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CONSERVATIVE NUMERICAL METHODS FOR ADVANCED MODEL KINETIC EQUATIONS

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Abstract. *A new conservative discrete ordinate method for nonlinear model kinetic equations is proposed. The conservation property with respect to the collision integral is achieved by satisfying at the discrete level approximation conditions used in deriving the model collision integrals. Additionally to the conservation property, the method ensures the correct approximation of the heat fluxes. Numerical examples of a hypersonic plane flow with large gradients are provided for the Shakhov and Rykov model kinetic equations.*

1 INTRODUCTION

Rarefied gas flows are often described by nonlinear model kinetic equations, which are constructed by replacing the exact collision integral by an approximate model collision integral. Examples include the Krook or BGK,[2] Holway[5] and Shakhov[12,14] model equations for monatomic gases as well as Holway[5] and Rykov[10] model equations for diatomic gases. Numerical solution of these equations requires the use of conservative methods suitable in a broad range of Knudsen numbers and for both steady and unsteady flow regimes. For simple monatomic BGK and Holway model conservative discrete ordinate methods were proposed equations;[4,9] however, these cannot be extended directly to the Shakhov and Rykov models. A rather sophisticated correction procedure was applied in[3] to the Shakhov model collision integral at each time step in such a way as to satisfy the conservation property. Its generalization to other models has not been reported. No conservative method has so far been developed for diatomic models.

The purpose of this paper is to present an exceedingly simple and universal approach to construction of conservative discrete ordinate methods for model kinetic equations. The approach is an extension of[16] and is based on the approximation of the constrains used in deriving the model equations. Therefore, it can be used for virtually any model kinetic equation. We provide a detailed explanation of the idea as applied to the Shakhov model equation and then extend it to the Rykov model equation.

As a numerical example, we consider a supersonic transverse flow over a flat plate at near-continuum regime using both model equations. The presented results illustrate the sensitivity of the method to the choice of the molecular velocity mesh as well as provide a study of distribution of the macroparameters.

2 Monatomic gases

2.1 The model of Shakhov

For monatomic gases a general approach to construction of model kinetic equations was proposed in[11,12,14] and is based on the idea of approximating the exact Boltzmann kinetic equation in terms of momentum equations. Since the differential parts of the exact and model equations are the same, the approximation condition means that first few moments J_φ of exact collision integral $J(f, \boldsymbol{\xi})$ coincide with the first few moments of the model collision integral $Q(f, \boldsymbol{a}, \xi)$:

$$\int \phi Q(f, \boldsymbol{a}, \xi) d\boldsymbol{\xi} = \int \phi J(f, \boldsymbol{\xi}) d\boldsymbol{\xi} = J_\varphi, \tag{1}$$

Here $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)$ is the molecular velocity vector, t is time, $\boldsymbol{r} = (x_1, x_2, x_3)$ is the spatial coordinate, $\boldsymbol{a}$ is an unknown vector of macroparameters which depends on the chosen model equation,

$$\varphi = 1, \quad \xi_i, \quad \xi^2, \quad \xi_i\xi_j, \quad \xi_i\xi_j\xi_k, \ldots$$

Alternatively one can use

$$\varphi = 1, \quad v_i, \quad v^2, \quad v_iv_j, \quad v_iv_jv_k, \ldots, \quad \boldsymbol{v} = \boldsymbol{\xi} - \boldsymbol{u}.$$

As is common in construction of model kinetic equations for the monatomic gas it is assumed that the approximation condition (1) should be satisfied for the maxwellian molecules only. Then the moments J_φ can be evaluated analytically and we can express the vector $\boldsymbol{a}$ via the integrals of the velocity distribution function:

$$\boldsymbol{U}(\boldsymbol{a}) = \int \boldsymbol{b}(\boldsymbol{\xi}) f d\boldsymbol{\xi}, \tag{2}$$

where $\boldsymbol{U}$ is a certain function of macroparameters and $\boldsymbol{b}(\boldsymbol{\xi})$ is a vector function of the molecular velocity $\boldsymbol{\xi}$. As a result, a sequence of model kinetic equations can be developed by increasing the order of moments for which the approximation condition holds.

