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Abstract

An effective deterministic method based on the Fast Fourier Transform (FFT) for the Boltzmann equation with Maxwell molecules is considered. The global existence, uniqueness and boundness of the discrete solution is proved. The analytical form of the first 13 moments of the solution is derived. An effective procedure for the conservation of the macroscopic quantities is described. The results of some numerical tests are presented.

Contents

1 Introduction

In this paper we continue the study of the numerical solution of the spatially homogeneous Boltzmann equation [4] with Maxwell molecules using a difference scheme which we have proposed in [2] (see also [9]). This scheme is based on the uniform discretisation of the velocity space and the Fast Fourier Transform (FFT) [5],[8]. The main advantage of this scheme is that it requires only $O(N^{4/3})$ arithmetical operations per time step, where N denotes the whole number of discrete velocities in use. However there are some difficulties. First of all our scheme is not completely conservative, only the conservation of mass is guaranteed automatically. The correction suggested in [2] leads to a scheme conserving some values which are connected to the usual macroscopic quantities via Fourier transform. Thus, the scheme does not conserve the momentum and energy exactly but also does not allow these quantities to vary much. The initial and asymptotic values for the temperature are correct but in-between we can observe some deviation.
In the present paper we report a considerable theoretical and numerical progress achieved by using this scheme. The treatment of the problem consists of two main steps. First, we derive a large system of ordinary differential equations for the Fourier transform of the unknown function evaluated at some knots in the frequency space. We show that this system has the unique, global solution which is bounded from above by the numerical density. Furthermore, we prove the necessary and sufficient conditions for that the asymptotic solution of this system is discrete Maxwellian. After that we show how to force the system to be completely conservative. It is remarkable, that the additional numerical work due to conservative properties is only of the order $O(N^{1/3})$. Then we consider slightly implicit difference scheme for this system and show that it still has the above properties naturally adapted to the discrete case.
The paper is organised as follows. In Section 2, we give a brief description of the difference scheme suggested in[2] and prove its properties as we have formulated before. In Section 3, we derive the exact formulae for the time relaxation of the first 13 moments of the system. In Section 4, we use these formulae and discuss the conservation of momentum and energy. Finally, in Section 5, we present the results of some numerical experiments and draw some conclusions.

2 Fourier transform for the Boltzmann equation

We consider the following initial value problem for spatially homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t}(v,t) \quad = \quad Q(f,f),\ t>0,\ v\in\mathbb{R}^3_v,\ f(v,0)=f_0(v)>0, \tag{1}$$

where

$$Q(f,f)=\int_{\mathbb{R}^3_w}\int_{S^2} B(v,w,e)\left(f(v',t)f(w',t)-f(v,t)f(w,t)\right)dw\,de. \tag{2}$$

We use the following notions in (2)

- $v,w\in\mathbb{R}^3$ are pre-collision velocities;
- dw is the volume element in $\mathbb{R}^3_w$;
- $e\in S^2\subset\mathbb{R}^3$ is a unit vector;
- de is the surface element on the unit sphere S^2;
- $u=v-w\in\mathbb{R}^3$ is the relative velocity of collision partners;
- v',w' are post-collision velocities defined by $v'=U+\frac{1}{2}|u|e,\ w'=U-\frac{1}{2}|u|e,\ U=\frac{1}{2}(v+w)$;
- $B(v,w,e)$ is the differential collision cross-section.

The differential collision cross-section depends on the physical model of interaction between particles. Here we consider the special case of so called pseudo-Maxwellian molecules with

$$B(v,w,e)=g\left(\frac{(u,e)}{|u|}\right),$$

where $g(\mu)$ is some on the interval $[-1,1]$ non-negative and piecewise continuous function. The most simple choice, which we will use, is

$$B(v,w,e)=\frac{1}{4\pi}.$$

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

$$f_\infty(v) = \frac{\rho}{(2\pi T)^{3/2}} e^{-\dfrac{|v-V|^2}{2T}}.$$

The Fourier transform of the function $f(v,t)$ is defined as

$$\varphi(\xi,t) = [\mathcal{F}f](\xi) = \int_{\mathbb{R}^3_v} f(v,t)e^{\imath(v,\,\xi)}dv. \tag{6}$$

The inverse Fourier transform $\mathcal{F}^{-1}$ is then

$$f(v,t) = [\mathcal{F}^{-1}\varphi](v) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3_v} \varphi(\xi,t)e^{-\imath(v,\,\xi)}dv.$$

The simplified Boltzmann equation (cf. [1]) for the function $\varphi(\xi,t)$ is

$$\frac{\partial\varphi}{\partial t}(\xi,t) = \frac{1}{4\pi}\int_{S^2}\left(\varphi\left(\frac{\xi+|\xi|e}{2},t\right)\varphi\left(\frac{\xi-|\xi|e}{2},t\right) - \varphi(0,t)\varphi(\xi,t)\right)de. \tag{7}$$

This equation is subjected to the initial condition

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

The formulation of conservation laws (3),(4) and (5) in terms of the function $\varphi(\xi,t)$ is given by

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

Since the function $f(v,t)$ is up the factor ρ a probability distribution function, the function $\varphi(\xi,t)$ fulfils the following well known necessary conditions

$$\begin{aligned}|\varphi(\xi,t)| &\le \varphi(0,t)=\rho\in\mathbb{R},\\ \varphi(\xi,t) &= \overline{\varphi(-\xi,t)},\ \forall\xi\in\mathbb{R}^3.\end{aligned}$$

We begin the numerical solution of the equation (7) by the restriction of the $\mathbb{R}^3$ space of the variable ξ to the lattice

$$h_\xi\mathbb{Z}^3=\left\{\xi_k\in\mathbb{R}^3,\ \xi_k=h_\xi k,\ k\in\mathbb{Z}^3\right\}. \tag{8}$$

The next step is the numerical solution of the integral equation (7) over the unit sphere S^2. The main problem here is the following. For the given point ξ_k only some of $e\in S^2$ provide points $\xi_+,\ \xi_-$ such that

