DIFFERENCE SCHEME FOR THE BOLTZMANN EQUATION BASED ON FAST FOURIER TRANSFORM

A. Bobylev and S. Rjasanow

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Difference Scheme for the Boltzmann Equation Based on Fast Fourier Transform

A. Bobylev [*], Victoria (Canada)
S. Rjasanow, Saarbrücken (Germany)

Abstract

The initial value problem for the spatially homogenous Boltzmann equation with Maxwell molecules is considered. A difference scheme for this problem is developed using Fast Fourier Transform and a study of different numerical effects is presented.

1 Introduction

In this paper we present numerical results for the approximate solution of the spatially homogeneous Boltzmann equation [3] with Maxwell molecules using a difference scheme. This scheme is based on the uniform discretization of the velocity space and the very effective Fast Fourier Transform (FFT) [4],[9]. It is well-known [1] that the Boltzmann equation for Maxwell molecules can be drastically simplified by using the Fourier transform in the velocity space. On the other hand, this paper seems to be the first using this simplification for numerical solution of the Boltzmann equation.

The paper is organized as follows. In Section 2, we formulate the initial value problem for the Boltzmann equation. Furthermore, we introduce the Fourier transform of the unknown function and the corresponding integral equation on the unit sphere. The conservation laws of the Boltzmann equation are reformulated in terms of the Fourier transform. In Section 3, we introduce a uniform grid in the velocity space and describe how to use FFT to compute the corresponding discrete Fourier transform efficiently. In Section 4, our difference scheme for the integral equation on the unit sphere is introduced and analyzed. In Section 5, we deal with the approximation of the conservation laws of the Boltzmann equation. Finally, in Section 6, we present the results of our numerical experiments and draw some conclusions.

[*]Permanent adress : Keldysh Institute of Applied Mathematics, Miusskaja sq. 4, 125047 Moscow

2 Boltzmann equation and Fourier transform

In this section we formulate the problem and give a short summary of some important properties of the Boltzmann equation.
We consider the following initial value problem for spatially homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t}(v,t) = Q(f,f),\ t>0,\ v\in\mathbb{R}^3_v; \tag{1}$$

$$Q(f,f) = \int_{\mathbb{R}^3_w}\int_{S^2} |u|\sigma\left(|u|,\frac{(u,e)}{|u|}\right)(f(v',t)f(w',t)-f(v,t)f(w,t))dwde;$$

$$f(v,0) = f_0(v)>0. \tag{2}$$

We use the following notations in (2)

- $v,w\in\mathbb{R}^3$ are pre-collision velocities;
- dw is the volume element in $\mathbb{R}^3_w$;
- $e\in\mathbb{R}^3$ is a unit vector;
- de is the surface element on the unit sphere S^2;
- $u=v-w\in\mathbb{R}^3$ denotes the relative velocity of collision partners;
- v',w' are post-collisional velocities defined by
  $v'=0.5(v+w+|u|e),\ w'=0.5(v+w-|u|e)$;
- $\sigma\left(|u|,\frac{(u,e)}{|u|}\right)de$ is the so called differential collision cross-section.

For Maxwellian molecules (or better pseudo-Maxwellian molecules) the product

$$|u|\sigma\left(|u|,\frac{(u,e)}{|u|}\right)$$

is independent of the relative velocity $|u|$ and will be denoted as

$$|u|\sigma\left(|u|,\frac{(u,e)}{|u|}\right)=g\left(\frac{(u,e)}{|u|}\right).$$

The function $g(\mu)$ is assumed to be non-negative and piecewise continuous on the interval $[-1,1]$.
One of the most important properties of the Boltzmann equation is conservation of the density ρ.

$$\rho(t) = \int_{\mathbb{R}^3_v} f(v,t)dv = \int_{\mathbb{R}^3_v} f_0(v)dv = \rho, \tag{3}$$

of the bulk velocity V

$$\rho(t)V(t) = \int_{\mathbb{R}^3_v} vf(v,t)dv = \int_{\mathbb{R}^3_v} vf_0(v)dv = \rho V, \tag{4}$$

and of the energy density per unit volume

$$W(t) = \frac{1}{2}\int_{\mathbb{R}^3_v} |v|^2 f(v,t)dv = \frac{1}{2}\int_{\mathbb{R}^3_v} |v|^2 f_0(v)dv = W, \tag{5}$$

during the time evolution of the function $f(v,t)$ from the initial function $f_0(v)$ to the final Maxwell distribution

$$f_\infty(v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(\frac{-|v-V|^2}{2T}\right). \tag{6}$$

The temperature T in (6) is given by

$$T = \frac{1}{3\rho}(2W - \rho|V|^2).$$

The Fourier transform $\varphi(\xi,t)$ of the distribution function $f(v,t)$ is defined by

$$\varphi(\xi,t) = \int_{\mathbb{R}^3_v} f(v,t)\exp(\imath(v,\xi))dv. \tag{7}$$

After rather long calculations (see [1]) one can obtain a simplified equation for the function $\varphi(\xi,t)$:

$$\frac{\partial\varphi}{\partial t}(\xi,t) = \int_{S^2} g\left(\frac{(\xi,e)}{|\xi|}\right)\left(\varphi\left(\frac{\xi+|\xi|e}{2},t\right)\varphi\left(\frac{\xi-|\xi|e}{2},t\right) - \varphi(0,t)\varphi(\xi,t)\right)de. \tag{8}$$

