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FINITE DIFFERENCE METHOD FOR NUMERICAL SOLUTION OF THE INITIAL AND BOUNDARY VALUE PROBLEM FOR BOLTZMANN'S SIXMOMENT SYSTEM OF EQUATIONS

Boltzmann's one-dimensional non-linear non-stationary moment system of equations in the third approximation is presented, in which the first, third and fourth equations corresponds to the laws of conservation of mass, momentum and energy, respectively. This system contains six equations and represents a nonlinear system of hyperbolic type equations. For the Boltzmann's six-moment system of equations an initial and boundary value problem is formulated. The macroscopic boundary condition contains the moments of the incident particles distribution function on the boundary and moments of the reflected particles distribution function from the boundary. The boundary condition depends on the temperature of the wall (boundary).

In this work, using the finite-difference method, an approximate solution of the mixed problem for the Boltzmann system of moment equations is constructed in the third approximation under the boundary conditions obtained by approximating the Maxwell boundary condition. For given values of the coefficients included in the moments of the nonlinear collision integral and the parameter depending on the wall temperature, as well as for fixed values of the initial conditions, a numerical experiment was carried out. As a result, the approximate values of the particle distribution function incident on the boundary and reflected from the boundary, as well as the density, temperature and average velocity of gas particles, as moments of the particle distribution function, are obtained.

Key words: Boltzmann's moment system of equations, microscopic Maxwell boundary condition, macroscopic Maxwell-Auzhan boundary conditions.

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Бөлшектердің шекарадан айна және диффузия шағылысу жағдайында Больцманның алты моменттік теңдеулер жүйесі

Больцманның бір өлшемді сызықсыз стационар емес моменттік теңдеулер жүйесінің үшінші жуықтауы келтірілген, онда бірінші, үшінші және төртінші теңдеулер тиісінше массаның, импульстің және энергияның сақталу заңдарына сәйкес келеді. Бұл жүйе алты теңдеуден тұрады және гиперболалық типті теңдеулердің сызықсыз жүйесін құрайды. Больцманның алты моменттік теңдеулер жүйесі үшін алғашқы-шекаралық есеп құрастырылды. Макроскопиялық шекаралық шарт шекараға түскен бөлшектердің таралу функциясының моменттерін және шекарадан шағылысқан бөлшектердің таралу функциясының моменттерін қамтиды. Шекаралық шарт қабырғаның (шекараның) температурасынан тәуелді.

Жұмыста ақырлы-айырым әдісімен Максвелдің шекаралық шартын аппроксимациялау арқылы алынған шекаралық шартты қанағаттандыратын Больцманның теңдеулер жүйесінің үшінші жуықтауы үшін қойылған аралас есептің жуық сан шешуі алынған. Сызықсыз соқтығысу интегралының моменттеріндегі коэффициенттер мен шекараның температурасынан тәуелді параметрдің берілген мәндеріне сай және алғашқы шарттың нақты мәндері үшін сан эксперимент жүргізілді. Нәтижесінде, шекараға түскен (құлаған) және шекарадан шағылысқан молекулалардың үлестіру функциясының, сонымен бірге, газ молекулалар тығыздығының, температурасының және орта жылдамдығының жуық мәндері анықталды.

Түйін сөздер: Больцманның моменттік теңдеулер жүйесі, Максвелдің микроскопиялық шекаралық шарты, Максвел-Аужанның макроскопиялық шекаралық шарты.

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Метод конечных разностей для численного решения начально-краевой задачи для шестимоментной системы уравнений Больцмана

Приведена одномерная нелинейная нестационарная система моментных уравнений Больцмана в третьем приближении, в которой первое, третье и четвертое уравнения соответствуют законам сохранения массы, импульса и энергии соответственно. Эта система содержит шесть уравнений и представляет нелинейную систему уравнений гиперболического типа. Для шестимоментной системы уравнений Больцмана сформулирована начально-краевая задача. Макроскопическое граничное условие содержит моменты функции распределения падающих на границу частиц и функции распределения отраженных от границы частиц. Граничное условие зависит от температуры стенки (границы).