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

again belong to the lattice (8). To be precise, we introduce an equivalence relation on the set $\mathbb{Z}^3$

$$k\sim m \text{ iff } |k|=|m| \text{ and } (k+m)/2\in\mathbb{Z}^3 \tag{9}$$

and define the disjoint decomposition of $\mathbb{Z}^3$ in the equivalence classes

$$\mathrm{Cl}(k)=\left\{m:\ m\in\mathbb{Z}^3,\ m\sim k\right\}. \tag{10}$$

The number of elements in the class $\mathrm{Cl}(k)$ will be denoted by $n_k=\#\mathrm{Cl}(k)$. The approximation of the equation (7) on the lattice (8) can now be written as

$$\frac{\partial\varphi_k(t)}{\partial t}=\frac{1}{n_k}\sum_{m\in\mathrm{Cl}(k)}\left(\varphi_{\frac{k+m}{2}}(t)\varphi_{\frac{k-m}{2}}(t)-\rho\varphi_k(t)\right),\ k\in\mathbb{Z}^3. \tag{11}$$

The initial conditions for the infinite system of ordinary differential equations (11) are defined through the given function $\varphi_0(\xi)$ and fulfil

$$
\begin{aligned}
\varphi_k(0) &= \varphi_0(\xi_k), && (12)\\
|\varphi_k(0)| &\le \varphi_0(0) = \rho, && (13)\\
\varphi_k(0) &= \overline{\varphi_{-k}(0)},\ k \in \mathbb{Z}^3. && (14)
\end{aligned}
$$

We begin with the analytical study of the system (11) subjected to the initial conditions (12) having properties (13) and (14).

Lemma 1 *The system (11) conserves the values*

$$
\begin{aligned}
\varphi_0(t) &= \rho, && (15)\\
\varphi_{e_j}(t) &= \varphi_{e_j}(0) = \overline{\varphi_{-e_j}(t)} = \overline{\varphi_{-e_j}(0)},\ j = 1,2,3, && (16)
\end{aligned}
$$

where e_j *denotes the* $j-th$ *column of the* 3×3 *identity matrix.*

Proof:
The equivalence class Cl(0) contains only one element, the vector 0 itself. Thus, we get from (11) the following initial value problem for the function $\varphi_0(t)$

$$\dot{\varphi}_0(t) = \varphi_0^2(t) - \rho\varphi_0(t), \quad \varphi_0(0) = \rho.$$

The unique solution of this problem is $\varphi_0(t) = \rho$ and (15) is proved.
The equivalence classes for the vectors e_j contain each exactly two elements

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

The corresponding initial value problems are

$$\dot{\varphi}_{\pm e_j}(t) = \frac{1}{2}\left(\varphi_{\pm e_j}(t)\varphi_0(t) + \varphi_0(t)\varphi_{\pm e_j}(t) - 2\rho\varphi_{\pm e_j}(t)\right) = 0,$$

because of (15). This proves the lemma.

■

Therefore three complex values and one real value are conserved by the system (11). Our next step is to introduce an appropriate substitution to this system. Let us denote the values $\varphi_{\pm e_j}$ by

$$\varphi_{\pm e_j}(t) = \rho a_j e^{\imath h_\xi u_j},\ j = 1,2,3,$$

where the values a_j satisfy

$$0 \le a_j \le 1,\ \ j = 1,2,3$$

because of (12) and $u = (u_1, u_2, u_3)^T$ is some real vector. The following substitution

$$\varphi_k(t) = \rho e^{\imath h_\xi(u,k)} \tilde{\varphi}_k(\tilde{t}),\ \ \tilde{t} = \rho\, t \tag{17}$$

transforms the system (11) to the form

$$\frac{\partial \tilde{\varphi}_k(\tilde{t})}{\partial \tilde{t}} = \frac{1}{n_k} \sum_{m \in \mathrm{Cl}(k)} \left(\tilde{\varphi}_{\frac{k+m}{2}}(\tilde{t}) \tilde{\varphi}_{\frac{k-m}{2}}(\tilde{t}) - \tilde{\varphi}_k(\tilde{t}) \right),\ \ k \in \mathbb{Z}^3, \tag{18}$$

having the initial conditions

$$\tilde{\varphi}_0(0) \ = \ 1, \tag{19}$$

$$\tilde{\varphi}_{\pm e_j}(0) \ = \ a_j,\ \ j = 1,2,3\,, \tag{20}$$

and the corresponding initial conditions for the other components satisfying

$$\begin{aligned} |\tilde{\varphi}_k(0)| \ &\le \ 1, \\ \tilde{\varphi}_k(0) \ &= \ \overline{\tilde{\varphi}_{-k}(0)} \end{aligned} \tag{21}$$

because of (13),(14). For simplicity we omit the both tilde symbols by $\tilde{\varphi}_k(\tilde{t})$ in order not to overload the formulae having in mind the substitution (17). There are several possibilities to prove the existence of global solution of the system (18). May be the most elegant is using the "Wild-Sum" [11].

Lemma 2 *There is the global solution of the system (18) which satisfies*

$$|\varphi_k(t)| \le 1,\ \ t \ge 0,\ \ k \in \mathbb{Z}^3. \tag{22}$$

Proof:
If we substitute

$$\varphi_k(t) = e^{-t} \psi_k(\tau),\ \ \tau = 1 - e^{-t},\ \ \tau \in [0,1),\ \ k \in \mathbb{Z}^3$$

then the system (18) transforms into

$$\frac{\partial \psi_k(\tau)}{\partial \tau} = \frac{1}{n_k} \sum_{m \in \mathrm{Cl}(k)} \psi_{\frac{k+m}{2}}(\tau) \psi_{\frac{k-m}{2}}(\tau) = S(\psi_k, \psi_k),\ \ k \in \mathbb{Z}^3, \tag{23}$$

with obvious initial conditions

$$\psi_k(0) = \varphi_k(0), \ k \in \mathbb{Z}^3$$

and having the property (cf. (21))

$$|\psi_k(0)| \le 1, \ k \in \mathbb{Z}^3.$$

The bilinear operator $S(\psi_k, \zeta_k)$ is defined as

$$S(\psi_k, \zeta_k) = \frac{1}{n_k} \sum_{m \in \mathrm{Cl}(k)} \psi_{\frac{k+m}{2}} \zeta_{\frac{k-m}{2}}$$

and satisfies

$$|S(\psi_k, \zeta_k)| \le 1 \tag{24}$$

for $|\psi_k| \le 1, \ |\zeta_k| \le 1$. We will look for the solution of the system (23) in the form of power series

$$\psi_k(\tau) = \sum_{j=0}^{\infty} \alpha_j^{(k)} \tau^j, \ k \in \mathbb{Z}^3 \tag{25}$$

and remark that

$$|\alpha_0^{(k)}| = |\psi_k(0)| \le 1. \tag{26}$$

The time derivative of the function $\psi_k(\tau)$ is of the form

$$\frac{\partial \psi_k(\tau)}{\partial \tau} = \sum_{j=0}^{\infty} (j+1) \alpha_{j+1}^{(k)} \tau^j, \ k \in \mathbb{Z}^3 \tag{27}$$

and we obtain from (23) and (27) the following recursive relation for the coefficients $\alpha_j^{(k)}$

$$\alpha_{j+1}^{(k)} = \frac{1}{j+1} \sum_{m=0}^{j} S(\alpha_m^{(k)}, \alpha_{j-m}^{(k)}), \ j = 1, 2, \ldots . \tag{28}$$