The equation (8) is subjected to the initial condition

$$\varphi(\xi,0) = \int_{\mathbb{R}^3_v} f_0(v)\exp(\imath(v,\xi))dv = \varphi_0(\xi). \tag{9}$$

This equation will be the main object of our numerical investigations in the next sections. In order to be able to solve the Boltzmann equation numerically via Fourier transform (7) we need a formulation of conservation laws (3),(4) and (5) in terms of the function $\varphi(\xi,t)$. These relations can be easily obtained :

$$\begin{aligned} \rho &= \varphi(0,t) = \varphi_0(\xi)\mid_{\xi=0}; && (10)\\ \rho V &= -\imath \mathrm{grad}_\xi \varphi(0,t) = -\imath \mathrm{grad}_\xi \varphi_0(\xi)\mid_{\xi=0}; && (11)\\ W &= -\frac{1}{2}\Delta_\xi \varphi(0,t) = -\frac{1}{2}\Delta_\xi \varphi_0(\xi)\mid_{\xi=0}. \end{aligned}$$

Thus, in our numerical procedure we should ensure good approximation and conservation of the function $\varphi(\xi,t)$, its gradient and its Laplacian at zero.

3 Numerical realization of the Fourier Transform

We begin our numerical study of the initial value problem (8),(9) with discretization of the velocity space $\mathbb{R}^3_v$. First, we consider a cube

$$\begin{aligned} Q_L &= \left\{v : v \in \mathbb{R}^3_v,\ -L(n) \le v_j - V_j \le L(n),\ j = 1,2,3\right\}, && (12)\\ L(n) &= L n^{1-\alpha},\ L > 0,\ n \in \mathbb{N},\ \alpha \in (0,1). && (13) \end{aligned}$$

and assume all subsequent functions to be $2L(n)$ periodic in all three variables $v_j,\ j = 1,2,3$. The next step is the discretization of the cube Q_L using the nodes

$$\begin{aligned} v_j &= h_v j,\ j = (j_1,j_2,j_3)^T \in Q_n,\\ h_v &= \frac{2L(n)}{n},\ n \in \mathbb{N},\ \text{and } n \text{ is even},\\ Q_n &= \{j \in \mathbb{Z}^3,\ -n/2 \le j_1,j_2,j_3 \le n/2\}. \end{aligned}$$

Furthermore, we introduce the index set $\tilde{Q}_n$ as a subset of all vectors in Q_n excluding those, which have at least one component equal to $-n/2$.
The function $f_0(v)$ can now be represented by a vector $f^0 \in \mathbb{R}^{3n}$ having the components

$$f^0_j = f_0(v_j),\ j \in \tilde{Q}_n. \qquad (14)$$

Note that (14) defines the vector f^0 for all $j \in Q_n$ because of the assumed $2L(n)$-periodicity of all functions.

We replace the continuous Fourier transform (9) by a discrete one

$$\varphi_0(\xi_k) \approx \varphi_k^0 \;=\; h_v^3 \sum_{j\in\tilde{Q}_n} f_j^0 \exp(\imath(v_j,\xi_k)) = h_v^3 \textstyle\sum_{j\in\tilde{Q}_n} f_j^0 \exp\left(\imath\frac{2L(n)}{n}(j,\xi_k)\right). \qquad (15)$$

(15) is nothing but the midpoint quadrature formula for the integral (9). An appropriate choice for the nodes ξ_k is

$$\xi_k = \frac{\pi}{L(n)}k = h_\xi k,\ k \in Q_n. \qquad (16)$$

The described choice of discretization parameters guarantees that

$$\begin{aligned} h_v &\to 0,\ h_v = O(n^{-\alpha}),\ n\to\infty, \\ L(n) &\to \infty,\ L(n) = O(n^{1-\alpha}),\ n\to\infty, \\ h_\xi &\to 0,\ h_\xi = O(n^{-1+\alpha}),\ n\to\infty, \end{aligned}$$

and the expression for the values φ_k^0 then takes the form

$$\varphi_k^0 = h_v^3 \sum_{j\in\tilde{Q}_n} f_j^0 \exp\left(\imath\frac{2\pi}{n}(j,k)\right),\ k\in\tilde{Q}_n. \qquad (17)$$

It is necessary to rearrange the summation (17) in order to get an expression which is suitable for the FFT. For this purpose we introduce the following notation

$$j'(j) = (j_1', j_2', j_3')^T \in \mathbb{Z}^3,\ j_l' = \begin{cases} j_l & : \ j_l \geq 0 \\ n + j_l & : \ j_l < 0 \end{cases},\ l = 1,2,3.$$

Thus, we get

$$\varphi_{k'}^0 = h_v^3 \sum_{j_3'=0}^{n-1} \exp\left(\imath\frac{2\pi}{n}j_3'k_3'\right) \sum_{j_2'=0}^{n-1} \exp\left(\imath\frac{2\pi}{n}j_2'k_2'\right) \sum_{j_1'=0}^{n-1} f_{j'}^0 \exp\left(\imath\frac{2\pi}{n}j_1'k_1'\right). \qquad (18)$$

The computation of all the components $\varphi_k,\ k\in\tilde{Q}_n$ will require

$$O(n^3\log_2(n)) = O(N\log_2(N))$$

arithmetical operations, where $N = n^3$ denotes the whole number of nodes. Here we assume that n is chosen to be in the form $n = 2^{n_l}$. This amount of arithmetical operations is always considered to be "nearly" optimal in numerical analysis.