В работе с помощью конечно-разностного метода построено приближенное решение смешанной задачи для системы моментных уравнений Больцмана в третьем приближении при граничных условиях, полученных аппроксимацией граничного условия Максвелла. При заданных значениях коэффициентов, входящих в моменты нелинейного интеграла столкновений и параметра, зависящего от температуры стенки, а также при фиксированных значениях начальных условий проведен численный эксперимент. В результате, приближенные значения падающих на границу и отраженных от границы функции распределения частиц, а также плотность, температура и средняя скорость частиц газа, как моменты функции распределения частиц, получены.

Ключевые слова: Система моментных уравнений Больцмана, микроскопические граничные условия Максвелла, макроскопические граничные условия Максвелла-Аужана.

1 Introduction

The physical state of a system consisting of monatomic molecules can be described with varying degrees of accuracy. The state of the system has a variable meaning depending on what information about the system is useful for the purposes in question. The state of the system is usually determined by the values of some variables – state parameters. Depending on how these options are chosen, information about the system can be quite detailed. In other words, the description of a physical system is possible with varying degrees of accuracy. In order for the description of a non-equilibrium state to be satisfactory with a sufficient level of precision, equations must be known that allow one to determine their changes in time from the given initial the state parameters' values. The particle distribution function can be used to describe the state of the system, which satisfies the nonlinear Boltzmann equation. Boltzmann equation satisfies the rules of mass, momentum, and energy conservation. These

conservation laws correspond to five partial differential equations, which contain thirteen unknowns. This system of equations is not closed, since the conservation equations include additional variables – stresses and heat flux. Assuming that the particle distribution function has a special form depending only on thermodynamic variables and their derivatives, one can express stresses and heat flux in terms of these thermodynamic variables. Thus, the system of conservation equations is brought to a closed form. Within the framework of such a scheme, various approximations are possible, leading, respectively, to the equations of Euler, Navier-Stokes, Barnett, etc. Moment equations, which are a series of nonlinear equations represented in partial derivatives, can be used to characterize the state of the system in the transition phase. Between the kinetic (Boltzmann equation) and hydrodynamic (Euler and Navier-Stokes equations, etc.) levels of characterizing the state of a gas lies the system of moment equations. Different basis function systems, the degree of arbitrariness of the particle distribution function, and the procedures for calculating the coefficients of the expansion of the particle distribution function in a Fourier series set apart the various moment approaches. Expanding the particle distribution function in terms of Hermite polynomials around a local Maxwellian distribution produced the Grad system of moment equations in [1] and [2]. By expanding the particle distribution function in terms of the eigenfunctions of the linearized collision operator [5],[6], the moment system of equations, which is distinct from the Grad system, was constructed in [3],[4]. The Boltzmann system of moment equations was the name given to this set of equations. The moment system's and the Boltzmann equation's structures are comparable. Calculating the collision integral's moments is the source of the entire challenge [7]. Solution The mixed value problem for the nonlinear nonstationary moment system of equations of Boltzmann's existence and uniqueness in three dimensions were established [3],[4].

The design and operation of aircraft at high altitudes requires the calculation of aerodynamic characteristics in a wide range of determining parameters (flight altitude, atmospheric parameters, flight speed, spacecraft orientation, aircraft configuration, etc.).

The aerodynamic characteristics of the flow around bodies in the upper layer of the atmosphere in the transition mode are obtained by calculation. On the basis of the kinetic theory of gases, computational investigations of the flow around bodies in the transitional regime are conducted. The condition at the moving boundary, more specifically the interaction of a gas with a moving solid surface, is important in aerospace engineering [8]. If the gas's initial state is known and the condition on the moving boundary is defined, the integro-differential Boltzmann equation can characterize the gas' evolution. The moment method stands out among the approximate methods for resolving the Boltzmann equation.

