Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Direct simulation of the uniformly heated granular Boltzmann equation

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submitted: 28th March 2003

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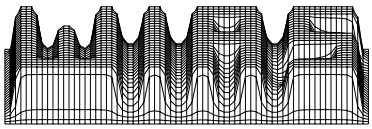
No. 834
Berlin 2003



1991 *Mathematics Subject Classification.* 82C40, 82C80, 65R20.

Key words and phrases. inelastic Boltzmann equation, granular flow, Monte Carlo algorithm.

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Abstract

In the present paper we give an overview of the analytical properties of the steady state solution of the spatially homogeneous uniformly heated granular Boltzmann equation. The asymptotic properties of this distribution (so called tails) are formulated for different models of interaction. A new stochastic numerical algorithm for this problem is presented and tested using analytical relaxation of the temperature. The "tails" of the steady state distribution are computed using this algorithm and the results are compared with the available analytical information.

Contents

1 Introduction

In recent years a significant interest has been focused on the study of kinetic models for rapid granular flows [17],[10],[15]. Depending on the external conditions (geometry, gravity, interactions with surface of a vessel) granular systems may be in a variety of regimes, displaying typical features of solids, liquids or gases and also producing novel statistical effects [28]. In the case of rapid, dilute flows, the binary collisions between particles may be considered the main mechanism of inter-particle interactions in the system. In such cases methods of the kinetic theory of rarefied gases, based on the Boltzmann-Enskog equation have been applied [18],[17],[16]. Experimental and numerical data from Molecular Dynamics simulations (MD) [3],[23] indicate that particle distribution functions are far from Maxwellian distributions when particles collide inelastically. Thus MD simulations of uniformly heated homogeneous granular flow show a clear deviation from Maxwellian state.

Physically realistic regimes include excitation from the moving boundary, through-flow of air, fluidised beds, gravity, and other special conditions.

We take a simple model for a driving mechanism, called thermal bath, in which particles are assumed to be "uniformly heated" by uncorrelated random accelerations between the collisions. Such a model has been initially studied in [31] in the one-dimensional case, and in [29] in general dimension.

The first reference to non Maxwellian steady state solution was published in [29], by Van Noije and Ernst, where by means of formal expansions in Sonine polynomials and ad-hoc closures, the authors conjectured the existence of steady state solution with overpopulated "tails", i.e. slow decay rate of the distribution function for large velocities. Steady state solutions were also studied by formal expansion methods for the Maxwell pseudo-molecules model in [9],[4],[5],[19],[20]. These methods are based on small energy dissipation expansions and Fourier transforms.

Existence, uniqueness and regularity of the time dependent and steady state solutions for the uniformly heated inelastic Boltzmann equation can be found in [5]. In addition, in [12], the authors proved rigorously the existence of radially symmetric steady state solutions for the Maxwell pseudo-molecules model.

Rigorous mathematical properties of corresponding stationary solutions for the uniformly heated inelastic Boltzmann equation for the hard spheres model have been recently discussed in [14].

We consider the spatially homogeneous uniformly heated Boltzmann equation for granular media

$$f_t - \beta \Delta f = \gamma Q_\alpha(f, f) \tag{1}$$

which describes the time evolution of the particle density $f(t, v)$

$$f \ : \ \mathbb{R}_+ \times \mathbb{R}^3 \to \mathbb{R}_+.$$

The right-hand side of the equations (1), known as the collision integral or the collision term, can be written in the weak form

$$\int_{\mathbb{R}^3} Q_\alpha(f, f)(v)\, \varphi(v)\, dv = \tag{2}$$

$$= \frac{1}{2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\int\limits_{S^2} B(|u|,\mu)f(v)f(w)\Big(\varphi(v')+\varphi(w')-\varphi(v)-\varphi(w)\Big)\,de\,dw\,dv\,,$$

where $\varphi : \mathbb{R}^3 \to \mathbb{R}$ is a test function. In (1), β and γ are some constants. The following notations have been used in (2): $v, w \in \mathbb{R}^3$ are velocities, $u = v - w$ is the relative velocity and $v', w' \in \mathbb{R}^3$ are the post-collisional velocities defined by

$$\begin{aligned} v' &= \frac{1}{2}(v+w) + \frac{1-\alpha}{4}u + \frac{1+\alpha}{4}|u|\,e\,, \\ w' &= \frac{1}{2}(v+w) - \frac{1-\alpha}{4}u - \frac{1+\alpha}{4}|u|\,e\,, \end{aligned} \tag{3}$$

where $e \in S^2 \subset \mathbb{R}^3$ is a unit vector, The quantity μ is

$$\mu = \frac{(u,e)}{|u|}\,.$$

The parameter $0 < \alpha \leq 1$ is called restitution coefficient. For $\alpha = 1$ the collisions are elastic and $Q_1(f,f)$ coincides with the classical Boltzmann collision operator for a simple, dilute gas of particles [11]. Some special models for the (isotropic) kernel B are as follows:

1. The **hard spheres model** is described by the kernel

$$B(|u|,\mu) = \frac{d^2}{4}|u|\,, \tag{4}$$

   where d denotes the diameter of the particles.