4 Difference scheme

The next and most important step is the numerical solution of the integral equation (8) over the unit sphere S^2. The main problem here is the following. The approximate values of the initial function $\varphi_0(\xi)$ are given on the fixed grid (16). For the given point ξ_k only some of $e \in S^2$ provide points ξ_+, ξ_- such that

$$\xi_+ = \frac{\xi_k + |\xi_k| e}{2}, \ \xi_- = \frac{\xi_k - |\xi_k| e}{2} \tag{19}$$

again belong to the grid (16). To be precise, we introduce an equivalence relation on the set Q_n

$$k \sim m \ \text{ iff } \ |k| = |m| \text{ and } (k+m)/2 \in Q_n$$

and define the disjoint decomposition of this set in the equivalence classes

$$\mathrm{Cl}(k) = \{m : \ m \in Q_n, \ m \sim k\}.$$

The number of these classes will be denoted by M_n and the number of elements in the class $\mathrm{Cl}(k)$ by $\#\mathrm{Cl}(k)$. The approximation of the equation (8) on the grid (16) can now be written as

$$\frac{\partial \varphi_k(t)}{\partial t} = \sum_{m \in \mathrm{Cl}(k)} \frac{4\pi}{\#\mathrm{Cl}(k)} g\left(\frac{(\xi_k, \xi_m)}{|\xi_k||\xi_m|}\right)\left(\varphi_{\frac{k+m}{2}}(t)\varphi_{\frac{k-m}{2}}(t) - \rho\varphi_k(t)\right), \ k \in Q_n \tag{20}$$

where ρ denotes the value φ_0^0. (20) is a large system of ordinary differential equations subjected to the initial conditions given by (18). This system has a form which is usual for the so called Discrete Velocity Models (DVM) for the Boltzmann equation [6], [7]. One of the obvious possibilities to solve this system numerically is the discretization of the time axis using the nodes

$$t_l = \tau l, \ \tau > 0, \ l = 0, 1, \ldots.$$

and a slightly implicit scheme for equation (20)

$$\varphi_k^{l+1} = \frac{\varphi_k^l}{1 + 4\pi\tau\rho} + \frac{4\pi\tau}{(1+4\pi\tau\rho)\#\mathrm{Cl}(k)} \sum_{m \in \mathrm{Cl}(k)} g\left(\frac{(\xi_k, \xi_m)}{|\xi_k||\xi_m|}\right)\varphi_{\frac{k+m}{2}}^l \varphi_{\frac{k-m}{2}}^l, \tag{21}$$

$$k \in Q_n, \ l = 0, \ldots.$$

In (21) φ_k^l approximates $\varphi_k(t_l)$ and the initial values φ_k^0 are given in (18). The next important questions are the following: how good is the approximation (20) of the unit sphere integral (8) and how much numerical work is necessary to realize one time step corresponding to (21)? The answer of the first question is one of the results of additive number theory obtained in [10], [8],[5]. The number of integer solutions of equation

$$m_1^2 + m_2^2 + m_3^2 = k_1^2 + k_2^2 + k_3^2 = |k|^2 = K \tag{22}$$

tends to infinity with $|k| \to \infty$ having almost the order $O(|k|^{1-\epsilon})$ for any $\epsilon > 0$. There are two exceptions. There is no solution of the equation (22) if $K = 4^i(8j+7)$. Such K cannot appear in our scheme because we have always at least two solutions (for $|k| \neq 0$) of the equation (22) namely $m = k$ and $m = -k$. The second exception is more serious. The number of solutions (22) remains the same if we increase k by factor 2. The significance of this pathology for our purpose is not clear and we would like to leave it for future research. The solutions of the equation (22) are well distributed on the sphere having the radius $|k|$ which implies that we are able to approximate an integral over the unit sphere with an arbitrary accuracy by $|k| \to \infty$ (see [2]).
The last remarks show that the number of elements in the $\mathrm{Cl}(k)$ is almost of order

$$\#\mathrm{Cl}(k) \sim O(n) = O(N^{1/3}).$$

The numerical work per time step is then of order $O(N^{4/3})$ which we consider to be acceptable for practical computations.
Before we begin the next important discussion concerning the conservation laws of the system (20) in the next section we illustrate the results of number theory in the **Table 1**. Here we show the number of equivalence classes M_n and the average number of elements in one class #Cl versa the discretization parameter n.

n	M_n	#Cl
4	20	3.2
8	68	7.5
16	254	16.1
32	1028	31.8
64	4262	61.5

Table 1. *Number of classes and average number of elements in one class versa discretization parameter n*

5 Conservation laws

Now we consider the discrete system (21) and discuss its conservation laws. First of all we remark that for $k = (0,0,0)^T$ only k itself belongs to $\mathrm{Cl}(k)$. Assuming $\varphi_0^l = \rho$ which is true for $l = 0$ we obtain for $l = 0, \ldots$

$$\varphi_0^{l+1} = \frac{\rho}{1 + 4\pi\tau\rho} + \frac{4\pi\tau\rho^2}{1 + 4\pi\tau\rho} = \rho.$$