The Shakhov[12,14] model kinetic equation is a generalization of the Krook[2] model equation in that the approximation condition (1) is satisfied not only for 1, ξ_i, ξ^2, $\xi_i\xi_j$, but also for $\xi_i\xi^2$. This ensures the correct relaxation of both the heat flux and stresses, leading thus to the correct continuum limit in the case of small Knudsen numbers. In particular, the model gives the correct Prandtle number. Comparisons of different monatomic model equations with experimental data and the finite-difference solution of the Boltzmann equation with the exact collision integral shows the Shakhov model to be more accurate than the BGK and Holway models.[15,19]

In the rest of the paper we use the non-dimensional form of the kinetic equations in which non-dimensional spatial variable r, time t, number density n, velocity u, temperature T, viscosity μ, heat flux q and distribution function f are given by

$$\begin{gathered} r' = \frac{r}{L}, \quad t' = \frac{t\sqrt{2RT_\infty}}{L}, \quad n' = \frac{n}{n_\infty}, \quad u' = \frac{u}{\sqrt{2RT_\infty}}, \quad T' = \frac{T}{T_\infty}, \\ \mu' = \frac{\mu}{\frac{5}{16}mn_\infty\sqrt{2\pi RT_\infty}\lambda_\infty}, \quad q' = \frac{q}{mn_\infty(2RT_\infty)^{3/2}}, \quad f' = \frac{f}{n_\infty(2RT_\infty)^{-3/2}}. \end{gathered} \tag{3}$$

Here L is a typical spatial scale of the problem, n_∞, T_∞ - some characteristic values of gas density and temperature; m is the molecule mass, λ_∞ is the mean free path. Below we shall use the conventional notation for all variables meaning the non-dimensional quantities.

In the non-dimensional form the Shakhov model equation is given by[12–14]

$$\begin{gathered} \frac{\partial f}{\partial t} + \boldsymbol{\xi}\frac{\partial f}{\partial \boldsymbol{r}} = Q(f, \boldsymbol{\xi}, \boldsymbol{a}) \quad Q(f, \boldsymbol{\xi}, \boldsymbol{a}) = \nu f^+ - \nu f, \quad \nu = \frac{8}{5\sqrt{\pi}}\frac{1}{\mathrm{Kn}}\frac{nT}{\mu}, \\ f^+ = f_M\left[1 + \frac{4}{5}(1-\mathrm{Pr})\frac{2\boldsymbol{q}\boldsymbol{v}}{nT^2}\left(\frac{v^2}{T} - \frac{5}{2}\right)\right], \quad f_M = \frac{n}{(\pi T)^{3/2}}\exp\left(-\frac{v^2}{T}\right). \end{gathered} \tag{4}$$

Here f_M is the locally-maxwellian function, $\mathrm{Kn} = \lambda_\infty/L$ and Pr are the Knudsen and Prandtle numbers, respectively. The vector of unknown parameters in the model collision integral $\boldsymbol{a} = (n, \boldsymbol{u}, T, \boldsymbol{q})^T$ containing number density n, temperature T and vectors of gas velocity $\boldsymbol{u}$ and heat flux $\boldsymbol{q}$ can be calculated as:

$$\boldsymbol{U}(\boldsymbol{a}) = \left(n, n\boldsymbol{u}, \frac{3}{2}nT + nu^2, 2\boldsymbol{q}\right) = \int (1, \boldsymbol{\xi}, \xi^2, \boldsymbol{v}v^2) f \, d\boldsymbol{\xi}. \tag{5}$$

2.2 Conventional discrete ordinate method and conservation property

A standard approach to solve the model kinetic equation with given boundary and initial conditions is the so-called discrete ordinate method. Its main idea is to replace the exact integration with respect to molecular velocity $\boldsymbol{\xi}$ over all velocity space by an approximate numerical integration over a finite domain using a discrete set of points. Let β be an index of the three-dimensional molecular velocity mesh, $\boldsymbol{\xi}_\beta$ be a node in this mesh, $f_\beta = f(t, \boldsymbol{r}, \boldsymbol{\xi}_\beta)$. Then the model kinetic equation is replaced by a system of equations for f_β:

$$\frac{\partial}{\partial t} f_\beta + \frac{\partial}{\partial \boldsymbol{r}}\left(\boldsymbol{\xi}_\beta f_\beta\right) = Q_\beta, \quad Q_\beta = Q(f_\beta, \boldsymbol{\xi}_\beta, \boldsymbol{a}) \tag{6}$$

which are connected via macroparameters defined as integrals over the entire molecular velocity space. Each of equations (6) can now be solved using a modern high order non-oscillatory scheme. For example, a semi-discrete scheme can be written as

$$\frac{\partial}{\partial t} f_\beta = -D_h(\boldsymbol{\xi}_\beta f_\beta) + Q_\beta, \tag{7}$$

where D_h is a conservative numerical approximation to the advection operator. Conventionally, macroparameters are evaluated by direct approximation of the form

$$\left(n, n\boldsymbol{u}, \frac{3}{2}nT + nu^2, 2\boldsymbol{q}\right) = \sum_{\beta} \left(1, \boldsymbol{\xi}, \xi^2, \boldsymbol{v}v^2\right)_{\beta} f_{\beta} A_{\beta}. \tag{8}$$

Here A_β are weights of the integration rule used in the numerical scheme. Normally one uses a tensor product of one-dimensional quadrature to perform the three-dimensional integration in the molecular velocity space, e.g. the simplest choice corresponds to the first order quadrature and is given by $A_\beta = \Delta\xi^3$.