2. The **Maxwell pseudo-molecules** are given by

$$B(|u|,\mu) = \frac{1}{4\,\pi}\,.$$

   The collision kernel $B(|u|,\mu)$ here does not depend on the relative speed $|u|$.

3. The **Variable Hard Spheres model** (cf. [2]) (VHS) has an isotropic kernel

$$B(|u|,\mu) = C_\lambda |u|^\lambda\,,\ 0 \leq \lambda \leq 1. \tag{5}$$

   The model includes, as particular cases, the hard spheres model for $\lambda = 1$ and a case of the Maxwell pseudo–molecules with $\lambda = 0$.

The equation (1) is subjected to the initial condition

$$f(0,v) = f_0(v)\,.$$

All relevant physical values of the gas flow are computed as the first 13 moments of the distribution function or their combinations. These moments are:

the density

$$\varrho(t) = \int\limits_{\mathbb{R}^3} f(t,v)\,dv\,, \tag{6}$$

the momentum

$$m(t) = \int\limits_{\mathbb{R}^3} v\, f(t,v)\, dv\,, \tag{7}$$

the momentum flow

$$M(t) = \int\limits_{\mathbb{R}^3} vv^T f(t,v)\, dv\,, \tag{8}$$

and the energy flow

$$r(t) = \frac{1}{2}\int\limits_{\mathbb{R}^3} v|v|^2 f(t,v)\, dv\,. \tag{9}$$

Note that the matrix $M(t)$ is symmetric and therefore defined by its upper triangle. Using these moments we define the bulk velocity

$$V(t) = \frac{m}{\varrho}, \tag{10}$$

the internal energy and the temperature

$$e(t) = \frac{1}{2\,\varrho}\left(\mathrm{tr}M - \varrho|V|^2\right),\ T(t) = \frac{2}{3}e\,, \tag{11}$$

the pressure

$$p(t) = \varrho\, T\,,$$

the stress tensor

$$P(t) = M - \varrho\, VV^T$$

and the heat flux vector

$$q(t) = r - \left(M + \left(\frac{1}{2}\mathrm{tr}M - \varrho|V|^2\right) I\right) V\,.$$

Note that in the spatially homogeneous case we consider the following important conservation properties hold. The density

$$\varrho(t) = \int\limits_{\mathbb{R}^3} f(t,v)\, dv = \int\limits_{\mathbb{R}^3} f_0(v)\, dv = \varrho_0 \tag{12}$$

and the momentum

$$m(t) = \int\limits_{\mathbb{R}^3} v\, f(t,v)\, dv = \int\limits_{\mathbb{R}^3} v\, f_0(v)\, dv = m_0$$

remain constant during the relaxation. Thus, corresponding to (10) also the bulk velocity

$$V(t) = V_0 = \frac{m_0}{\varrho_0}$$

is conserved quantity. Without loss of generality we assume $\varrho_0 = 1$ and $V_0 = 0$ for further discussions.

In contrast to the classical Boltzmann equation for elastic collisions, inelastic collisions ($0 < \lambda < 1$) dissipate energy. Thus the temperature (cf. (11))

$$T(t) = \frac{1}{3} \int\limits_{\mathbb{R}^3} |v|^2 f(t,v)\, dv\,.$$

is a function of time. Taking $\varphi(v) = |v|^2$ in (2) we obtain (cf. [14])

$$|v'|^2 + |w'|^2 - |v|^2 - |w|^2 = -\frac{1-\alpha^2}{4}\,(1-\mu)\,|u|^2\,.$$

The second Green's formula leads to

$$\int\limits_{\mathbb{R}^3} \Delta f(t,v)\,|v|^2 dv = \int\limits_{\mathbb{R}^3} f(t,v) \Delta |v|^2 dv = 6 \int\limits_{\mathbb{R}^3} f(t,v)\, dv = 6\varrho_0 = 6\,.$$