The system of moment equations contains all the macroscopic quantities that are of primary interest when it comes to rarefied gas theory. Therefore, moment equations are sufficient to determine the macroscopic quantities characterizing the state of gas molecules. However, boundary conditions must be formulated for a set of partial differential equations. As a result, the issue of estimating the Boltzmann equation's boundary condition approximation emerges. Additionally, the moment equations' ensuing problem needs to be properly phrased.

In [9], the macroscopic boundary conditions for the Boltzmann's nonstationary one-dimensional moment system of equations were used to approximate the Maxwell's microscopic boundary conditions for the Boltzmann's nonlinear equation. Maxwell-Auzhan conditions

were given to new macroscopic boundary conditions.

In problems of atmospheric optics, the theory of radiative transfer, and the rarefied gas dynamics moment equations are often used. As a result, it is a crucial and pressing issue to design approximate solutions to the mixed problem for the system of moment equations.

2 Materials and methods

2.1 Numerical experiment for Boltzmann's six-moment one-dimensional system of equations with macroscopic boundary conditions

We investigate the mixed problem for the third approximation of the Boltzmann system of moment equations under the approximate Maxwell boundary condition. The third approximation of the mixed problem for the Boltzmann system of moment equations is created through the finite-difference method.

We take into account the third approximation of the Boltzmann's moment system equations [4]

$$\begin{aligned}
& \frac{\partial \varphi_{00}}{\partial t} + \frac{1}{\alpha} \frac{\partial \varphi_{01}}{\partial x} = 0, \\
& \frac{\partial \varphi_{02}}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial x} \left(\frac{2}{\sqrt{3}} \varphi_{01} + \frac{3}{\sqrt{5}} \varphi_{03} - \frac{2\sqrt{2}}{\sqrt{15}} \varphi_{11} \right) = J_{02}, \\
& \frac{\partial \varphi_{10}}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial x} \left(-\sqrt{\frac{2}{3}} \varphi_{01} + \sqrt{\frac{5}{3}} \varphi_{11} \right) = 0, \\
& \frac{\partial \varphi_{01}}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial x} \left(\varphi_{00} + \frac{2}{\sqrt{3}} \varphi_{02} - \sqrt{\frac{2}{3}} \varphi_{10} \right) = 0, \\
& \frac{\partial \varphi_{03}}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial x} \frac{3}{\sqrt{5}} \varphi_{02} = J_{03}, \\
& \frac{\partial \varphi_{11}}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial x} \left(-\frac{2\sqrt{2}}{\sqrt{15}} \varphi_{02} + \sqrt{\frac{5}{3}} \varphi_{10} \right) = J_{11}, \\
& x \in (-a, a), \quad t > 0,
\end{aligned} \tag{1}$$

where $\varphi_{00} = \varphi_{00}(t, x)$, $\varphi_{01} = \varphi_{01}(t, x)$, \dots , $\varphi_{11} = \varphi_{11}(t, x)$ are the coefficients of particle distribution function's expansion to Fourier series;

$$I_{02} = (\sigma_2 - \sigma_0)(\varphi_{00}\varphi_{02} - \varphi_{01}^2/\sqrt{3})/2,$$

$$I_{03} = \frac{1}{4}(\sigma_3 + 3\sigma_1 - 4\sigma_0)\varphi_{00}\varphi_{03} + \frac{1}{4\sqrt{5}}(2\sigma_1 + \sigma_0 - 3\sigma_3)\varphi_{01}\varphi_{02},$$

$$I_{11} = (\sigma_1 - \sigma_0)(\varphi_{00}\varphi_{11} + \frac{1}{2}\sqrt{\frac{5}{3}}\varphi_{10}\varphi_{01} - \frac{\sqrt{2}}{\sqrt{15}}\varphi_{01}\varphi_{02}) -$$

are the nonlinear collision integral's moments, where $\sigma_0, \sigma_1, \sigma_2, \sigma_3$ are constants, $\alpha = \frac{1}{R\Theta}$, Θ is the reflective wall temperature and Θ is the constant. Three homogeneous equations that represent the laws of conservation of mass, momentum, and energy can be found in the system of equations (1).