It is well known that the conservation laws for mass, momentum and energy of the gas can be obtained by multiplying the kinetic equation by collision invariants 1, $\boldsymbol{\xi}$, ξ^2 and integrating over the entire molecular velocity space. It is natural to require that this property be maintained at the discrete level by the numerical method (7),(8). The discrete relations expressing conservation of mass, momentum and energy in the computations are obtained by multiplying (7) by the collision invariants and summing them with the weights A_β:

$$\frac{\partial}{\partial t}\boldsymbol{R} + D_h(\boldsymbol{\Pi}) = \boldsymbol{\delta}.$$

Here the vector of conserved quantities $\boldsymbol{R}$, the flux tensor Π_{ij} and the numerical source term $\boldsymbol{\delta}(\boldsymbol{a}, \mathrm{Kn})$ on the right hand side are given by

$$\boldsymbol{R} = \sum_{\beta} \boldsymbol{l}_{\beta} f_{\beta} A_{\beta}, \quad \boldsymbol{\Pi} = \sum_{\beta} \boldsymbol{l}_{\beta} \boldsymbol{\xi}_{\beta}^T f_{\beta} A_{\beta}, \quad \boldsymbol{\delta} = \sum_{\beta} \boldsymbol{l}_{\beta} Q_{\beta} A_{\beta}, \quad \boldsymbol{l} = (1, \boldsymbol{\xi}, \xi^2)^T.$$

It is obvious, that $\boldsymbol{R}$ coincides with first five components of $\boldsymbol{U}$ defined by (8).

Following[1] we call the numerical method (7) conservative with the respect to the collision integral if the numerical source term vanishes: $\boldsymbol{\delta} \equiv \boldsymbol{0}$. Basically, conservative methods mimic the conservation property of the collision integral on a given molecular velocity grid. They do not produce non-physical sources of mass, momentum and energy and therefore in the limit of small Knudsen numbers the kinetic solution approaches the solution of Navier-Stokes equations away from boundaries. On the contrary, for non-conservative methods very fine meshes in the molecular velocity space are needed to keep the conservation error small when the Knudsen number decreases.

It can be easily seen that for any choice of the quadrature weights A_β and cell size $\Delta\xi$ the conventional discrete ordinate method, given by (7), (8) is not conservative with the estimate of the numerical source

$$|\boldsymbol{\delta}| \approx \nu O\left(\Delta\xi^r\right) \approx \frac{1}{\mathrm{Kn}} O\left(\Delta\xi^r\right). \tag{9}$$

From (9) it is obvious that for a given molecular velocity mesh $\boldsymbol{\delta} \to \infty$ as $\mathrm{Kn} \to 0$. In the case of small Knudsen numbers $\boldsymbol{\delta}$ can be very large. In practical calculations one cannot afford a fine mesh for $\boldsymbol{\xi}$ due to excessive memory requirements. As a result, computing flows with small Knudsen number may become difficult. For example, it follows from the above argument that the free-stream conditions cannot be preserved exactly.

2.3 Construction of the conservative method

The conservative method is obtained by modifying the discrete collision integral in the following way:

$$\frac{\partial f_\beta}{\partial t} = -D_h(\boldsymbol{\xi}_\beta f_\beta) + Q(f_\beta, \boldsymbol{\xi}_\beta, \tilde{\boldsymbol{a}}), \tag{10}$$

where the modified vector of macroparameters $\tilde{\boldsymbol{a}}$ is obtained as a solution of the discrete approximation to (1)

$$\sum_\beta \phi_\beta Q(f_\beta, \boldsymbol{\xi}_\beta, \tilde{\boldsymbol{a}}) A_\beta = J_\varphi. \tag{11}$$

For the Shakhov model equation it is convenient to use $\phi = 1,\ \boldsymbol{\xi},\ \xi^2,\ \boldsymbol{v}v^2$. Then first five equations in (11) represent conservation of mass, momentum and energy of colliding molecules; the corresponding moments J_φ vanish. The conservation conditions (11) can be written as:

$$\sum_\beta \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \xi^2 \\ \boldsymbol{v}v^2 \end{pmatrix}_\beta Q_\beta A_\beta = - \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \\ -(4/3)\nu\mathbf{q} \end{pmatrix}. \tag{12}$$

The nonlinear system (12) for $(n, \boldsymbol{u}, T, \boldsymbol{q})$ can be easily solved by the Newton iteration method. The iteration process requires an initial guess which is provided by the conventional expressions (8). Usually, it is sufficient to make one or two iterations since the Newton process converges very rapidly.