Thus, $\varphi_0^l = \rho,\ l = 0, \ldots$ remains constant for all l by induction and we obtain the first conservation law of the system (21). This conservation law corresponds to (10) and is completely correct.
The next conservation laws we obtain for $k = \pm e_j,\ j = 1,2,3$, where e_j denotes the $j-$th column of the unit matrix. The corresponding classes are

$$\mathrm{Cl}(\pm e_j) = \{e_j, -e_j\},\ j = 1,2,3.$$

For $k = \pm e_j,\ j = 1,2,3$ we obtain from (21) the next six (!) conservation laws of this system

$$\begin{aligned} \varphi_k^{l+1} &= \frac{\varphi_k^l}{1 + 4\pi\tau\rho} + \frac{4\pi\tau}{2(1 + 4\pi\tau\rho)}(\varphi_k^l\varphi_0^l + \varphi_0^l\varphi_k^l) = \varphi_k^l, \\ k &= \pm e_j,\ j = 1,2,3,\ l = 0, \ldots . \end{aligned}$$

Thus, the values of $\varphi_k^l = \varphi_k^0$ are conserved during the computations. With the help of these values we can conserve an appropriate approximation of the gradient of the function $\varphi(\xi, t)$ using, e.g., the central differences

$$\frac{1}{2h_\xi}(\varphi_{e_1}^0 - \varphi_{-e_1}^0, \varphi_{e_2}^0 - \varphi_{-e_2}^0, \varphi_{e_3}^0 - \varphi_{-e_3}^0)^T \approx \mathrm{grad}\varphi(\xi, 0)\mid_{\xi=0}. \tag{23}$$

This approximation corresponds to the conservation law (11) and is also correct. But having now seven conserved values $\varphi_0^0,\ \varphi_k^0,\ k = \pm e_j,\ j = 1,2,3$ we are also able to approximate each second order partial derivative of the function $\varphi(\xi, t)$ at zero

$$\frac{\varphi_{e_j}^0 - 2\varphi_0^0 + \varphi_{-e_j}^0}{h_\xi^2} \approx \left.\frac{\partial^2\varphi(\xi, t)}{\partial\xi_j^2}\right|_{\xi=0},\ j = 1,2,3.$$

with almost the same accuracy as in (23).

It is now clear that the difference scheme (21) will never converge to an approximation of the Maxwell distribution (6) and, therefore, it is necessary to modify this scheme at least for $k = \pm e_j,\ j = 1, 2, 3$ for which the approximation of the unit sphere integral is so poor. The corresponding grid points ξ_k are close to zero and our idea now is to use an asymptotic expansion (for $|\xi| \to 0$) for the function $\varphi(\xi, t)$ instead of the scheme (21).
First we introduce some additional notations. The flow of momentum will be denoted by

$$M(t) = \int_{\mathbb{R}^3_v} vv^T f(v,t)dv = -H\varphi(\xi,t)\mid_{\xi=0}, \tag{24}$$

where $H\varphi(\xi, t)$ denotes the Hessian of the function $\varphi(\xi, t)$.
This tensor is connected with the stress tensor $P(t)$ by

$$M(t) = \rho VV^T + P(t), \tag{25}$$

where V is the bulk velocity defined in (11). Finally, we rewrite the stress tensor $P(t)$ in the form

$$P(t) = U(t) + pI, \tag{26}$$

where

$$p = \frac{1}{3}\mathrm{tr}P(t)$$

denotes the pressure and the tensor $U(t)$ is therefore trace free.
We begin our asymptotic analysis with a Taylor expansion of the function $\varphi(\xi, t)$ for small $|\xi|$:

$$\begin{aligned}
\varphi(\xi,t) &= \varphi(0,t) + (\mathrm{grad}\varphi(\xi,t)\mid_{\xi=0},\xi) + \frac{1}{2}(H\varphi(\xi,t)\mid_{\xi=0}\xi,\xi) + O(|\xi|^3) = \\
&= \rho + \imath\rho(V,\xi) - \frac{1}{2}(M(t)\xi,\xi) + O(|\xi|^3) = \qquad (27)\\
&= \rho + \imath\rho(V,\xi) - \frac{\rho}{2}(V,\xi)^2 - \frac{1}{2}p|\xi|^2 - \frac{1}{2}(U(t)\xi,\xi) + O(|\xi|^3). \qquad (28)
\end{aligned}$$

Here we have used the relations (10),(11),(24),(25) and (26). From (28) is clear that the time dependence of the function $\varphi(\xi, t)$ on time t is quite weak for small $|\xi|$. The difference scheme should be of third order accuracy to be able to resolve this dependence.

The time derivative of the function $\varphi(\xi,t)$ can now be written as

$$\frac{\partial\varphi(\xi,t)}{\partial t} = -\frac{1}{2}(\dot{U}(t)\xi,\xi) + O(|\xi|^3). \tag{29}$$

Let us denote the weighted averaging of some function $s(e)$, $e \in S^2$ over the unit sphere by $< s(e) > (\xi)$

$$< s(e) > (\xi) = \int_{S^2} g\left(\frac{(\xi,e)}{|\xi|}\right) s(e)de.$$

The right-hand-side of equation (8) can herewith be written as

$$< \varphi(\xi_+,t)\varphi(\xi_-,t) - \rho\varphi(\xi,t) >, \tag{30}$$

where ξ_+ and ξ_- are defined in (19). The expression in the brackets can be computed up to third order in $|\xi|$ using (27),(24),(25) and (26) as follows

$$\begin{aligned}
\varphi(\xi_+,t)\varphi(\xi_-,t) - \rho\varphi(\xi,t) &= \frac{\rho}{2}\left((M(t)\xi,\xi) - (M(t)\xi_+,\xi_+) - (M(t)\xi_-,\xi_-)\right) - \\
&- \rho^2(V,\xi_+)(V,\xi_-) + O(|\xi|^3) = \\
&= \rho(M(t)\xi_+,\xi_-) - \rho^2(VV^T\xi_+,\xi_-) + O(|\xi|^3) = \\
&= \rho(P(t)\xi_+,\xi_-) + O(|\xi|^3) = \\
&= \frac{\rho}{4}\left((U(t)\xi,\xi) - |\xi|^2(U(t)e,e)\right) + O(|\xi|^3) = \\
&= \frac{\rho}{4}|\xi|^2\sum_{k,l=1}^{3} u_{kl}(t)(\omega_l\omega_k - e_le_k) + O(|\xi|^3).
\end{aligned} \tag{31}$$