Thus we get by induction from (26),(24) and (28)

$$|\alpha_j^{(k)}| \le 1, \ j = 0, 1, \ldots, \ k \in \mathbb{Z}^3. \tag{29}$$

The power series (25) converge therefore absolute for all $\tau \in [0, 1)$. This completes the proof.

■

Remark 1 *The inequalities (29) imply also*

$$|\varphi_k(t)| = \left| e^{-t} \sum_{j=0}^{\infty} \alpha_j^{(k)} (1-e^{-t})^j \right| \leq e^{-t} \sum_{j=0}^{\infty} (1-e^{-t})^j = 1, \ k \in \mathbb{Z}^3,$$

i.e. the initial property (21) remains valid for all $t \geq 0$.

Remark 2 *The initial property (14) also remains valid for all* $t \geq 0$

$$\varphi_k(t) = \overline{\varphi_{-k}(t)}, \ k \in \mathbb{Z}^3,$$

because of $Cl(k) = Cl(-k)$ *and if* $m \in Cl(-k)$ *then* $-m \in Cl(-k)$. *Thus, the equations for* $\varphi_k(t)$ *and* $\varphi_{-k}(t)$ *are identical but the initial conditions are as in (14).*

The form of the system (18) allows to construct the solution recursively using the classes (9),(10). There are some preliminary remarks necessary. The recursion will be according to the squared length of the integer vector k

$$M = |k|^2 = k_1^2 + k_2^2 + k_3^2.$$

The system is already solved for $M = 0$ and $M = 1$ (cf. (15),(16)). Corresponding to results of additive number theory obtained in [10],[7],[6] the number of integer solutions of equation

$$m_1^2 + m_2^2 + m_3^2 = k_1^2 + k_2^2 + k_3^2 = |k|^2 = M \tag{30}$$

(i.e. the number of the elements in the equivalence class $\mathrm{Cl}(k)$) 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 (30) if

$$M = 4^i(8j+7), \ i,j \in \mathbb{N}. \tag{31}$$

Such M cannot appear in our scheme because we have always at least two solutions (for $|k| \neq 0$) of the equation (30) namely $m = k$ and $m = -k$. The second exception is that the number of solutions (30) remains the same if we increase k by factor 2. This exception does not play any role for the recursive consideration of our scheme. Let M be some natural number not of the form (31) and the system (18) is solved for all classes $\mathrm{Cl}(k)$ with $|k|^2 < M$. We consider now the equation (18) for some k with $|k|^2 = M$ and rewrite it using the properties $\pm k \in \mathrm{Cl}(k),\ \varphi_0(t) = 1$ as

$$\frac{\partial \varphi_k(t)}{\partial t} = -\left(1 - \frac{2}{n_k}\right)\varphi_k(t) + \frac{1}{n_k}\sum_{m\in \mathrm{Cl}(k),\, m\neq \pm k} \varphi_{\frac{k+m}{2}}(t)\varphi_{\frac{k-m}{2}}(t). \qquad (32)$$

Since

$$\left|\frac{k\pm m}{2}\right| < |k|,\ \forall m \in \mathrm{Cl}(k),\ m \neq \pm k,$$

(32) is a linear differential equation with a well defined right-hand side because of induction assumption. The unique solution of this initial value problem is therefore trivially guaranteed. Using the abbreviations

$$\lambda_k = 1 - \frac{2}{n_k},\ S_k(t) = \frac{1}{n_k}\sum_{m\in \mathrm{Cl}(k),\, m\neq \pm k} \varphi_{\frac{k+m}{2}}(t)\varphi_{\frac{k-m}{2}}(t)$$

we rewrite the equation (32) as follows

$$\dot{\varphi}_k(t) + \lambda_k \varphi_k(t) = S_k(t)$$

where the source $S_k(t)$ is known. The solution of this equation is

$$\varphi_k(t) = \varphi_k(0)e^{-\lambda_k t} + \int_0^t e^{-\lambda_k (t-\tau)} S_k(\tau)d\tau.$$

If $|\varphi_k(t)| \leq 1$ for $|k| < M$ (this is true for $M = 0, 1$ because of (19),(20)) then

$$|S_k(t)| \leq \frac{n_k - 2}{n_k} = \lambda_k$$

and therefore

$$\begin{aligned} |\varphi_k(t)| &\leq |\varphi_k(0)|e^{-\lambda_k t} + \int_0^t e^{-\lambda_k (t-\tau)}|S_k(\tau)|d\tau \\ . &\leq e^{-\lambda_k t} + \left(1 - e^{-\lambda_k t}\right) = 1 \end{aligned}$$

for $|k| = M$. Thus we again have proved the property (22). The solution $\varphi_k(t)$ is in general a sum of negative exponents probably multiplied by some polynomials (if some resonance case occurs). Thus, we deduce that the asymptotic solutions

$$\varphi_k = \lim_{t\to\infty} \varphi_k(t), \;\; k \in \mathbb{Z}^3$$

exist and fulfils the following system of algebraic equations

$$\varphi_0 \;\; = \;\; 1, \tag{33}$$

$$\varphi_{e_{\pm j}} \;\; = \;\; a_j, \;\; j = 1,2,3, \tag{34}$$

$$\varphi_k \;\; = \;\; \frac{1}{n_k - 2} \sum_{m\in \mathrm{Cl}(k),\, m\neq \pm k} \varphi_{\frac{k+m}{2}} \varphi_{\frac{k-m}{2}}, \;\; |k| > 1. \tag{35}$$

Note that this system is of triangle form, i.e. the solution is given by the initial values (33),(34) and the recursion (35). In the next lemma we prove an important criteria that the asymptotic solution is a discrete Maxwellian.