It is obvious that the modified method (10), (11) is conservative by construction for any choice of the quadrature weights A_β, including the first order quadrature, and any value of the Knudsen number Kn. However, since $\boldsymbol{a} = \tilde{\boldsymbol{a}} + O\left(\Delta\xi^r\right)$ the use of higher-order quadratures results in a better initial guess (8) and thus faster convergence of iterations. Naturally, smaller values of Kn require more iterations. The choice of the cell size of the molecular velocity mesh $\Delta\xi$ also plays a role: the smaller $\Delta\xi$ is the faster iterations converge; normally we use $\Delta\xi \leq \sqrt{T}/2$. See the section of numerical results for a numerical study of the influence of $\Delta\xi$ on the accuracy of the results.

The conservation property holds for the macroparameters $\boldsymbol{a}$ defined by the conventional expression (8). Although on a sufficiently fine molecular velocity mesh $\boldsymbol{a}$ and $\tilde{\boldsymbol{q}}$ differ only slightly, on a coarse mesh $\tilde{\boldsymbol{a}}$ is a more accurate approximation to the macroparameters. Therefore, while presenting results of computations, we always use the modified vector $\tilde{\boldsymbol{a}}$ rather than $\boldsymbol{a}$.

Since the model collision integral Q is an infinitely smooth function of all variables the formal approximation order of the modified discrete ordinate method (10) is equal to that of the conventional one. The Krook model collision integral does not contain the values of $\boldsymbol{q}$ and thus it is sufficient to use only the first five equations in (12), see.[4,9]

3 Extension to diatomic gases

3.1 The model of Rykov

For the diatomic gas the distribution function now depends not only on t, $\boldsymbol{r}$, $\boldsymbol{\xi}$, but also on the energy of rotational movement e. The Rykov model kinetic equation is given by:[10]

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\frac{\partial f}{\partial \boldsymbol{r}} = Q(f, \boldsymbol{\xi}, \boldsymbol{a}), \quad Q(f, \boldsymbol{\xi}, \boldsymbol{a}) = \nu_r f^r + \nu_t f^t - (\nu_r + \nu_t) f. \tag{13}$$

Here ν_r, ν_t are the frequencies of nonelastic and elastic collisions; f^r, f^t are the distribution functions of molecules after nonelastic and elastic collisions, respectively. Let us introduce the following reduced distribution functions[10]

$$f_0(t, r, \xi) = \int_0^\infty f\, de, \quad f_1(t, r, \xi) = \int_0^\infty ef\, de.$$

Multiplying (13) by 1, e and integrating with respect to e we obtain the following non-dimensional system for f_0, f_1:

$$\frac{\partial f_k}{\partial t} + \boldsymbol{\xi}\frac{\partial f_k}{\partial \boldsymbol{r}} = H_k, \quad H_k(f_k, \boldsymbol{\xi}, \boldsymbol{a}) = \nu_r f_k^r + \nu_t f_k^t - (\nu_r + \nu_t) f_k, \quad k = 0, 1. \tag{14}$$

where

$$\nu_r = \frac{8}{5\sqrt{\pi}}\frac{1}{\mathrm{Kn}_\infty}\frac{nT_t}{\mu_t}\frac{1}{Z}, \quad \nu_t = \frac{8}{5\sqrt{\pi}}\frac{1}{\mathrm{Kn}_\infty}\frac{nT_t}{\mu_t}\left(1 - \frac{1}{Z}\right),$$

$$f_0^r = f_M(T)\left[1 + \frac{8}{15}\omega_0\frac{\boldsymbol{q}^t}{p}\frac{\boldsymbol{v}}{T}\left(\frac{v^2}{T} - \frac{5}{2}\right)\right], \quad f_0^t = f_M(T_t)\left[1 + \frac{8}{15}\frac{\boldsymbol{q}^t}{p_t}\frac{\boldsymbol{v}}{T_t}\left(\frac{v^2}{T_t} - \frac{5}{2}\right)\right]$$

$$f_1^r = Tf_0^r + 4\omega_1(1-\delta)Tf_M(T)\frac{\boldsymbol{q}^r\boldsymbol{v}}{pT}, \qquad f_1^t = T_r f_0^t + 4(1-\delta)T_r f_M(T_t)\frac{\boldsymbol{q}^r\boldsymbol{v}}{p_t T_r}.$$

$$\frac{5}{2}T = \frac{3}{2}T_t + T_r, \quad p_t = nT_t, \quad p = nT, \quad \delta = 1/1.55.$$