Here we have used the notation ω for the unit vector in the direction of ξ. The averaging (30) therefore reduces to the averaging of the matrix $\omega\omega^T - ee^T$ which we will compute in two steps. The average of the matrix $\omega\omega^T$ is almost trivial

$$\begin{aligned}
< \omega\omega^T > &= \omega\omega^T < 1 >= 2\alpha\omega\omega^T, \\
\alpha &= \pi\int_{-1}^{1} g(\mu)d\mu.
\end{aligned} \tag{32}$$

For averaging the matrix ee^T we assume first that $\omega = (0,0,1)^T$ and compute

$$
\begin{aligned}
< ee^T > (\omega) &= \int_0^{2\pi} \int_0^{\pi} g(\cos\theta) e(\phi,\theta) e(\phi,\theta)^T \sin\theta d\theta d\phi = \\
&= \mathrm{diag}(\alpha-\beta, \alpha-\beta, 2\beta), \\
\beta &= \pi \int_{-1}^{1} g(\mu)\mu^2 d\mu.
\end{aligned}
$$

For general ω we introduce an orthogonal rotation matrix $Q(\omega)$ having the property

$$
Q(\omega)\omega = (0,0,1)^T,
$$

or equivalent

$$
Q(\omega)^T (0,0,1)^T = \omega.
$$

The average of the matrix ee^T can now be computed as

$$
\begin{aligned}
< ee^T > (\omega) &= \int_{S^2} g\left((\omega, e)\right) ee^T de = \\
&= \int_{S^2} g\left((\omega, Q^T e')\right) Q^T e' (e')^T Q de' = \\
&= Q^T \int_{S^2} g\left(((0,0,1)^T, e')\right) e'(e')^T de' Q = \\
&= Q^T \mathrm{diag}(\alpha-\beta, \alpha-\beta, 2\beta) Q = \\
&= (\alpha-\beta) I + (3\beta-\alpha) Q^T (0,0,1)^T (0,0,1) Q = \\
&= (\alpha-\beta) I + (3\beta-\alpha) \omega\omega^T. \qquad (33)
\end{aligned}
$$

Combining (32) and (33) we obtain

$$
< \omega\omega^T - ee^T > = 3(\alpha-\beta)\left(\omega\omega^T - \frac{1}{3} I\right).
$$

Thus, we get from (31)

$$
\begin{aligned}
< \varphi(\xi_+, t)\varphi(\xi_-, t) &- \rho\varphi(\xi, t) > = \\
&= \frac{3\rho}{4} |\xi|^2 (\alpha-\beta) \sum_{k,l=1}^{3} u_{kl}(t)(\omega_l\omega_k - \frac{1}{3}\delta_{lk}) + O(|\xi|^3) = \\
&= \frac{3\rho}{4} (\alpha-\beta)\left((U(t)\xi, \xi)\right) + O(|\xi|^3).
\end{aligned}
$$

The last equation together with (29) leads neglecting terms of the order $O(|\xi|^3)$ to an equation for the tensor $U(t)$:

$$-\frac{1}{2}\dot{U}(t) = \frac{3\rho}{4}(\alpha - \beta)U(t),$$

or

$$U(t) = U(0)\exp(-at), \tag{34}$$

$$a = \frac{3\rho}{2}(\alpha - \beta) = \frac{3\rho\pi}{2}\int_{-1}^{1} g(\mu)(1-\mu^2)d\mu. \tag{35}$$

(34),(35) give the exact explicit evolution of all second order moments for the Boltzmann equation with Maxwell molecules. The final asymptotic expansion of the function $\varphi(\xi, t)$ for small $|\xi|$ can now be written in the form

$$\begin{aligned}
\varphi(\xi,t) &\approx \rho + \imath\rho(V,\xi) - \frac{\rho}{2}(V,\xi)^2 - \frac{1}{2}p(\xi,\xi) - \frac{1}{2}(U(0)\xi,\xi)\exp(-at) = \\
&= \varphi_0(\xi)\exp(-at) + \left(\rho + \imath\rho(V,\xi) - \frac{\rho}{2}(V,\xi)^2 - \frac{1}{2}p(\xi,\xi)\right)(1-\exp(-at)) = \\
&= \varphi_0(\xi)\exp(-at) + \rho\left(1 + \imath(V,\xi) - \frac{1}{2}(V,\xi)^2 - \frac{1}{2}T(\xi,\xi)\right)(1-\exp(-at)),
\end{aligned}$$

where $T = p/\rho$ denotes the temperature.
The special choice of $\xi = \xi_{\pm e_j},\ j = 1,2,3$ leads to

$$\varphi(\xi_{\pm e_j}, t) \approx \rho \pm \imath h_\xi \rho V_j - \frac{h_\xi^2}{2}\left(\rho V_j^2 + \rho T + u_{jj}(0)\exp(-at)\right), \tag{36}$$

or

$$\varphi(\xi_{\pm e_j}, t) \approx \varphi_0(\xi_{\pm e_j})\exp(-at) + \rho\left(1 \pm \imath h_\xi V_j - \frac{h_\xi^2}{2}\left(V_j^2 + T\right)\right)(1-\exp(-at)). \tag{37}$$

