} = \frac{1}{n} f^+, \quad \frac{\partial f^+}{\partial u_i} = \frac{2(\xi_i - u_i)}{T} f^+,$$

$$\frac{\partial f^+}{\partial T} = -\frac{1}{2} \frac{3T - 2((\xi_x^2 - u_1)^2 + (\xi_y^2 - u_2)^2 + (\xi_z^2 - u_3)^2)}{T^2} f^+, \tag{27}$$

$$f^+ = f_m = \frac{n}{(\pi T)^{3/2}} \exp\left(-\frac{(\xi_x - u_1)^2 + (\xi_y^2 - u - 2)^2 + (\xi_z^2 - u_3)^2}{T} \right).$$

For the Shakhov's model these derivatives are more complicated. However, one can use some special software, such as the MAPLE package, to obtain the corresponding expressions.

In the case of the spatially two- and one-dimensional flows system (23) becomes smaller as the number of the unknown macroparameters decreases.

7 Restoring conservation at the boundary

A similar procedure can be used while treating boundary conditions. The density and temperature of reflected molecules should be computed as a solution of system (19). Let us introduce the following notation:

$$S_1 = \sum_{klm,\, \xi_n < 0} (\xi_x)_{klm} f_{klm} C_{klm}, \tag{28}$$

$$S_2 = \sum_{klm,\, \xi_n < 0} (\xi_x \xi^2)_{klm} f_{klm} C_{klm}, . \tag{29}$$

We note that S_1, S_2 do not depend on the unknown parameters n_w, T_w.

When the temperature of reflected molecules T_w is given (cold body), the expression for the density n_w is especially simple:

$$n_w = n_w(T_w) = -\frac{(\pi T_w)^{3/2} S_1}{\sum\limits_{klm,\, \xi_n > 0} \left(\xi_n \exp\left(-\xi^2/T_w\right) \right)_{klm} C_{klm}}. \tag{30}$$

For the heat-insulated body we have to solve system (19). Using (30) we eliminate n_w from the equations. Then for the distribution function of reflected molecules f_w we obtain the following expression:

$$f_w(\vec{\xi}) = -\frac{S_1}{\sum\limits_{klm,\, \xi_n > 0} \left(\xi_n \exp\left(-\xi^2/T_w\right) \right)_{klm} C_{klm}} \exp\left(-\frac{\xi^2}{T_w} \right). \tag{31}$$

Inserting the above expression for f_w into the second equation in (19) we arrive at the following equation for the temperature of reflected molecules T_w

$$\sum_{klm,\,\xi_n>0} (\xi_n)_{klm} \left(-S_1\xi^2 + S_2\right)_{klm} \exp\left(-\frac{\xi^2_{klm}}{T_w^2}\right) C_{klm} = 0. \tag{32}$$

This equation can be easily solved using a standard Newton iteration algorithm. The initial guess is again provided by the conventional expressions (17). Having found T_w we evaluate n_w from (30).

8 Numerical example

Consider the uniform distribution of macroparameters with $n = 5$, $u = 2$, $v = w = 0$, $T = 1$, $\vec{q} \equiv 0$. Then the Jacobian matrix (26) has size 3×3. For the sake of simplicity we use the BGK model. Let us also take $\mathrm{Kn} = 10^{-10}$ and $\nu = n$. In this case the solution is $f \equiv f_m$ and macroparameters are equal to the initial values.

The integration with respect to $\vec{\xi}$ is performed in the boundaded domain $|\xi_i| \le 6$ with $\Delta\xi = 0.6$ (20 grid points for each component of $\vec{\xi}$). Let us use the simplest first order integration rule so that $A_{klm} \equiv 1$.

Let us do iterations (24). All calculations will be made with double precision. The initial approximation is

$$n^{(0)} = 4.99999999892187,$$

$$u^{(0)} = 1.99999999897941,$$

$$T^{(0)} = 0.999999996908553.$$

It is obvious that the so-obtained values of density, mean velocity and temperature are very close to the exact one. However the vector b is very large.

$$b(1) = -53.9064900402261,$$

$$b(2) = -362.959800787625,$$

$$b(3) = -2476.36555555463$$

The first iteration gives

$$n^{(1)} = 5.0000000000000,$$

$$u^{(1)} = 2.0000000000000,$$

$$T^{(1)} = 1.0000000000000,$$

and $b(1) = b(2) = b(3) = 0.000000000000000$.

We observe that the conservative algorithm of calculating macroparameters is not only exact for uniform flow but also ensures exact conservation for an arbitrary Knudsen number.

9 Conclusions

A fully conservative modification of the discrete ordinate method for the nonlinear model kinetic equation has been presented. Conservation is achieved by a new way of evaluating macroparameters of the gas and the boundary values of the velocity distribution function. Conservation laws are satisfied for an arbitrary Knudsen number on a fixed molecular velocity grid. Additionally, the correct evaluation of the heat flux is ensured in the limit of small Knudsen numbers.

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