Thus the following relation for time evolution of the temperature can be written

$$\frac{dT}{dt} = 2\beta - \gamma\,\frac{1-\alpha^2}{24} \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} B_1(|u|)|u|^2 f(v) f(w)\, dw\, dv\,,$$

where

$$B_1(|u|) = \int\limits_{S^2} (1-\mu) B(|u|,\mu)\, de\,.$$

In the special case of Maxwell pseudo-molecules ($\lambda = 0$ in (5)) we obtain

$$B_1(|u|) = 4\pi\, C_0$$

and the following ordinary differential equation for the temperature (cf. (2))

$$\frac{dT}{dt} = 2\beta - \gamma\,\pi\, C_0\,(1-\alpha^2)\,T$$

Thus the time relaxation of the temperature is

$$T(t) = T_0\, e^{-\gamma\,\pi\, C_0\,(1-\alpha^2)t} + T_\infty\, \left(1 - e^{-\gamma\,\pi\, C_0\,(1-\alpha^2)t}\right)\,, \tag{13}$$

where

$$T_0 = \frac{1}{3} \int\limits_{\mathbb{R}^3} |v|^2 f_0(v)\, dv\,,\; T_\infty = \frac{2\beta}{\gamma\,\pi\, C_0\,(1-\alpha^2)}\,. \tag{14}$$

The paper is organised as follows. In Section 2 we give an overview on the asymptotic properties of the steady state solution of the equation (1). In Section 3 we describe a new stochastic numerical algorithm for the uniformly heated inelastic Boltzmann equation. In the fourth and final Section we present the results of some numerical tests. Here we use the analytically known time relaxation of the temperature (13),(14) for the Maxwell pseudo-molecules model for a careful check of the accuracy. Finally, the "tails" of the steady state distribution are computed using this algorithm for different λ in (5) and the results are compared with the available analytical information.

2 Asymptotic properties of the steady state solution

Asymptotic properties of stationary solutions for the uniformly heated inelastic Boltzmann equation (1) have been recently discussed in many publications [29],[8],[12],[9],[14].

One of the most interesting related questions is the asymptotic behaviour of the steady state distribution function f_∞

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

for large $|v|$ (high energy tails). It is worth to note that there are no such solution for the uniformly heated elastic Boltzmann equation, since the kinetic energy will increase linearly in time.

It has been recently shown in [29],[13],[14] that a typical tail for the inelastic variable hard spheres model (5) is expected to be given by a formula

$$f_\infty(v) \sim \exp(-a|v|^b)\,,\ |v|\to\infty\,, \tag{15}$$

where a depends on the quotient of the energy dissipation rate and the heat bath temperature and b depends on the balance between the forced diffuse forcing term and the loss term of the collisional integral in the Boltzmann equation (1). For instance, for the inelastic hard spheres (4), the exponent, or tail order is $b = 3/2$. This fact was notice first in [29] by searching for the radially symmetric steady state solution of a pointwise partial differential equation which was obtained using high velocities estimates to the loss term of the collision integral neglecting the gain term. Some arguments which justify this fact at a physical level of rigour and using an a priori assumption (15) were presented in a recent paper by Ernst and Brito [13]. However, a rigorous pointwise lower estimate was obtained in [14] by means of strong comparison principle arguments, borrowing classical non-linear PDE techniques to obtain pointwise bounds for regular solutions.

Indeed, for the inelastic hard spheres model, the authors have proved in [14] the existence, uniqueness and regularity of the time dependent and steady state solutions for the uniformly heated inelastic Boltzmann equation (1). In particular they showed the existence of the steady state solution for the hard spheres model in the Schwartz space of rapidly decaying smooth functions, with a lower pointwise bound

$$f(v) \geq A\exp(-a|v|^{3/2})\,,\ |v|\geq R\,.$$

It is clear, however, that while Maxwell pseudo-molecules model is good for an approximate description of integral quantities (see, for example, [7] for a comparison of the

Maxwell pseudo-molecules and hard spheres models in a shear flow problem), they lead to different behaviour of the tails compared to the hard spheres model, which can be observed when looking for approximate high-energy solutions of the inelastic Boltzmann-Fokker-Planck model when neglecting the gain part of the collision integral.

We emphasise that the appearance of the "3/2" exponent is a specific feature of the the uniformly heated inelastic Boltzmann equation for the hard spheres model which can also be predicted by dimensional arguments (cf. [29]).

On the other hand, the uniformly heated inelastic Boltzmann equation for the Maxwell pseudo-molecules model results in a high-velocity tail with asymptotic behaviour

$$f_\infty(v) \sim \exp(-a|v|)\,,\ |v| \to \infty\,,$$

(see [5]). As a general rule, the exponents in the tails are expected to depend on the driving and collision mechanisms [1],[13],[6]. In fact, deviations of the steady states of granular systems from Maxwellian equilibria ("thickening of tails") is one of the characteristic features of dynamics of granular systems, and has been an object of intensive study in the recent years [22],[21],[27],[23].

However, when different exponent $\lambda \neq 0, 1$ in the VHS model (5) is considered as usually done for classical (elastic) Boltzmann equation, there is no rigorous proof of existence of steady state solutions.