We have two possibilities to change our difference scheme corresponding to the equations (36) or (37). The first one is the following. Since the exact values of the parameters ρ, V, T and $u_{jj}(0)$ are given by the initial function (2), we can use these exact values by setting

$$\varphi_0^l = \rho, \tag{38}$$

$$\varphi_{\pm e_j}^l = \rho \pm \imath h_\xi \rho V_j - \frac{h_\xi^2}{2}\left(\rho V_j^2 + \rho T + u_{jj}(0)\exp(-at_l)\right), \tag{39}$$

$$j = 1,2,3,\ l = 0,1,\ldots .$$

The corresponding values obtained by Fourier transform (17) will be ignored in this case. The second possibility is to define the numerical values ρ_h, V_h, T_h using φ_k^0 from (17) as

$$\begin{aligned}
\rho_h &= \varphi_0^0, \\
V_h &= \frac{1}{h_\xi \rho} \mathrm{Im}\left(\varphi_{e_1}^0, \varphi_{e_2}^0, \varphi_{e_3}^0\right)^T, \\
T_h &= \frac{2}{\rho_h h_\xi^2}\left(\rho - \frac{1}{3}\sum_{j=1}^{3} \mathrm{Re}(\varphi_{e_j}^0)\right) - \frac{1}{3}|V_h|^2
\end{aligned}$$

and to use the following approximation

$$\varphi_0^l = \rho_h, \tag{40}$$

$$\varphi_{\pm e_j}^l = \varphi_{\pm e_j}^0 \exp(-a t_l) + \rho_h \left(1 \pm i h_\xi (V_h)_j - \frac{h_\xi^2}{2}\left((V_h)_j^2 + T_h\right)\right)(1 - \exp(-a t_l)), \tag{41}$$

$$j = 1,2,3, \; l = 0,1,\ldots .$$

Combining the formula (21) for $k \neq 0, \pm e_j, \; j = 1,2,3$ with (38),(39) or with (40),(41) we obtain the final version of our difference scheme.

6 Numerical example

In this section we calculate an example of the relaxation using our difference scheme. The initial distribution $f_0(v)$ is given by

$$f_0(v) = \frac{1}{2(2\pi)^{3/2}}\left(\exp\left(-\frac{|v - 2e_1|^2}{2}\right) + \exp\left(-\frac{|v + 2e_1|^2}{2}\right)\right),$$

where e_1 denotes the first column of the unit matrix.
It is easy to see that the macroscopic parameters we need are defined as

$$\rho = 1, \; V = (0,0,0)^T, \; T = 7/3.$$

The parameter L in (13) is in our numerical tests as follows

$$L = \sqrt{2T}.$$

In general, we cannot expect that these values remain conserved during the computation. However, for this example the values of density and bulk velocity remain constant because of the symmetry considerations. In the first figure we show the time evolution of the temperature for $n = 4, 8, 16$ and $L(n) = L\sqrt{n}$.