Lemma 3 *The solution of the algebraic system (33),(34),(35) is a discrete Maxwellian*

$$\varphi_k = e^{-s|k|^2}, \;\; s \in \mathbb{R}, \;\; s > 0, \tag{36}$$

if and only if

$$a_1 = a_2 = a_3 = a, \;\; 0 < a < 1. \tag{37}$$

Proof:
The conditions (37) are trivially necessary because of the initial conditions (34). If (37) is fulfilled then we obtain

$$a = \varphi_{e_{\pm j}} = e^{-s|e_{\pm j}|^2} = e^{-s}$$

and therefore $s = -\ln(a)$. Thus, the form (36) of the solution is true for $M = 0, 1$. For $|k|^2 = M > 1$ we get from the induction assumption, recursion (35) and using $|k|^2 = |m|^2$

$$\begin{aligned} \varphi_k \;\; &= \;\; \frac{1}{n_k - 2} \sum_{m\in \mathrm{Cl}(k),\, m\neq \pm k} e^{-s\left|\frac{k+m}{2}\right|^2} e^{-s\left|\frac{k-m}{2}\right|^2} \\ &= \;\; \frac{1}{n_k - 2} \sum_{m\in \mathrm{Cl}(k),\, m\neq \pm k} e^{-s|k|^2} = e^{-s|k|^2}. \end{aligned}$$

The proof is herewith completed.

■

The next interesting question is to clearly the following question. Define some space of functions $\varphi_k(t) : \mathbb{Z}^3 \to \mathbb{C}$ so, that if the initial function $\varphi_k(0)$ belongs to this space then the time evolution of this function corresponding to the system (18) will belong to the same space for all times.

Definition 1 *Let $\varepsilon \geq 0$ be a non-negative number and the function φ_k fulfils*

$$\varphi_k : \mathbb{Z}^3 \;\to\; \mathbb{C}, \tag{38}$$

$$\varphi_0 \;=\; 1. \tag{39}$$

Then the class $A(\varepsilon)$ of functions (38),(39) is defined as

$$A(\varepsilon) = \left\{ \varphi_k : |\varphi_k| \leq e^{-\varepsilon|k|^2} \right\}.$$

Now we are able to formulate the last result of this section.

Lemma 4 *The Cauchy problem*

$$\begin{aligned} \frac{\partial \varphi_k(t)}{\partial t} &= \frac{1}{n_k} \sum_{m \in Cl(k)} \varphi_{\frac{k+m}{2}}(t) \varphi_{\frac{k-m}{2}}(t) - \varphi_k(t), \;\; k \in \mathbb{Z}^3, \\ \varphi_k(0) &\in A(\varepsilon) \end{aligned}$$

is uniquely solvable in $A(\varepsilon)$ for all $\varepsilon \geq 0$.

Proof:
Using the substitution

$$\varphi_k(t) = e^{-\varepsilon|k|^2} \psi_k(t)$$

we rewrite the system (40),(40) as

$$\begin{aligned} \frac{\partial \psi_k(t)}{\partial t} &= \frac{1}{n_k} \sum_{m \in \mathrm{Cl}(k)} \psi_{\frac{k+m}{2}}(t) \psi_{\frac{k-m}{2}}(t) - \psi_k(t), \;\; k \in \mathbb{Z}^3, \\ |\psi_k(0)| &\leq 1 \end{aligned}$$

which is identical with (18). Thus, there is the global solution $\psi_k(t)$ satisfying $|\psi_k(t)| \leq 1$ or equivalently $\psi_k(t) \in A(0)$. Then $\varphi_k(t) \in A(\varepsilon)$.

■

3 The exact time evolution of the moments

If $f(v)$ is a distribution function with

$$\int_{\mathbb{R}^3_v} f(v)\, dv = 1$$

then we denote the weighted averaging of a given function $g(v)$ as

$$< g(v) >_f = \int_{\mathbb{R}^3_v} g(v) f(v)\, dv.$$

We consider the following Maxwell distribution function

$$f_M(v) = \frac{1}{(2\pi T)^{3/2}} e^{-\dfrac{|v-V|^2}{2T}}.$$

Its first 13 moments can be computed as

$$\begin{aligned} < 1 >_{f_M} &= 1; \\ < v >_{f_M} &= V; \\ < vv^T >_{f_M} &= T\, I + VV^T; \\ < v|v|^2 >_{f_M} &= (5T + |V|^2)V \end{aligned}$$

I denotes here the 3×3 identity matrix. The following formulae are also useful

$$\begin{aligned} < v - V >_{f_M} &= 0; \\ < (v-V)(v-V)^T >_{f_M} &= T\, I; \\ < |v|^2 >_{f_M} &= \text{tr} < vv^T >_{f_M} = 3T + |V|^2; \\ < |v-V|^2 >_{f_M} &= \text{tr} < (v-V)(v-V)^T >_{f_M} = 3T; \\ < (v-V)|v-V|^2 >_{f_M} &= 0. \end{aligned}$$

The moments of the solution of the equation (1) satisfy the initial value problem for the following system of ordinary differential equations

$$
\begin{aligned}
\frac{d}{dt} < 1 >_f (t) &= 0; && (40)\\
\frac{d}{dt} < v >_f (t) &= 0; && (41)\\
\frac{d}{dt} < vv^T >_f (t) &= -\frac{1}{2} < vv^T >_f (t) + \frac{1}{2}\left(T\, I + VV^T\right) && (42)\\
\frac{d}{dt} < v|v|^2 >_f (t) &= -\frac{1}{3} < v|v|^2 >_f (t) && (43)\\
&- \frac{1}{3} < vv^T >_f (t)V + 2\left(T + \frac{1}{3}|V|^2\right) V.
\end{aligned}
$$

The initial values of the moments are defined by the initial distribution $f_0(v)$

$$
\begin{aligned}
< 1 >_f (0) &= < 1 >_{f_0} = 1;\\
< v >_f (0) &= < v >_{f_0} = V;\\
< vv^T >_f (0) &= < vv^T >_{f_0};\\
T &= \frac{1}{3}\mathrm{tr} < (v - V)(v - V)^T >_{f_0};\\
< v|v|^2 >_f (0) &= < v|v|^2 >_{f_0} .
\end{aligned}
$$