Here $\mu_t = \mu(T_t)$ - viscosity, T_t, T_r – translational and rotational temperatures, T – average temperature, $\mathbf{q}^t$, $\mathbf{q}^r$ – translational and rotational heat fluxes, $Z = Z(T_r, T_t)$ is ratio of the number of collisions to the number of rotational (nonelastic) collision. Expressions for μ and $Z(T_r, T_t)$ can be found in[6,7,10] and are omitted here to save space. These values of ω_0, ω_1 are found from the conditions that the heat conductivity coefficient obtained from the model kinetic equations is equal to its experimentally found value.[8]

3.2 Approximation conditions and macroparameters

For the Rykov model the vector $\boldsymbol{a}$ in the model collision integral is given by

$$\boldsymbol{a} = (n, \boldsymbol{u}, T_t, T_r, \boldsymbol{q}^t, \boldsymbol{q}^r)^T.$$

The approximation conditions (1) on the model collision integral which are used to determine the expressions for the vector $\boldsymbol{a}$ in terms of the distribution function can be written as follows:

$$\int \begin{pmatrix} H_0 \\ \boldsymbol{\xi} H_0 \\ \xi^2 H_0 + H_1 \\ H_1 \\ \boldsymbol{v} v^2 H_0 \\ \boldsymbol{v} H_1 \end{pmatrix} d\boldsymbol{\xi} = - \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \\ (3/2)\nu_r n (T_t - T) \\ (4/3 + 2(1-\omega_0)/3Z)\, Z\nu_r \mathbf{q}^t \\ (2\delta + 2(1-\omega_1)(1-\delta)/Z)\, Z\nu_r \mathbf{q}^r \end{pmatrix}. \tag{15}$$

The first six equations represent conservation laws of mass, momentum and energy and include the relaxation of translational and rotational temperatures to the average gas temperature. The last six equations represent the conditions for relaxation of translational and rotational heat fluxes.

Performing exact integration in(15) we obtain the following expressions for macroparameters:

$$\begin{gathered} \left(n, n\boldsymbol{u}, \frac{3}{2} n T_t + n\mathbf{u}^2\right) = \int (1, \boldsymbol{\xi}, \boldsymbol{\xi}^2) f_0 d\boldsymbol{\xi}, \\ \boldsymbol{q}^t = \frac{1}{2} \int \boldsymbol{v} v^2 f_0 d\boldsymbol{\xi}, \quad n T_r = \int f_1 d\boldsymbol{\xi}, \quad \boldsymbol{q}^r = \frac{1}{2} \int \boldsymbol{v} f_1 d\boldsymbol{\xi}. \end{gathered} \tag{16}$$

Note that when the rotational degrees of freedom are frozen ($Z = \infty$), the Rykov model reduces to the Shakhov model.

3.3 The conservative discrete ordinate method

The conservative version of the discrete ordinate method for the Rykov model is a direct extension of the monatomic version from the previous section. The basic idea is again to modify the vector of macroparameters in used in the model collision integral so that to ensure the conservation property.

Let us denote the values of f_k in the velocity nodes ξ_β by $f_{k,\beta} = f_k(t, \boldsymbol{r}, \boldsymbol{\xi}_\beta)$. The conservative discrete ordinate method (7) is now written as:

$$\frac{\partial f_{k,\beta}}{\partial t} = -D_h \left(\boldsymbol{\xi}_\beta f_{k,\beta}\right) + H_k(f_k, \boldsymbol{\xi}, \tilde{\boldsymbol{a}}), \quad k = 0, 1, \tag{17}$$

where the modified vector of macroparameters $\tilde{\boldsymbol{a}}$ is obtained by solving the following system of equations:

$$\sum_\beta \begin{pmatrix} H_0 \\ \boldsymbol{\xi} H_0 \\ \xi^2 H_0 + H_1 \\ H_1 \\ \boldsymbol{v} v^2 H_0 \\ \boldsymbol{v} H_1 \end{pmatrix}_\beta A_\beta = - \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \\ (3/2)\nu_r n (T_t - T) \\ (4/3 + 2(1-\omega_0)/3Z)\, Z\nu_r \mathbf{q}^t \\ (2\delta + 2(1-\omega_1)(1-\delta)/Z)\, Z\nu_r \mathbf{q}^r \end{pmatrix}. \tag{18}$$