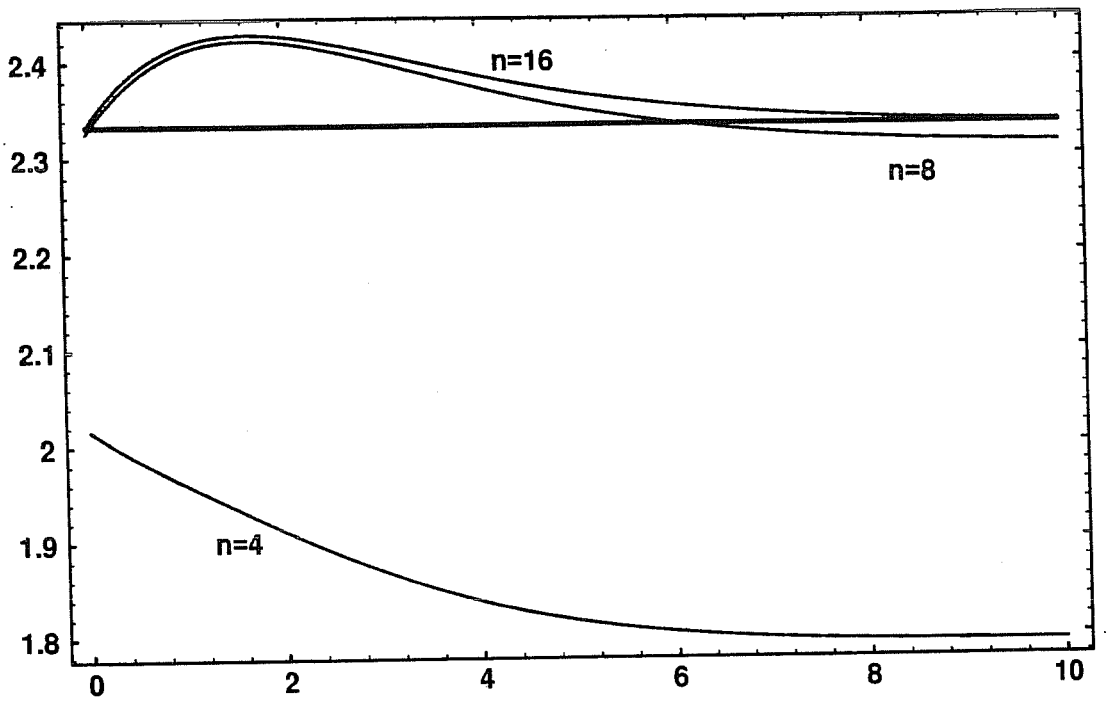

Figure 1: The time evolution of the temperature for different n

The thick solid line in the Figure 1 shows the ideal constant value of the temperature, while the other lines represent the numerical results. It is clear to see that only 4 points are not enough even for an appropriate approximation of the initial function. If we take 8 points then the initial value of the temperature is approximated quite good but not the asymptotic value. Our numerical tests show that for $n \geq 16$ both, the initial and asymptotic values of the temperature are very well approximated. However, the maximal error for $n = 16$ is about 3.7 %.

In the next figure we show the relaxation of components $p_{11}(t)$ and $p_{22}(t)$ of the stress tensor. The relaxation of the $p_{33}(t)$ is identical to that of $p_{22}(t)$ because of symmetry reasons. The dashed lines show here the exact curves defined as

$$
\begin{aligned}
p_{11}(t) &= 5\exp\left(-\frac{1}{2}t\right) + \frac{7}{3}\left(1 - \exp\left(-\frac{1}{2}t\right)\right), \\
p_{22}(t) &= \exp\left(-\frac{1}{2}t\right) + \frac{7}{3}\left(1 - \exp\left(-\frac{1}{2}t\right)\right).
\end{aligned}
$$

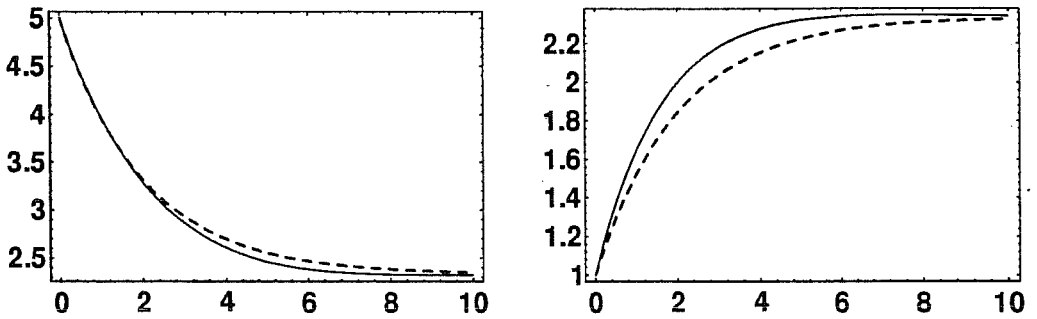

Figure 2: The time relaxation of components of the stress tensor

while the solid lines represent the numerical results obtained for $n = 16$. In **Table 2** we show the relative errors E_1 and E_2 defined as

$$E_j = \max_{0 \le l \le 100} \left| p_{jj}(t_l) - \tilde{p}^l_{jj} \right|, \ j = 1, 2, \ \tau = 0.1$$

where $\tilde{p}^l_{jj}$ denotes the numerical value at $t = t_l$.
This table shows that the corresponding error seems to be of the order $O(n^{-1/2})$ which corresponds to our choice $\alpha = 0.5$ in (12).

n	E_1	E_2
4	0.19921	0.19847
8	0.04685	0.09627
16	0.03640	0.08599
32	0.02478	0.06289
64	0.01853	0.04698

Table 2. *The relative error for the stress tensor*

Next we show the relaxation of the distribution function itself to the Maxwell distribution in Figure 3 and the corresponding iso-lines in the Figure 4. We have used the values of $f((v_1, v_2, 0)^T, t)$ to plot these figures.