The derivation of the system (40)-(43) can be done using the following well known identity

$$
\int_{\mathbb{R}^3} g(v) Q_+(f, f)(v) dv = <<< g(v') >_{S^2} >_{f(v)} >_{f(w)} . \qquad (44)
$$

where $v' = 0.5(v + w + |v - w|e)$ is the post-collisional velocity, $< g(e) >_{S^2}$ denotes the averaging of the function $g(e)$ over the unit sphere

$$
< g(e) >_{S^2} = \frac{1}{4\pi} \int_{S^2} g(e) de
$$

and $Q_+(f, f)(v)$ denotes the gain part of the collision integral

$$Q_+(f,f)(v) = \frac{1}{4\pi}\int_{\mathbb{R}^3}\int_{S^2} f(v')f(w')dw\,de.$$

We remark that in our case the loss part of the collision integral leads to

$$\int_{\mathbb{R}^3} g(v)Q_-(f,f)(v)dv =< 1 >_f (t) < g(v) >_f (t)$$

Therefore the averaging of the Boltzmann equation leads to

$$\begin{aligned}\frac{d}{dt} < g(v) >_f (t) &= <<< g(v') >_{S^2}>_{f(v)}>_{f(w)} (t)\\ &- < 1 >_f (t) < g(v) >_f (t)\end{aligned}$$

Now we will use this equation for $g(v) = 1$ and obtain

$$\frac{d}{dt} < 1 >_f (t) =<<< 1 >_{S^2}>_{f(v)}>_{f(w)} (t) - < 1 >_f (t) < 1 >_f (t) = 0.$$

Thus we obtain the equation (40) and conclude that

$$< 1 >_f (t) =< 1 >_f (0) =< 1 >_{f_0}= 1. \tag{45}$$

In the following we will need the following simple property

$$< e >_{S^2}= 0. \tag{46}$$

Using $g(v) = v$ as well as (45) and 4.36 we obtain

$$\begin{aligned}\frac{d}{dt} < v >_f (t) &= <<< \frac{1}{2}(v + w + |v - w|e) >_{S^2}>_{f(v)}>_{f(w)} (t) - < v >_f (t)\\ &= \frac{1}{2} < v >_{f(v,t)} + \frac{1}{2} < w >_{f(w,t)} - < v >_f (t) = 0. \end{aligned} \tag{47}$$

Thus we get

$$< v >_f (t) =< v >_f (0) =< v >_{f_0}= V. \tag{48}$$

Before we derive the equation for $g(v) = vv^T$ we will see that the averaging of $g(v) = |v|^2$ remains conserved.

$$\begin{aligned}
< \frac{1}{4}|v + w + |v - w|e|^2 >_{S^2} &= \frac{1}{4} < |v|^2 + |w|^2 + |v - w|^2 + 2(v, w) \\
&+ 2|v - w|(v, e) + 2|v - w|(w, e) >_{S^2} \\
&= \frac{1}{2}(|v|^2 + |w|^2)
\end{aligned}$$

The space averaging leads to the equation

$$\frac{d}{dt} < |v|^2 >_f (t) = 0$$

and therefore to the expression

$$< |v|^2 >_f (t) =< |v|^2 >_{f_M}= 3T + |V|^2. \tag{49}$$

Here we have used the Maxwell distribution

$$f_M(v) = \lim_{t\to\infty} f(v, t).$$

First nontrivial differential equation we will get for $g(v) = vv^T$. Here we will use that

$$< ee^T >_{s^2}= \frac{1}{3}I, \tag{50}$$

where I denotes the 3×3 identity matrix. The function to be averaged over the unit sphere is now

$$
\begin{aligned}
g\left(\frac{1}{2}(v+w+|v-w|e)\right) &= \frac{1}{4}\big(vv^T + vw^T + |v-w|(v+w)e^T \qquad (51)\\
&+ wv^T + ww^T + \\
&+ |v-w|e(v^T+w^T) + |v-w|^2 ee^T\big)
\end{aligned}
$$

The averaging of the third and sixth summands in (51) over the unit sphere disappears corresponding to (46) and we get using (50)

$$
\begin{aligned}
< g\left(\frac{1}{2}(v+w+|v-w|e)\right) >_{S^2} &= \frac{1}{4}\big(vv^T + vw^T + wv^T + ww^T\\
&+ \frac{1}{3}|v-w|^2 I\big)
\end{aligned}
$$

Thus we obtain after the double averaging over the space

$$
\begin{aligned}
\frac{1}{2}\big(< vv^T >_f (t) &+ < v >_f (t) < v >_f^T (t)\\
&+ \frac{1}{3}(< |v|^2 >_f (t) - |< v >_f (t)|^2) I\big). \qquad (52)
\end{aligned}
$$

Using (48) and (49) we get finally

$$
\frac{1}{2}\left(< vv^T >_f (t) + VV^T + T\,I\right)
$$

and therefore the equation (42). The derivation of the equation (43) is a bit longer but completely similar to the previous and we will omit this.
Thus the solution of the system (40)-(43) is

$$
\begin{aligned}
< 1 >_f (t) &= 1;\\
< v >_f (t) &= V;\\
< vv^T >_f (t) &= < vv^T >_{f_0} e^{-t/2} + (T\,I + VV^T)(1-e^{-t/2}); \qquad (53)\\
< v|v|^2 >_f (t) &= < v|v|^2 >_{f_0} e^{-t/3} + (5T + |V|^2)V(1-e^{-t/3})\\
&+ 2(< vv^T >_{f_0} - VV^T - T\,I)V(e^{-t/2} - e^{-t/3}). \qquad (54)
\end{aligned}
$$

As an example we consider the initial distribution $f_0(v)$ as a mixture of two different Maxwell distributions

$$f_0(v) = \alpha f_{M_1}(v) + (1-\alpha) f_{M_2}(v), \ 0 \le \alpha \le 1.$$

The parameters of the Maxwell distributions are V_1, T_1 and V_2, T_2. In this case we obtain

$$\begin{aligned}
< 1 >_{f_0} &= 1; \\
< v >_{f_0} &= V = \alpha V_1 + (1-\alpha) V_2; \\
< vv^T >_{f_0} &= (\alpha T_1 + (1-\alpha) T_2) I + \alpha V_1 V_1^T + (1-\alpha) V_2 V_2^T; \\
T &= \alpha T_1 + (1-\alpha) T_2 + \frac{1}{3}\alpha(1-\alpha)|V_1 - V_2|^2; \\
< v|v|^2 >_{f_0} &= \alpha(5T_1 + |V_1|^2) V_1 + (1-\alpha)(5T_2 + |V_2|^2) V_2.
\end{aligned}$$