We expect that a technical and tedious extension of the analytical methods developed in [14] for existence, regularity and pointwise lower estimates; and in [6] for the L^1–weighted tail control indicates that uniformly heated inelastic Boltzmann equation for the VHS model (5) results in a high-velocity tail with asymptotic behaviour

$$f_\infty(v) \sim \exp(-a|v|^{1+\lambda/2})\,,\ |v| \to \infty\,. \tag{16}$$

Our numerical results presented in Section 4 indicate that is the case.

3 Direct stochastic simulation

The main idea of all particle methods for the Boltzmann equation (1) is an approximation of the time dependent family of measures

$$f(t,v)dv\,,\ t \in \mathbb{R}_+\,,$$

by a family of point measures

$$\nu(t,dv) = \frac{1}{n}\sum_{j=1}^{n} \delta_{(v_j(t))}(dv)$$

defined by the system of particles

$$\Big(v_1 t), \ldots, v_n(t)\Big)\,. \tag{17}$$

Thus the weights of the particles are $1/n$ and $v_j(t) \in \mathbb{R}^3$ denote their velocities. The behaviour of the system (17) can be briefly described as follows. The first step is an approximation of the initial measure

$$f_0(v)\,dv$$

by a system of particles (17) for $t = 0$. Then particles are continuously subjected to a Gaussian white noise forcing and obtain the kinetic energy executing individual Brownian motion between the collisions. The velocity of a single particle after the time Δt of Brownian motion is given by

$$v_j(t + \Delta t) = v_j(t) + \sqrt{2\,\beta\,\Delta t}\;\xi\,, \tag{18}$$

where $\xi \in \mathbb{R}^3$ is a random variable distributed according to the normalised Gaussian. The inelastic collisions take place in randomly distributed discrete time points dissipating the kinetic energy of the particles. The "collision step" is the most crucial part of the whole procedure. The behaviour of the collision process is as follows: The waiting time τ between the collisions can be defined either as a random variable with the distribution

$$\text{Prob}\,\{\tau \geq t\} \quad = \quad \exp(-\hat{\pi}\,t)\,,$$

where

$$\hat{\pi} \quad = \quad \frac{1}{2\,n} \sum_{1 \leq i \neq j \leq n} B_{max}(i,j)$$

and

$$\int\limits_{S^2} B(|v_i - v_j|, \mu)\,de \quad \leq \quad B_{max}(i,j)\,, \tag{19}$$

or as a deterministic object by

$$\tau = \hat{\pi}^{-1}\,.$$

The majorant (19) can be obtained for the VHS-model (5) using the a-priori known maximal relative speed of particles U_{max}

$$\gamma \int\limits_{S^2} B(|v_i - v_j|, \mu)\,de = 4\,\pi\,\gamma\,C_\lambda\,|v_i(t) - v_j(t)|^\lambda \leq 4\,\pi\,\gamma\,C_\lambda\;(U_{max})^\lambda\;.$$

Thus we get a constant majorant

$$B_{max}(i,j) = B_{max} = 4\,\pi\,\gamma\,C_\lambda\;(U_{max})^\lambda$$

and

$$\hat{\pi} \quad = \quad 2\,\pi\,\gamma\,C_\lambda\,(n-1)\,(U_{max})^\lambda\;.$$

Then the collision partners (i.e. the indices i and j) must be chosen. Since the majorant $B_{max}(i,j) = B_{max}$ in (19) is a constant, the parameter i is to be chosen according to the probability $1/n$, i.e. uniformly from the set $\{1, \ldots, n\}$. Given i, the parameter j is chosen according to the probability $1/(n-1)$, i.e. uniformly from the set $\{1, \ldots, n\} \setminus \{i\}$.

Given i and j, the collision is fictitious with probability

$$1 - \left(\frac{|v_i - v_j|}{U_{max}}\right)^\lambda\,, \tag{20}$$

otherwise the vector e is uniformly distributed on the surface of the unit sphere S^2 and the post-collisional velocities v_i' and v_j' can be computed corresponding to the collision transformation (3). Note that the velocities v_i and v_j of the collision partners have to be updated corresponding to (18) before computing the probability of fictitious collision according to (20). The majorant U_{max} for the maximal relative velocity of the particle system can be obtained using the numerical bulk velocity

$$V = \frac{1}{n} \sum_{j=1}^{n} v_j \tag{21}$$

as follows

$$\max_{i,j} |v_i - v_j| \leq \max_{i,j} \Big(|v_i - V| + |V - v_j| \Big) = 2 \max_{i} |v_i - V| = U_{max} \, .$$

Thus we are now able to formulate the whole stochastic algorithm for the numerical solution of the equation (1) on the time interval $[0, t_{max}]$.