The system (18) is a direct approximation of (15) on the given molecular velocity mesh and is solved by the Newton iteration method. The first guess is provided by the conventional expressions of the form:

$$\begin{gathered} \left(n, n\boldsymbol{u}, \frac{3}{2} n T_t + n\mathbf{u}^2\right) = \sum_\beta (1,\, \boldsymbol{\xi},\, \xi^2)_\beta f_{0.\beta} A_\beta, \\ \boldsymbol{q}^t = \frac{1}{2} \sum_\beta \boldsymbol{v}_\beta v_\beta^2 f_{0,\beta} A_\beta, \quad n T_r = \sum_\beta f_{1,\beta} A_\beta, \quad \boldsymbol{q}^r = \frac{1}{2} \sum_\beta \boldsymbol{v}_\beta f_{1,\beta} A_\beta. \end{gathered} \tag{19}$$

As for the monatomic model, the method given by (18) remains conservative for any Kn and A_β. The choice of the quadrature and $\Delta\xi$ is motivated by the same arguments as for the Shakhov model.

4 Numerical examples

To illustrate the robustness of the proposed conservative procedure for evaluating macroparameters, we study transverse flow of a rarefied gas past a zero-thickness plate of finite width L. Both monatomic and diatomic flows are considered. A detailed setup of the problem can be found in.[13,17] The free stream is characterized by the density n_∞, velocity U_∞, temperature T_∞. We introduce a coordinate system with the x axis aligned with the normal to the plate, and y and z axes directed along the plate and spanwise. The plate is assumed to be homogeneous. Then the distribution function does not depend on z. The boundary condition of complete temperature accommodation of molecules to the surface temperature T_w is used throughout.

We incorporated the proposed conservative procedure into a implicit finite-volume TVD scheme for the kinetic equation, described in.[18] This scheme can be used for arbitrary Knudsen numbers, including free-molecular regime, in which the discontinuities of the distribution functions play important role, and the continuum region, in which the second order of accuracy is essential to correctly model the flow in the boundary layer. The fourth-order composite Simpson rule is used for constructing the weights A_β and evaluating integrals with respect to the molecular velocity. For the monatomic gas we use $\mathrm{Pr} = 2/3$ in the Shakhov model and $\mu = T^{1/2}$ (hard spheres). The diatomic gas is taken to be nitrogen.

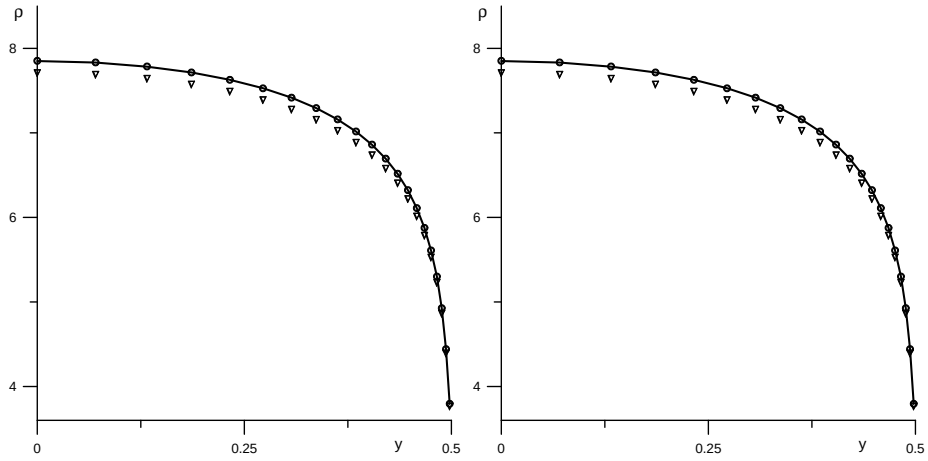

Figure 1: Density and pressure distribution over the upwind ($x = 0-$) side of the plate for Kn = 0.003 and $\Delta\xi = 0.25$ (solid line), 0.45 (circles), 0.9 (triangles).

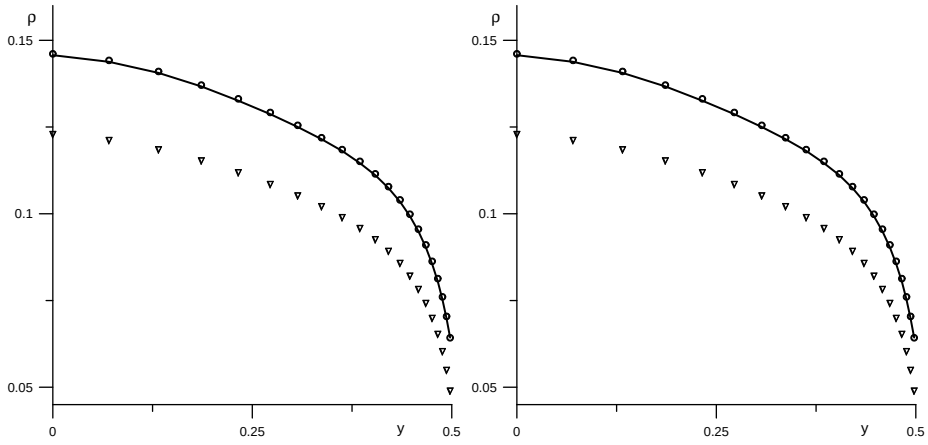

Figure 2: Density and pressure distribution over the downwind ($x = 0+$) side of the plate for Kn = 0.003 and $\Delta\xi = 0.25$ (solid line), 0.45 (circles), 0.9 (triangles)