The last formulae ere extremely useful for the numerical tests because they provide the explicite time evolution of the most important moments of the distribution function. For the following simple but nontrivial choice

$$V_1 = (-2, 2, 0)^T, \ V_2 = (2, 0, 0)^T, \ T_1 = T_2 = 1, \ \alpha = 1/2$$

we obtain

$$
\begin{aligned}
< 1 >_f (t) &= 1; \\
< v >_f (t) &= V = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; \\
< vv^T >_f (t) &= \begin{pmatrix} 5 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix} e^{-t/2} + \frac{1}{3} \begin{pmatrix} 8 & 0 & 0 \\ 0 & 11 & 0 \\ 0 & 0 & 8 \end{pmatrix} (1 - e^{-t/2}); \qquad (55) \\
T &= 8/3; \\
< v|v|^2 >_f (t) &= \begin{pmatrix} -4 \\ 13 \\ 0 \end{pmatrix} e^{-t/3} + \frac{1}{3} \begin{pmatrix} 0 \\ 43 \\ 0 \end{pmatrix} (1 - e^{-t/3}) \qquad (56) \\
&- \frac{1}{3} \begin{pmatrix} 12 \\ 4 \\ 0 \end{pmatrix} (e^{-t/2} - e^{-t/3}).
\end{aligned}
$$

4 Conservation properties

In this section we propose a possible modification of our system of ordinary differential equations (11) for the knots $\pm e_l,\ l = 1, 2, 3$ in order to conserve the macroscopic quantities ρ_h and V_h as well as to force the second moments $(m_h(t))_{ll},\ l = 1, 2, 3$ to follow the exact curves (53). Then the conservation of the energy density W_h will also be guaranteed. Because of the obvious practical reasons we begin the numerics by the discretisation of the velocity space $\mathbb{R}^3_v$. Let V_h be an approximation of the bulk velocity V which can be obtained numerically or exactly from the initial distribution $f_0(v)$. Then we will need two discretisation parameters $L > 0$ and $n \in \mathbb{N}$. The parameter L should be chosen so that it is possible to neglect the values of the distribution function $f(v, t)$ in outside of the cube

$$
\{v : (V_h)_l - L \le v_l \le (V_h)_l + L,\ l = 1, 2, 3\},\ 2L = h_v n,\ h_v = \frac{2L}{n}. \qquad (57)
$$

It is convenient to choose the parameter n as a power of two because of the especially efficient FFT procedure in this case. The set of discrete velocities is now $\{V_h + v_k = h_v k,\ k \in Q_n\}$, where Q_n denotes the set of three-dimensional integer vectors whose components belong to the set $\{-n/2+1,\dots,n/2\}$. If we denote $f_k(t)$ as the approximation of $f(v_k,t)$ then the numerical form of the macroscopic quantities is

$$\rho_h = h_v^3 \sum_{j\in Q_n} f_j(t), \tag{58}$$

$$\rho_h(V_h)_l = h_v^3 \sum_{j\in Q_n} (v_j)_l f_j(t),\ \ l=1,2,3, \tag{59}$$

$$(m_h(t))_{ll} = h_v^3 \sum_{j\in Q_n} ((v_j)_l)^2 f_j(t),\ \ l=1,2,3, \tag{60}$$

$$W_h = \frac{1}{2}\left((m_h(t))_{11} + (m_h(t))_{22} + (m_h(t))_{33}\right). \tag{61}$$

Using the definition of the discrete velocities and the following numbering of its components $(0,1,\dots,n/2,-n/2+1,\dots,-1)$ first in $x-, y-$ and finally in $z-$direction we represent these quantities as the following scalar products

$$\rho_h = h_v^3(g^{(0)}, f(t)), \tag{62}$$

$$g^{(0)} = e\otimes e\otimes e \in \mathbb{R}^N, \tag{63}$$

$$\rho_h(V_h)_1 = h_v^3(V_h)_1(g^{(0)}, f(t)) + h_v^3(g^{(1)}, f(t)), \tag{64}$$

$$g^{(1)} = a\otimes e\otimes e \in \mathbb{R}^N, \tag{65}$$

$$(m_h(t))_{11} = h_v^3((V_h)_1)^2(g^{(0)}, f(t)) + 2h_v^3(V_h)_1(g^{(1)}, f(t)) + h_v^3(g^{(2)}, f(t)), \tag{66}$$

$$g^{(2)} = b\otimes e\otimes e \in \mathbb{R}^N. \tag{67}$$

Here $\otimes$ denotes the Kronecker product. The $n-$dimensional vectors e, a and b are defined as follows

$$e = (1,1,\dots,1)^T \in \mathbb{R}^n, \tag{68}$$

$$a = h_v(0,1,\dots,n/2-1,0,-n/2+1,\dots,-1)^T \in \mathbb{R}^n, \tag{69}$$

$$b = h_v^2(0^2,1^2,\dots,(n/2-1)^2,(n/2)^2,(-n/2+1)^2,\dots,(-1)^2)^T \in \mathbb{R}^n. \tag{70}$$

Using (62) in (64) and then (62),(64) in (66) we rewrite these conditions as

$$\rho_h = h_v^3(g^{(0)}, f(t)), \tag{71}$$

$$0 = h_v^3(g^{(1)}, f(t)), \tag{72}$$

$$(m_h(t))_{11} - \rho_h(V_h)_1 = h_v^3(g^{(2)}, f(t)). \tag{73}$$

The meshsizes h_v and h_ξ are connected via the relation $h_v h_\xi = 2\pi/n$. Then we are able to rewrite (71),(72) and (73) in terms of the discrete Fourier transform $\varphi(t)$ of the vector $f(t)$

$$\varphi(t) = h_v^3 D F_3 f(t), \; F_3 = F_1 \otimes F_1 \otimes F_1. \tag{74}$$