Algorithm

1. initial distribution

   1.1 set time to zero $t = 0$;

   1.2 for $j = 1, \ldots, n$ generate the particles (v_j, t_j) with

   1.2.1 v_j distributed according to $f_0(v)$,

   1.2.2 $t_j = 0$;

   1.3 compute the bulk velocity V corresponding to

$$V = \frac{1}{n} \sum_{j=1}^{n} v_j \, ;$$

   1.4 compute the majorant U_{max} corresponding to

$$U_{max} = 2 \max_{i} |v_i - V|$$

2. repeat until $t \geq t_{max}$

   2.1 compute the time counter τ

$$\tau = \frac{1}{2 \, \pi \, \gamma \, C_\lambda \, (n-1) \, (U_{max})^\lambda} \ln(-r_1) \, ;$$

   2.2 update the time of the system

$$t := t + \tau \, ;$$

   2.3 define the index i

$$i = [r_2 \cdot n] + 1;$$

2.4 define the index j repeating

$$j = [r_3 \cdot n] + 1$$

until $j \neq i$;

2.5 update the velocities v_i and v_j corresponding to (18)

$$v_i := v_i + \sqrt{2\,\beta\,(t - t_i)}\;\xi_1\,,\;\; v_j := v_j + \sqrt{2\,\beta\,(t - t_j)}\;\xi_2\,;$$

2.6 update the times of the particles i and j

$$t_i = t\,,\;\; t_j = t\,;$$

2.7 update the majorant U_{max}

$$U_{max} = \max\Big\{U_{max}\,, |v_i - V|\,, |v_j - V|\Big\};$$

2.8 decide whether the collision is fictitious. If

$$r_4 \leq 1 - \left(\frac{|v_i - v_j|}{U_{max}}\right)^{\lambda}$$

then continue with Step 2.1, else

2.9 compute the post-collisional velocities

$$\begin{aligned} v_i &:= \frac{1}{2}(v_i + v_j) + \frac{1-\alpha}{4}(v_i - v_j) + \frac{1+\alpha}{4}|v_i - v_j|\,e\,, \\ v_j &:= \frac{1}{2}(v_i + v_j) - \frac{1-\alpha}{4}(v_i - v_j) - \frac{1+\alpha}{4}|v_i - v_j|\,e\,. \end{aligned}$$

2.10 update the majorant U_{max}

$$U_{max} = \max\Big\{U_{max}\,, |v_i - V|\,, |v_j - V|\Big\}$$

and continue with Step 2.1.

3. final step

3.1 update the velocities of all particles

$$v_i := v_i + \sqrt{2\,\beta\,(t_{max} - t_i)}\;\xi_i\,,\;\; i = 1, \ldots, n\,;$$

3.2 compute the numerical moments of the distribution

$$m_\varphi(t_{max}) = \frac{1}{n}\sum_{j=1}^{n} \varphi(v_j)\,,\;\; \varphi(v) = 1\,, v\,, vv^T\,, v|v|^2\,.$$

In the above algorithm, the random numbers r_1, r_2, r_3 and r_4 are uniformly distributed on the interval $(0, 1)$ while the three-dimensional vectors ξ_i are distributed according to the normalised Gaussian. The vector e used in Step 2.9 is uniformly distributed on the unit sphere S^2

Remark 1 *The above algorithm is not completely conservative, i.e. the bulk velocity will change during the time. However our numerical tests show only very small deviation of the bulk velocity from its initial value defined in (21).*

Remark 2 *If the moments of the distribution function are to be computed in some discrete points* $t_m = m\Delta t\,, m = 1, \ldots M\,, \Delta t = t_{max}/M$ *then it is necessary to stop the process at time* $t \geq t_m$*, to update all velocities as in Step 3.1 of the algorithm and then to compute (Step 3.2) and to store the moments for further use.*

Concerning the convergence of the stochastic particle methods for the classical, elastic Boltzmann equation we refer to [30]. In [25] more general Boltzmann like equations are considered. However the additional uniform heating of the particle system we consider here is not automatically covered and we let this important theoretical aspect for the future work.

4 Numerical examples and tests

4.1 Statistical notions

First we introduce some definitions and notations that are helpful for the understanding of stochastic numerical procedures. Functionals of the form (cf. (6)-(9))

$$F(t) = \int\limits_{\mathbb{R}^3} \varphi(v)\, f(t,v)\, dv\,. \tag{22}$$

are approximated by the random variable

$$\xi^{(n)}(t) = \frac{1}{n}\sum_{i=1}^{n} \varphi(v_i(t))\,, \tag{23}$$

here $(v_1(t), \ldots, v_n(t))$ are the velocities of the particle system. In order to estimate and to reduce the random fluctuations of the estimator (23), a number N of independent ensembles of particles is generated. The corresponding values of the random variable are denoted by

$$\xi_1^{(n)}(t), \ldots, \xi_N^{(n)}(t)\,.$$

The **empirical mean value** of the random variable (23)

$$\eta_1^{(n,N)}(t) = \frac{1}{N}\sum_{j=1}^{N} \xi_j^{(n)}(t) \tag{24}$$

is then used as an approximation to the functional (22). The error of this approximation is

$$e^{(n,N)}(t) = |\eta_1^{(n,N)}(t) - F(t)|$$

and consists of the following two components.