The system of equations (1) under the boundary conditions obtained by approximating the Maxwell boundary condition write in vector-matrix form

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{1}{\alpha} C \frac{\partial w}{\partial x} &= I_1(u, w) \\ \frac{\partial w}{\partial t} + \frac{1}{\alpha} C' \frac{\partial u}{\partial x} &= I_2(u, w), \quad t \in (0, T], \quad x \in (-a, a), \end{aligned} \quad (2)$$

$$u \Big|_{t=0} = u_0(x), \quad w \Big|_{t=0} = w_0(x), \quad x \in [-a, a], \quad (3)$$

$$\frac{1}{\alpha} (Cw^- + Du^-) \Big|_{x=-a} = \frac{1}{\alpha\beta} (Cw^+ - Du^+) \Big|_{x=-a} - \frac{(1-\beta)}{\alpha\beta\sqrt{\pi}} F, \quad t \in [0, T], \quad (4)$$

$$\frac{1}{\alpha} (Cw^- - Du^-) \Big|_{x=a} = \frac{1}{\alpha\beta} (Cw^+ + Du^+) \Big|_{x=a} + \frac{(1-\beta)}{\alpha\beta\sqrt{\pi}} F, \quad t \in [0, T], \quad (5)$$

where

$$C = \begin{pmatrix} 1 & 0 & 0 \\ \frac{2}{\sqrt{3}} & \frac{3}{\sqrt{5}} & -\frac{2\sqrt{2}}{\sqrt{15}} \\ -\sqrt{\frac{2}{3}} & 0 & \sqrt{\frac{5}{3}} \end{pmatrix}, \quad D = \frac{1}{\sqrt{\pi}} \begin{pmatrix} \sqrt{2} & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{3}} \\ \sqrt{\frac{2}{3}} & 2\sqrt{2} & -1 \\ -\frac{1}{\sqrt{3}} & -1 & 3\sqrt{2} \end{pmatrix}$$

$$I_1(u, w) = (0, I_{02}, 0)', \quad I_2(u, w) = (0, I_{03}, I_{11})',$$

$$u = (\varphi_{00}, \varphi_{02}, \varphi_{10})', \quad w = (\varphi_{01}, \varphi_{03}, \varphi_{11})', \quad F = \left(\frac{1}{4\sqrt{2}}, \frac{1}{8\sqrt{6}}, \frac{1}{8\sqrt{3}} \right)',$$

C' is the transpose matrix, while D is the positive definition matrix;

$u_0(x) = (\varphi_{00}^0(x), \varphi_{02}^0(x), \varphi_{10}^0(x))'$, $w_0(x) = (\varphi_{01}^0(x), \varphi_{03}^0(x), \varphi_{11}^0(x))'$ are the moments of initial function provided; w^+ , u^+ are the falling vectors to the moments of the boundary distribution function; w^- , u^- are the reflection vector from the moments of the boundary distribution function. Pure mirror reflection is represented by the value of $\beta \in [0, 1]$ and parameter value of $\beta = 1$.

Through straightforward calculations, it is feasible to verify

$$\det C_1 = \det \begin{pmatrix} 0 & C \\ C' & 0 \end{pmatrix} \neq 0,$$

hence the matrix C_1 has eigenvalues are real, with an equal number of positive and negative eigenvalues. Macroscopic boundary conditions correspond to the number of positive and negative eigenvalues of matrix C_1 . Correctness of the problem (2) – (5) in $C([0, T]; L^2[-a, a])R$ was proved in [10-11].

As a result, system (2) is a hyperbolic type system of nonlinear partial differential equations. To define approximate solution of the problem (2) – (5) we use finite-difference method.