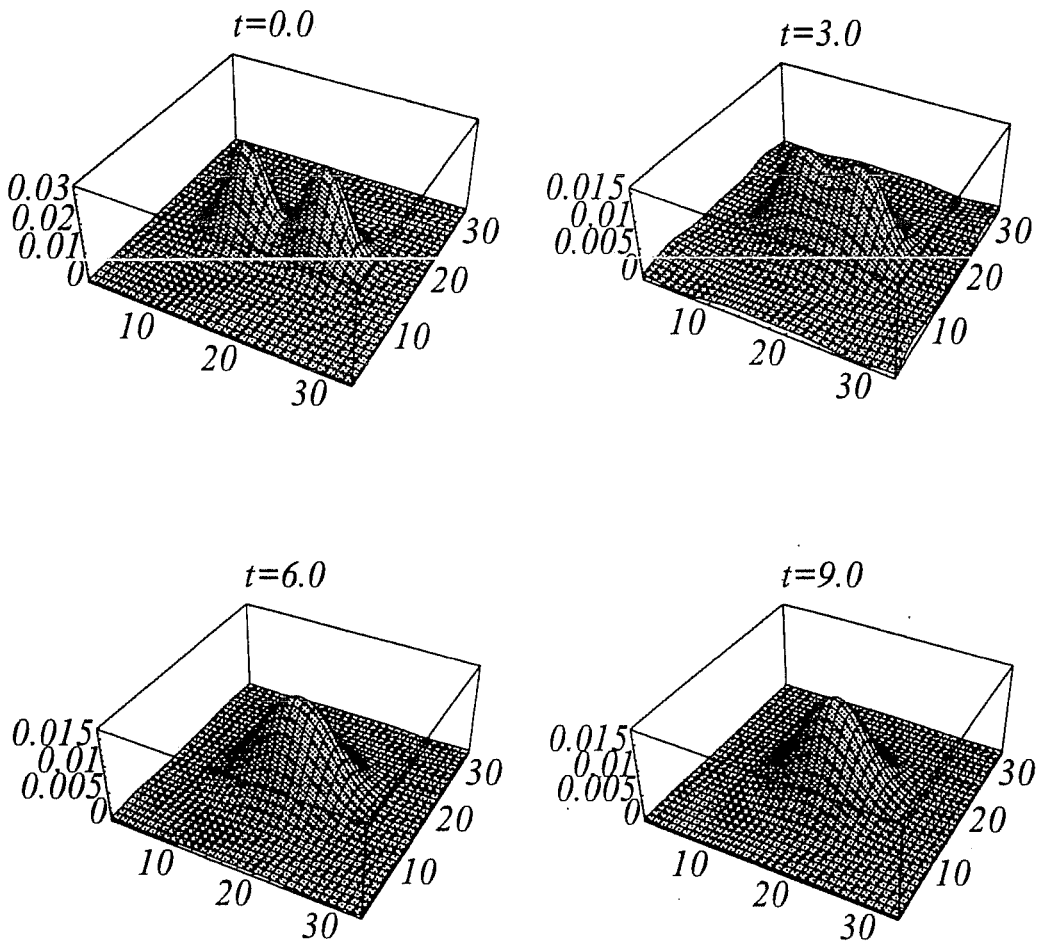

Figure 3: The time relaxation of the distribution function

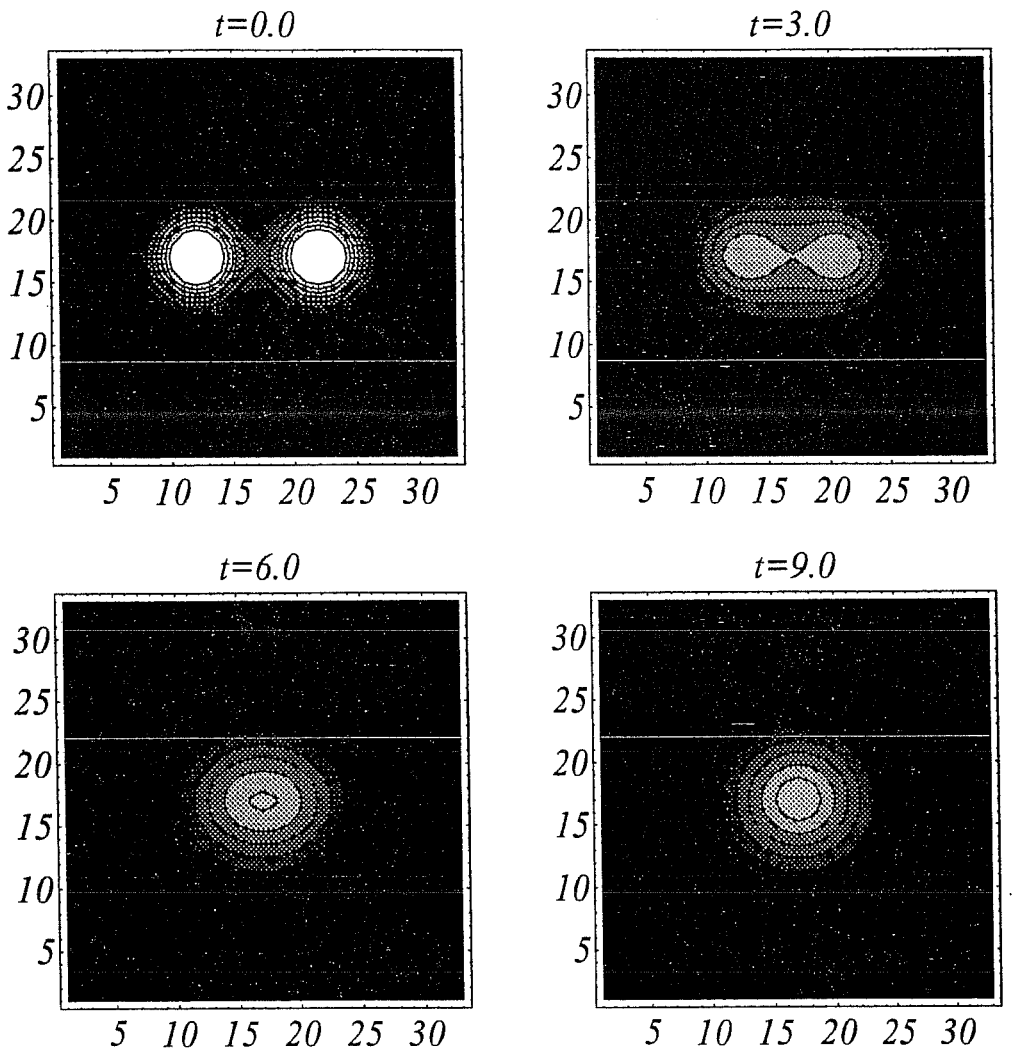

Figure 4: The iso-lines of the distribution function

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