The **systematic error** is the difference between the mathematical expectation of the random variable (23) and the exact value of the functional, i.e.

$$e_{sys}^{(n)}(t) = E\xi^{(n)}(t) - F(t)\,.$$

The **statistical error** is the difference between the empirical mean value and the expected value of the random variable, i.e.

$$e_{stat}^{(n,N)}(t) = \eta_1^{(n,N)}(t) - E\xi^{(n)}(t)\,.$$

A **confidence interval** for the expectation of the random variable $\xi^{(n)}(t)$ is obtained as

$$I_p = \left[\eta_1^{(n,N)}(t) - \lambda_p\sqrt{\frac{\mathrm{Var}\,\xi^{(n)}(t)}{N}}\,,\ \eta_1^{(n,N)}(t) + \lambda_p\sqrt{\frac{\mathrm{Var}\,\xi^{(n)}(t)}{N}}\right], \tag{25}$$

where

$$\mathrm{Var}\,\xi^{(n)}(t) := E\left[\xi^{(n)}(t) - E\xi^{(n)}(t)\right]^2 = E\left[\xi^{(n)}(t)\right]^2 - \left[E\xi^{(n)}(t)\right]^2 \tag{26}$$

is the **variance** of the random variable (23), and $p \in (0,1)$ is the **confidence level**. This means that

$$\mathrm{Prob}\left\{E\xi^{(n)}(t) \notin I_p\right\} = \mathrm{Prob}\left\{|e_{stat}^{(n,N)}(t)| \geq \lambda_p\sqrt{\frac{\mathrm{Var}\,\xi^{(n)}(t)}{N}}\right\} \sim p\,.$$

Thus, the value

$$c^{(n,N)}(t) = \lambda_p\sqrt{\frac{\mathrm{Var}\,\xi^{(n)}(t)}{N}}$$

is a probabilistic upper bound for the statistical error.

In the calculations we use a confidence level of $p = 0.999$ and $\lambda_p = 3.2$. The variance is approximated by the corresponding empirical value (cf. (26)), i.e.

$$\mathrm{Var}\,\xi^{(n)}(t) \sim \eta_2^{(n,N)}(t) - \left[\eta_1^{(n,N)}(t)\right]^2,$$

where

$$\eta_2^{(n,N)}(t) = \frac{1}{N}\sum_{j=1}^{N}\left[\xi_j^{(n)}(t)\right]^2$$

is the **empirical second moment** of the random variable (23).

4.2 Relaxation of the temperature

In this subsection we begin to test the **Algorithm** using an analytically known relaxation of the temperature (cf. (13),(14)) in case of Maxwell pseudo-molecules.

Example 3 *We use the following Maxwell distribution*

$$f_0(v) = \frac{1}{(2\,\pi)^{3/2}}\, e^{-\frac{|v|^2}{2}} \tag{27}$$

as the initial condition and the following set of parameters in (1)

$$\alpha = \frac{1}{2}\,,\ \beta = 1\,,\ \gamma = 4\,,\ C_0 = \frac{1}{4\,\pi}\,.$$

Thus we obtain

$$T_0 = 1\,,\ T_\infty = \frac{8}{3}$$

and

$$T(t) = e^{-\frac{3}{4}\,t} + \frac{8}{3}\left(1 - e^{-\frac{3}{4}\,t}\right) \tag{28}$$

Thus the temperature increases monotonically in time.

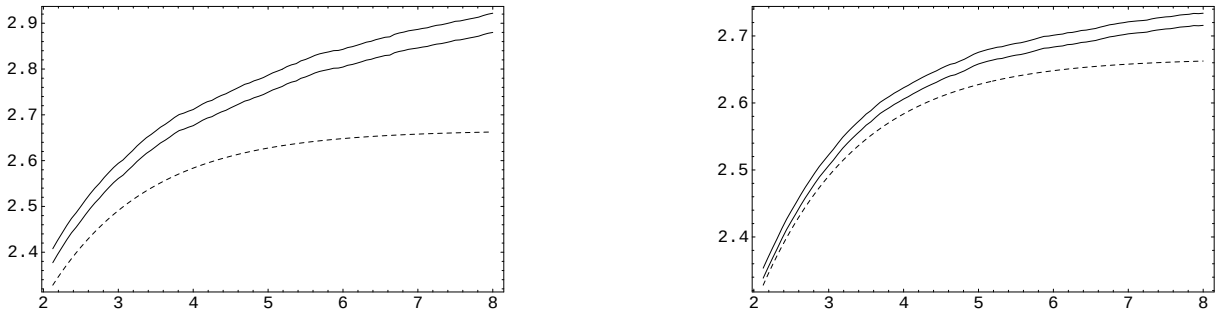

Figure 1. Analytical and numerical solutions for $n = 64$ and $n = 256$.