We first study influence of the cell size in the molecular velocity mesh on the accuracy of the solution for the non-dimensional freestream velocity $U_\infty = 3$ and plate temperature $T_w = 2$; the dimensional value of the free-stream temperature is 59.475 K. We consider in addition to the basic molecular velocity mesh with $\Delta\xi = 0.45$ two more meshes: a coarse mesh with $\Delta\xi = 0.9$ and a fine mesh with $\Delta\xi = 0.25$. The results obtained with the finest mesh are used as the reference. Figs. 1 – 2 present distribution of density and pressure over the both sides of the plate for Kn = 0.003 as a function of $\Delta\xi$. We see that solutions on two finest meshes ($\Delta\xi = 0.45$ and $\Delta\xi = 0.25$) are virtually identical. However, for the downwind side the use of $\Delta\xi = 0.9$ still gives a visible error. Thus, we conclude that

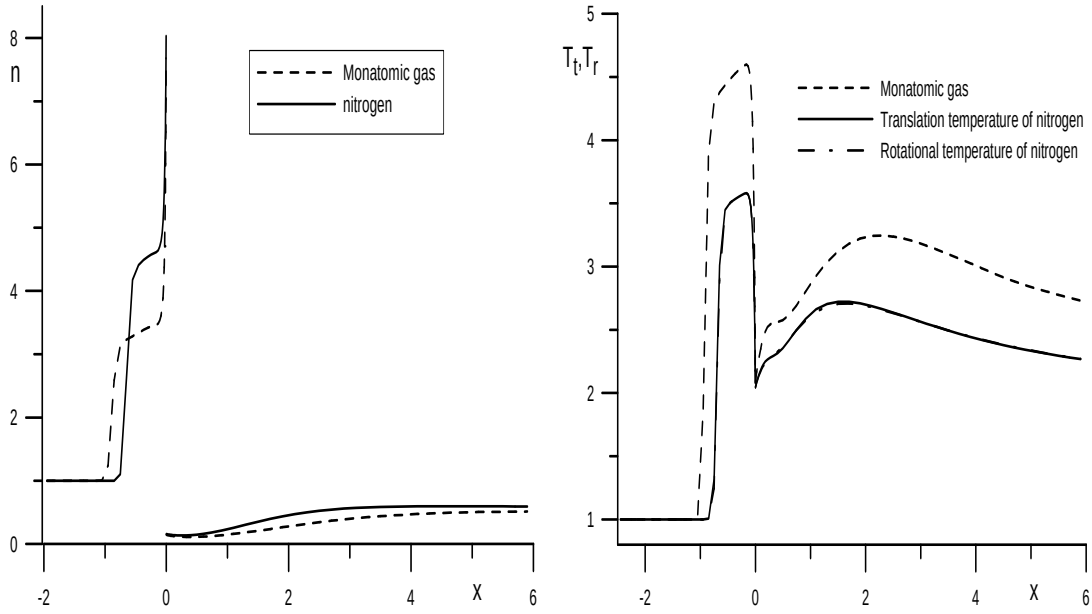

Figure 3: Density and temperature profiles along the symmetry line for Kn = 0.003

for small Kn it is sufficient to use $\Delta\xi \approx 0.5$. The use of smaller $\Delta\xi$ is justified only if an accurate computation of the low-density region behind the plate for transitional and large Knudsen numbers is necessary.