Here F_1 denotes the matrix of one-dimensional Fourier transform having the elements

$$f_{lm} = e^{\imath \frac{2\pi}{n} lm}, \; l, m = 0, \ldots, n-1. \tag{75}$$

Note the obvious property of these elements

$$f_{lm} = \overline{f_{l,n-m}}, \; m = 1, \ldots, n/2. \tag{76}$$

D denotes in (74) the following diagonal matrix

$$D = \mathrm{diag}\left(e^{\imath h_\xi (V_h, j)}, \; j \in Q_n \right). \tag{77}$$

$$F_3 F_3^* = n^3 I, \tag{78}$$

we rewrite (74) as

$$f(t) = \frac{1}{(2L)^3} F_3^* D^{-1} \varphi(t) \tag{79}$$

and the scalar products (71),(72) and (73) as

$$\begin{aligned}
\rho_h &= \frac{1}{n^3}(g^{(0)}, F_3^* D^{-1}\varphi(t)) = \frac{1}{n^3}(F_3 g^{(0)}, D^{-1}\varphi(t)), && (80)\\
0 &= \frac{1}{n^3}(g^{(1)}, F_3^* D^{-1}\varphi(t)) = \frac{1}{n^3}(F_3 g^{(1)}, D^{-1}\varphi(t)), && (81)\\
(m_h(t))_{11} - \rho_h (V_h)_1 &= \frac{1}{n^3}(g^{(2)}, F_3^* D^{-1}\varphi(t)) = \frac{1}{n^3}(F_3 g^{(2)}, D^{-1}\varphi(t)). && (82)
\end{aligned}$$

The analytic form of the Fourier transforms of the vectors (63), (65) and (67) was obtained in our recent paper [3]. Here we give only the final result. Using

(81) and (82) we obtain the final formulae for the functions $\varphi_{e_l}(t)$, $l = 1,2,3$

$$
\begin{aligned}
\mathrm{Im}(D^{-1}\varphi)_{e_l}(t) &= \tan\frac{\pi}{n}\sum_{m=2}^{n/2-1}(-1)^m\cot\left(\frac{\pi}{n}m\right)\mathrm{Im}(D^{-1}\varphi)_{m\,e_l}(t), &(83)\\
\mathrm{Re}(D^{-1}\varphi)_{e_l}(t) &= \sin^2\frac{\pi}{n}\left(-\frac{(m_h(t))_{11}-\rho_h(V_h)_1}{h_v^2}+\frac{n^2+2}{12}\rho_h+\frac{1}{2}(D^{-1}\varphi)_{n/2\,e_l}(t)\right.\\
&+\left.\sum_{m=2}^{n/2-1}(-1)^m\sin^{-2}\left(\frac{\pi}{n}m\right)\mathrm{Re}(D^{-1}\varphi)_{m\,e_l}(t)\right), &(84)\\
(D^{-1}\varphi)_{-e_l} &= \overline{(D^{-1}\varphi)_{e_l}},\ l=1,2,3. &(85)
\end{aligned}
$$

Thus, the formulae (83),(84) and (85) allow to define the functions $\varphi_{e_l}(t)$, $l = 1,2,3$ so, that all numerical moments of the distribution function are conserved during the computation. Remarkable is also very low computational work required by the formulae (83),(84) and (85), which is of the capital order $O(n)$ because only the knots placed on the axeses are involved.

5 Numerical examples

In this section we solve the initial value problem (11),(12) in Q_n using the following slightly implicit scheme

$$
\begin{aligned}
\varphi_k^{j+1} &= \frac{1}{1+\tau\rho}\varphi_k^j+\frac{\tau}{n_k(1+\tau\rho)}\sum_{m\in\mathrm{Cl}(k)}\varphi^j_{\frac{k+m}{2}}\varphi^j_{\frac{k-m}{2}} &(86)\\
\varphi_k^0 &= \varphi_0(\xi_k),\, k\in Q_n. &(87)
\end{aligned}
$$

Here $\tau > 0$ denotes the time discretisation parameter and φ_k^j the approximation of $\varphi_k^(t_j = \tau j)$. This scheme is obviously unconditionally stable and of the first order of approximation with respect to time step τ.
For the numerical tests we consider the initial distribution $f_0(v)$ as in (55),(55)

$$
f_0(v) = \frac{1}{2(2\pi)^{3/2}}\left(\exp\left(-\frac{|v-V_1|^2}{2}\right)+\exp\left(-\frac{|v-V_2|^2}{2}\right)\right),
$$

where

$$
V_1 = (2,2,0)^T,\ V_1 = (-2,2,0)^T.
$$

The time evolution of the second and third moments of the distribution function $f(v,t)$ is given in (55),(56). We remark that the moments of the numerical solution follow the time evolution of the main diagonal elements of the $< vv^T >_f (t)$ tensor exactly. Therefore we concentrate our attention on the only non-trivial component $\left(< vv^T >_f\right)_{12}(t)$ of the tensor (55) and on the first component of the vector (56).
There are three discretisation parameters in our method: the size L of the cube (57), the number n of knots in one direction and the time step τ. The parameter L can be chosen using the initial distribution. First we compute the (conserved !) temperature which is $T = 8/3$ in our case. Then we use $L = \sqrt{-2T\ln(\varepsilon)}$ in order to guarantee the accuracy ε by approximation of the final Maxwellian. This leads in our case for $\varepsilon = 10^{-6}$ to the rough value $L = 9$. This very high accuracy should allow to see the role of two other parameters of discretisation more precisely.
In the next tables we present the maximal error by computing of $\left(< vv^T >_f\right)_{12}(t)$ and of $(< v|v|^2 >_f)_1 (t)$ on the time interval $(0, 12)$ which is sufficient for the almost complete relaxation. The number of time steps is denoted by N_τ there

N_τ	$n = 16$	$n = 32$	$n = 64$
50	$9.75 \cdot 10^{-2}$	$9.39 \cdot 10^{-2}$	$9.30 \cdot 10^{-2}$
100	$4.54 \cdot 10^{-2}$	$4.30 \cdot 10^{-2}$	$4.24 \cdot 10^{-2}$
200	$2.26 \cdot 10^{-2}$	$2.13 \cdot 10^{-2}$	$2.09 \cdot 10^{-2}$
400	$1.31 \cdot 10^{-2}$	$1.23 \cdot 10^{-2}$	$1.21 \cdot 10^{-2}$

Table 1: The error for $\left(< vv^T >_f\right)_{12}(t)$.