Divide the segment $[0, T]$ into N_1 equal parts, and divide the segment $[-a, a]$ into N_2 equal parts. Let us consider the grid functions $u_{ij} = u(t_i, x_j)$ and $w_{ij} = w(t_i, x_j)$. We approximate the differential problem (2) – (5) by the following finite-difference scheme [12, 13]

$$\frac{u_{i+1,j}^{n+1} - u_{ij}^{n+1}}{\tau} + \frac{1}{\alpha} C \frac{w_{ij}^{n+1} - w_{i,j-1}^{n+1}}{h} = I_1(u_{ij}^n, w_{ij}^n), \quad (6)$$

$$i = 0, 1, \dots, N_1 - 1; \quad j = 1, \dots, N_2;$$

$$\frac{w_{i+1,j}^{n+1} - w_{ij}^{n+1}}{\tau} + \frac{1}{\alpha} C' \frac{u_{i,j+1}^{n+1} - u_{i,j}^{n+1}}{h} = I_2(u_{ij}^n, w_{ij}^n), \quad (7)$$

$$i = 0, 1, \dots, N_1 - 1; \quad j = N_2 - 1, \dots, 0;$$

$$u_{0j}^{n+1} = u_j^0, \quad w_{0j}^{n+1} = w_j^0, \quad j = 0, 1, \dots, N_2; \quad (8)$$

$$\frac{1}{\alpha} (Cw^- - Du^-)_{i,0}^{n+1} = \frac{1}{\alpha\beta} (Cw^+ + Du^+)_{i,0}^n - \frac{1-\beta}{\alpha\beta\sqrt{\pi}} F, \quad i = 0, 1, \dots, N_1, \quad (9)$$

$$\frac{1}{\alpha} (Cw^- + Du^-)_{i,N_2}^{n+1} = \frac{1}{\alpha\beta} (Cw^+ - Du^+)_{i,N_2}^n + \frac{1-\beta}{\alpha\beta\sqrt{\pi}} F, \quad i = 0, 1, \dots, N_1, \quad (10)$$

τ is time step, h is spatial variable step.

From the difference equations (6) – (7) it follows that the derivatives on t and x are approximated by the first order.

In order to find a numerical solution of the problem (6) – (10), we use the iterative method. We start the iterative process by n and continue calculations until we achieve the following conditions

$$|u_{ij}^{n+1} - u_{ij}^n| < \varepsilon, \quad |w_{ij}^{n+1} - w_{ij}^n| < \varepsilon, \quad i = 0, 1, \dots, N_1 - 1; \quad j = 1, \dots, N_2,$$

where ε is a given sufficiently small number.

Numerical experiment.

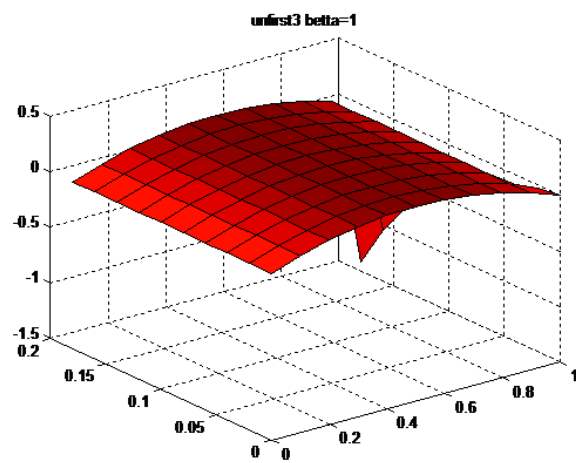
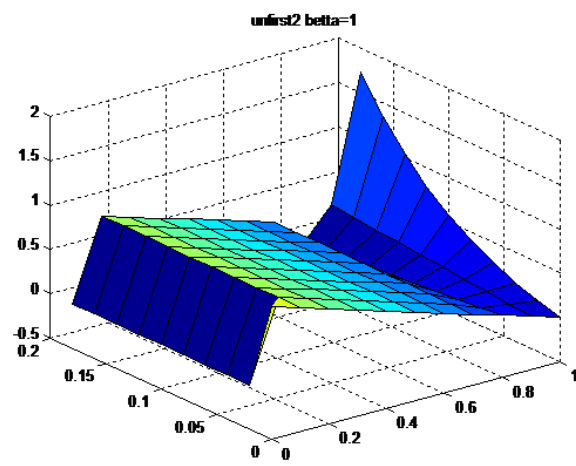
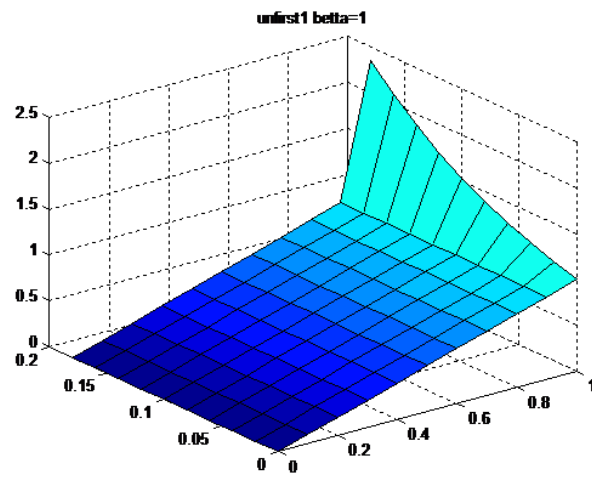
With the following data, a numerical experiment was performed: $[-a, a] \cong [0, 1]$,