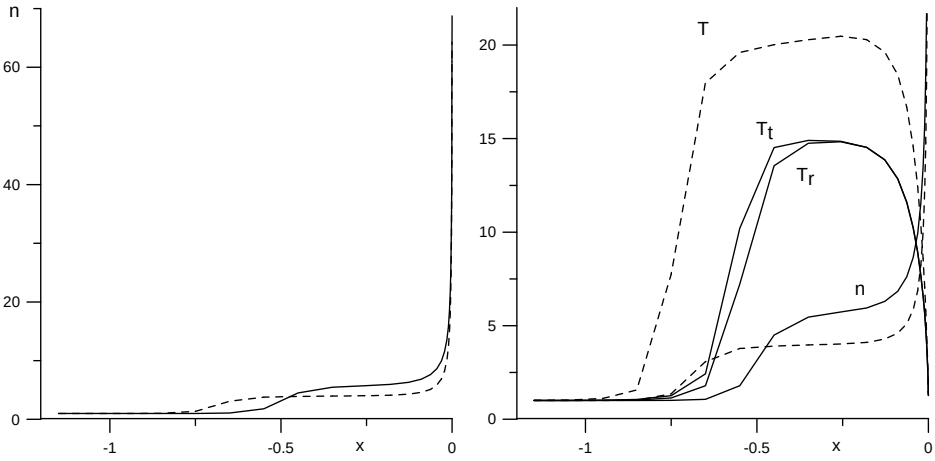

Figure 4: Density and temperature in front of the plate for $U_\infty = 7$, $T_w = 1$ Kn = 0.01; dashed line - monatomic solution.

4.1 Comparison of monatomic and diatomic results

We study the influence of the Knudsen number and degrees of freedom (monatomic versus diatomic gas) on distribution of macroparameters.

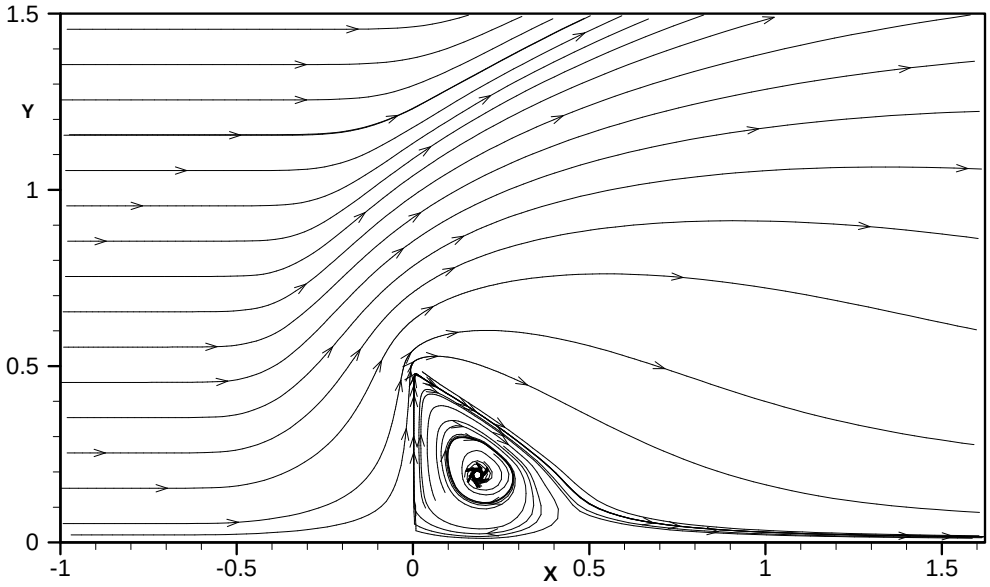

Figure 5: Streamlines for the diatomic solution and $U_\infty = 7$, $T_w = 1$, Kn $= 0.01$.

We first consider the case $U_\infty = 3$, $T_w = 2$. Fig. 3 shows the density and temperature profiles along the symmetry line (normal to the plate) for Kn $= 0.003$. We observe a standard flow pattern with a bow shock wave and exceedingly thin boundary layer with very sharp gradients of density and temperature. The temperature jump is negligible and the flow is in equilibrium everywhere except at the shock front and the Knudsen layer.

We next consider the case of a hypersonic flow over the cold plate with $S_\infty = 7$, $T_w = 1$; the dimensional value of the free-stream temperature is 276.133K. Fig. 4 shows the distribution of density and temperatures in front of the plate for Kn $= 0.01$. For convenience, the temperature plot contains the density distributions cut at $y = 25$. We see a well-defined bow shock wave as well as an extremely thin boundary layer with exceedingly steep gradients of macroparameters. Despite this, the method works well and produces the correct solution. As expected, monatomic and diatomic distributions are different. Fig. 5 shows streamlines for the diatomic solution and the same Knudsen number. We clearly see the formation of the recirculation zone as the Knudsen number is decreased.

5 Conclusions

A fully conservative modification of the discrete ordinate method for the nonlinear model kinetic equations of Shakhov and Rykov has been presented. Conservation is achieved by a new way of evaluating macroparameters of the gas. Conservation laws are satisfied for an arbitrary Knudsen number. Additionally, the correct evaluation of the heat flux is ensured in the limit of small Knudsen numbers. The numerical results provided show that the proposed modification work well for high-speed flows with sharp

gradients.

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