N_τ	$n = 16$	$n = 32$	$n = 64$
50	$1.95 \cdot 10^{-1}$	$1.87 \cdot 10^{-1}$	$1.86 \cdot 10^{-1}$
100	$9.07 \cdot 10^{-2}$	$8.60 \cdot 10^{-2}$	$8.48 \cdot 10^{-2}$
200	$4.51 \cdot 10^{-2}$	$4.26 \cdot 10^{-2}$	$4.20 \cdot 10^{-4}$
400	$2.62 \cdot 10^{-2}$	$2.47 \cdot 10^{-2}$	$2.44 \cdot 10^{-4}$

Table 2: The error for $(< v|v|^2 >_f)_1 (t)$.

The above tables illustrate quite clear the first order of the scheme with respect to τ. On the other hand the increase of accuracy with respect to n is rather low. It is due to the very rough approximation of the integral over the unit sphere in (7) for small $|\xi|$. Thus, the equivalence class for $(1,1,0)^T$

contains only four elements $(\pm 1, \pm 1, 0)^T$ independent of n. Corresponding to the asymptotic $\#\mathrm{Cl}(k) = O(|k|^{1-\epsilon}$, the best accuracy we can expect here, is $O(n^{-1/2})$ even for $|\xi| \to \infty$. Fortunately, the accuracy is very sufficient already for $n = 16$. The main reason for this is probably the fact that the points with small $|\xi|$ are directly connected via (86) to the points $\pm e_j$, $j = 1, 2, 3$ which are corrected corresponding to (83), (84).
It is possible to improve the accuracy with respect to τ using high order solvers (i.e. Runge-Kutta methods) for the system of ordinary differential equations (11) in Q_n. But this does not seem to be very reasonable because the numerical solution of the spatially homogeneous Boltzmann equation only makes sense in connection with the usual splitting procedure for the spatially inhomogeneous Boltzmann equation. This splitting is of the first order of accuracy with respect to the time step τ.
Finally we show the convergence history for above moments in the following figures. The thin solid lines indicate the numerical solutions obtained for $N_\tau = 50, 100, 200, 400$ (from below) while the dashed line shows the analytical solution (55) in first and (56) in the second figure.

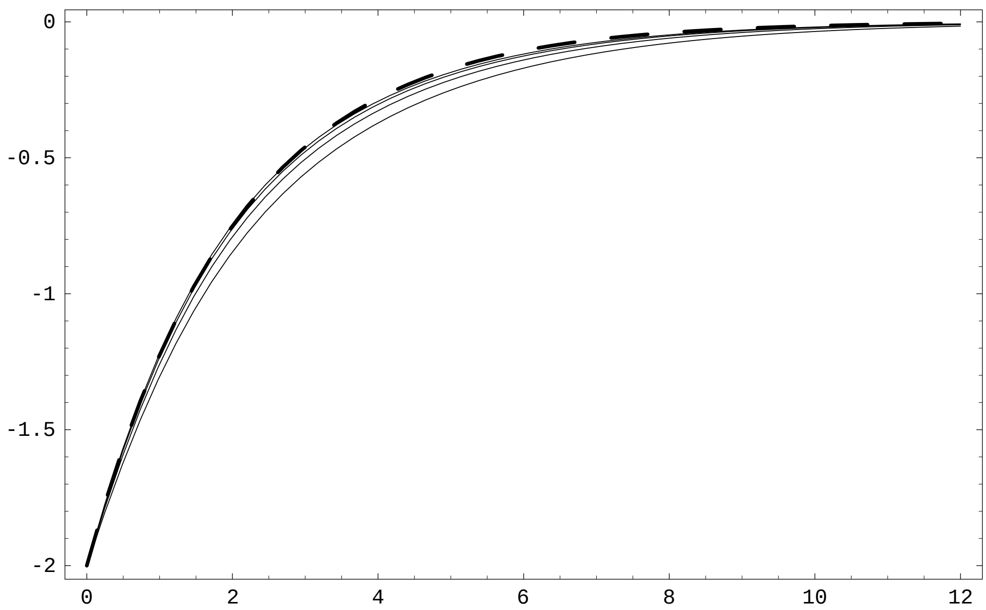

Figure 1 The analytical and numerical solutions for $\left(< vv^T >_f\right)_{12}(t)$ and $N_\tau = 50, 100, 200, 400$.

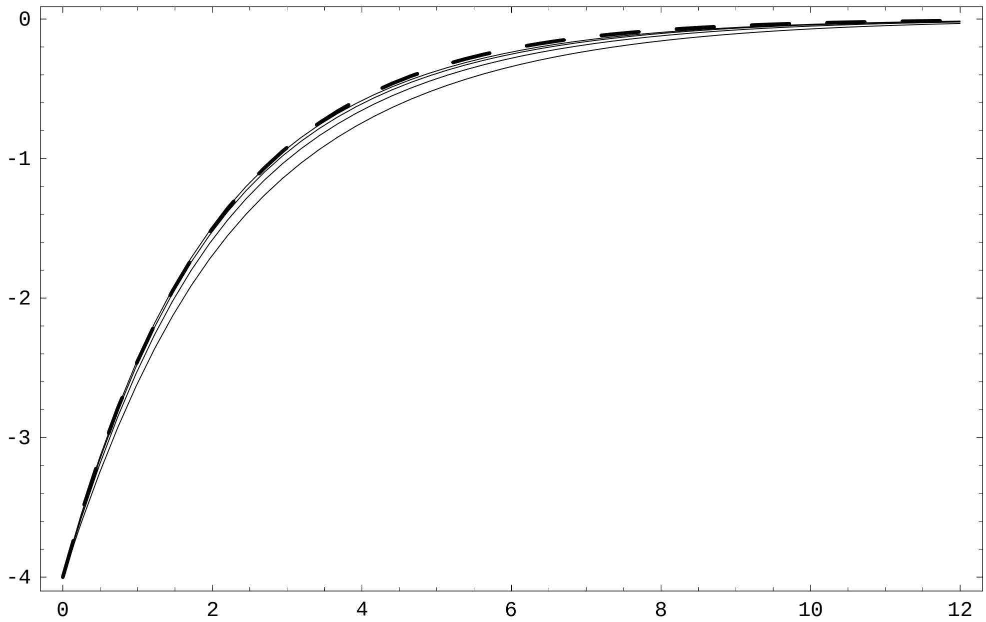

Figure 2 The analytical and numerical solutions for $\left(< v|v|^2 >_f\right)_1 (t)$ and $N_\tau = 50, 100, 200, 400$

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