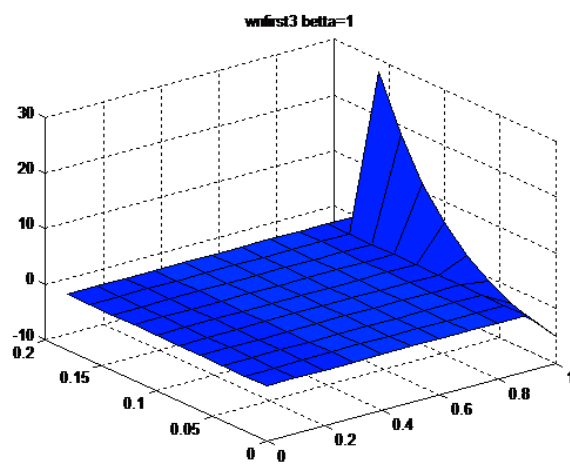
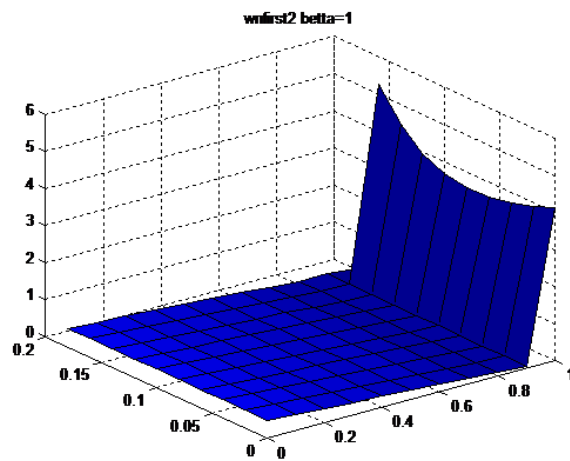
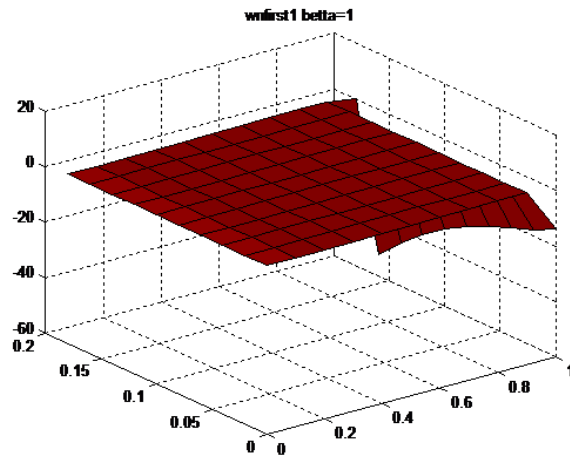
$$u_0(x) = \begin{pmatrix} x \\ 1-x \\ x(1-x) \end{pmatrix}, \quad w_0(x) = \begin{pmatrix} 1+x \\ (1-x)/2 \\ x(1-x)/2 \end{pmatrix}, \quad x \in [0, 1],$$