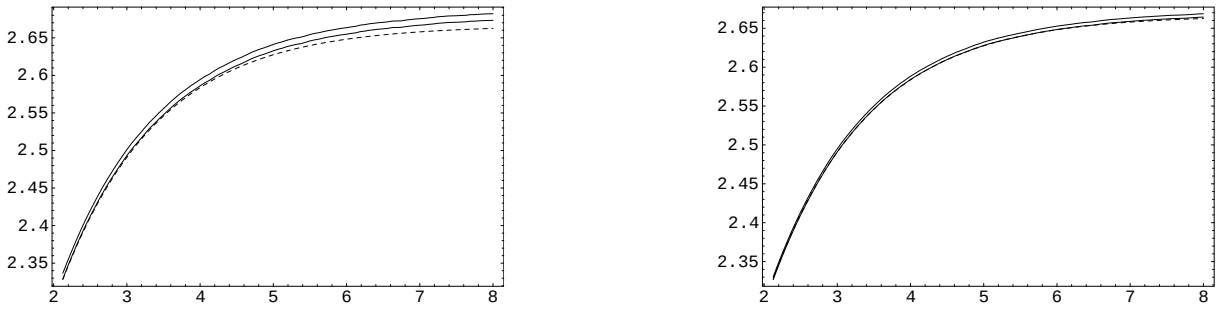

Figure 2. Analytical and numerical solutions for $n = 1024$ and $n = 4096$.

In **Figures 1 and 2**, the thick dashed line represent the course of the analytical solution (28) on the time interval $[2.0, 8.0]$ while the pairs of thin solid lines represent the confidence intervals (25) obtained using 10 000 independent ensembles generated by the stochastic **Algorithm** formulated in Section 3. It is almost impossible to see any difference between the numerical and the analytical solution in a figure for $n = 16\,384$, so we present the corresponding results in a form of table.

n	E_{max}	CF	$\|V\|_\infty$
64	0.895 E-01	-	0.672 E-02
256	0.235 E-01	3.81	0.516 E-02
1 024	0.571 E-02	4.11	0.211 E-02
4 096	0.150 E-02	3.81	0.141 E-02
16 384	0.305 E-03	4.92	0.355 E-03

Table 1. Numerical convergence, Example 3.

The second column of **Table 1** shows the maximal error of the temperature on the whole time interval computed as

$$E_{max} = \max_{0 \le m \le M} \left| \frac{T(t_m) - T_m}{T(t_m)} \right| , \tag{29}$$

where $T(t_m)$ are the exact values of the temperature at time point t_m and T_m is the computed temperature. The third column of Table 1 shows the "convergence factor", i.e. the quotient between the errors in two consecutive lines. This column clearly indicates the linear convergence of the error, i.e. $E_{max} = O(n^{-1})$. The maximum of the norm of the bulk velocity

$$\|V\|_\infty = \max_{0 \le m \le M} |V(t_m)|$$

is presented in the fourth column of Table 1. Thus this error is well controlled.

Example 4 *We use the Maxwell distribution (27) as the initial condition and the following set of parameters in (1)*

$$\alpha = \frac{1}{2}\,,\ \beta = \frac{1}{8}\,,\ \gamma = 4\,,\ C_0 = \frac{1}{4\,\pi}\,.$$

Thus we obtain

$$T_0 = 1\,,\ T_\infty = \frac{1}{3}$$

and

$$T(t) = e^{-\frac{3}{4}\,t} + \frac{1}{3}\left(1 - e^{-\frac{3}{4}\,t}\right) \tag{30}$$

Thus the temperature decreases now monotonically in time.

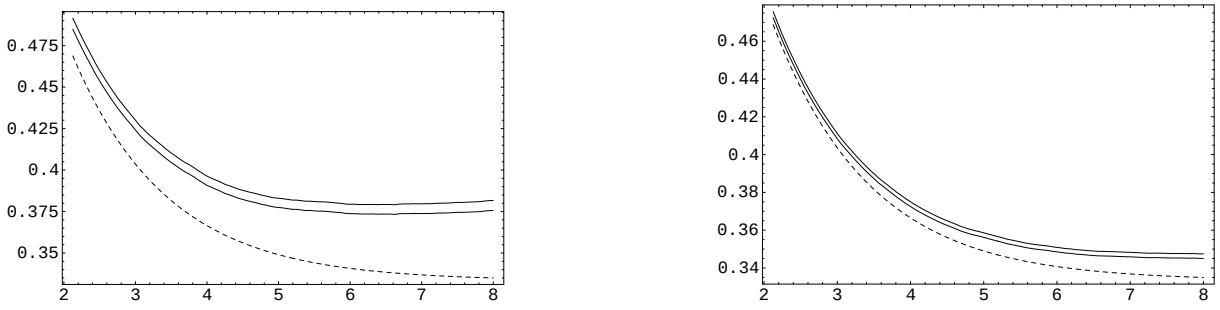

Figure 3. Analytical and numerical solutions for $n = 64$ and $n = 256$.