$$\alpha = 38.681, \quad \sigma_0 = 1.333, \quad \sigma_1 = \sigma_3 = 0, \quad \sigma_2 = -0.266;$$

$$h = \frac{1}{10}, \quad \tau = \frac{2}{100}.$$

Interval $[0, 1]$ is divided into 10 equal parts, h is the step in the spatial variable x , τ is the time step. The relation $\frac{\tau}{h}$ satisfied the stability condition. Let us present the graphs of the vectors u and w for value of $\beta = 1$.





3 Conclusion

The moments φ_{00} , φ_{01} , φ_{10} expressed by the macroscopic characteristics of the gas such that density, average speed and temperature. More exactly, we have following equalities $\varphi_{00} = \rho$, $\varphi_{01} = \alpha\rho V$, $\varphi_{10} = \sqrt{\frac{3}{2}}\rho - \sqrt{\frac{2}{3}}\alpha^2\rho(\frac{3}{2}k\theta + \frac{1}{2}V^2)$, where ρ is the gas density, V is the gas average speed, θ is the gas temperature and $\alpha = 38.681$ is the constant. On the plot $\text{unfirst1} = \varphi_{00}$, $\text{unfirst3} = \varphi_{10}$, $\text{wnfirst1} = \varphi_{01}$. $\beta = 1$ corresponds to pure specular reflection. The value of the parameter β appreciable affected to the values of moments φ_{00} , φ_{01} , φ_{10} . Moreover we define approximate values of

$$\varphi_3(t, x, v) = f_0(\alpha|v|) \sum_{2n+1=0}^3 \varphi_{n1}(t, x)g_{n1}(\alpha v),$$

$f_0(\alpha|v|)$ – is global Maxwell distribution, more exactly we define following functions

$$\begin{aligned} \varphi_3^\pm(t, \mp a, v) &= \varphi_{00}^\pm(t, \mp a)g_{00}(\alpha v) + \varphi_{01}^\pm(t, \mp a)g_{01}(\alpha v) + \varphi_{02}^\pm(t, \mp a)g_{02}(\alpha v) + \\ &+ \varphi_{10}^\pm(t, \mp a)g_{10}(\alpha v) + \varphi_{03}^\pm(t, \mp a)g_{03}(\alpha v) + \varphi_{11}^\pm(t, \mp a)g_{11}(\alpha v), \end{aligned}$$

where $\varphi_3^+(t, \mp a, v)$ is the distribution function of falling to the boundary particles, $\varphi_3^-(t, \mp a, v)$ is the distribution function of reflecting from boundary particles,

$$\begin{aligned} g_{00}(\alpha v) &= 1, \quad g_{01}(\alpha v) = \alpha|v| \cos \theta, \quad g_{02}(\alpha v) = \frac{1}{\sqrt{3}} \left(\frac{\alpha|v|}{\sqrt{2}} \right)^2 (3 \cos^2 \theta - 1), \\ g_{10}(\alpha v) &= \sqrt{\frac{2}{3}} \left(\frac{3}{2} - \frac{\alpha^2 v^2}{2} \right), \quad g_{03}(\alpha v) = \sqrt{\frac{2}{15}} \left(\frac{\alpha|v|}{\sqrt{2}} \right)^3 (5 \cos^3 \theta - 3 \cos \theta), \\ g_{11}(\alpha v) &= \sqrt{\frac{4}{5}} \frac{\alpha|v|}{\sqrt{2}} \left(\frac{5}{2} - \frac{\alpha^2 v^2}{2} \right) \cos \theta. \end{aligned}$$

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