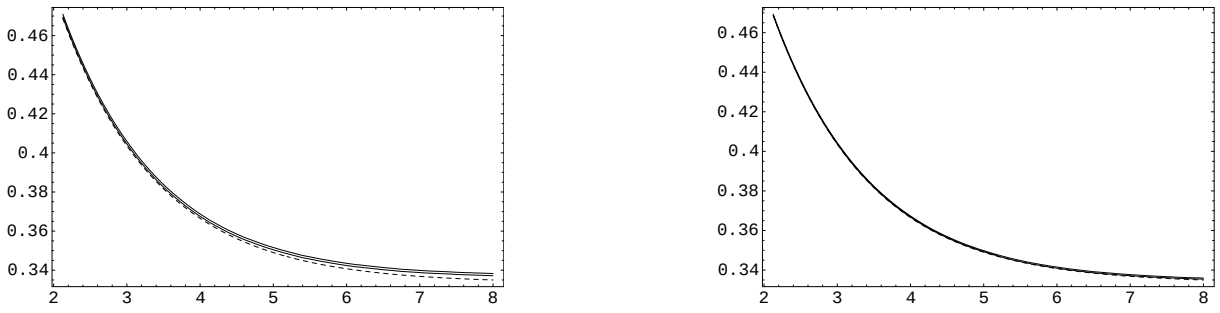

Figure 4. Analytical and numerical solutions for $n = 1024$ and $n = 4096$.

The curves in **Figures 3 and 4** have the same meaning as in **Figures 1 and 2**. The relative error of the temperature (30) computed corresponding to (29) is presented in Table 2.

n	E_{max}	CF	$\|V\|_\infty$
64	0.130 E-00	-	0.306 E-02
256	0.336 E-01	3.87	0.188 E-02
1 024	0.823 E-02	4.08	0.874 E-02
4 096	0.211 E-02	3.90	0.581 E-02
16 384	0.455 E-03	4.64	0.148 E-02

Table 2. Numerical convergence, Example 4.

Example 5 *This example illustrates the time relaxation of the temperature for the hard spheres model (4). We use again the Maxwell distribution (27) as the initial condition and the following set of parameters in (1)*

$$\alpha = \frac{1}{2}\,,\ \beta = 0.125\,,\ \gamma = 4\,,\ C_1 = \frac{1}{4\,\pi}\,.$$

We solve the equation (1) using the Algorithm 3 on the time interval $[0.0, 2.0]$

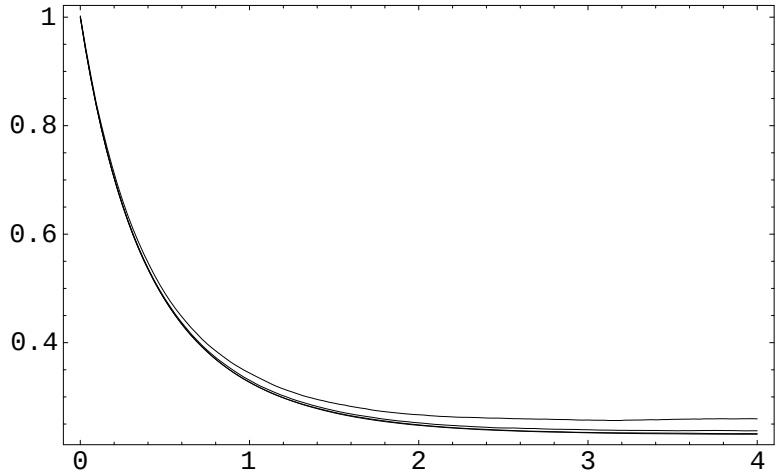

Figure 5. Courses of the numerical solutions for $n = 64, 256, 1024$ and $n = 4096$ (from above).

In **Figure 5**, the time relaxation of the empirical mean values (cf. (24)) for the temperature obtained for different number n of particles using $N = 1\,000$ independent ensembles are presented. It can be clearly seen that the curves converges by increasing the number of particles to some final curve of the temperature also for the hard spheres model.

4.3 Asymptotic tails

In this subsection we will show the asymptotic behaviour of the steady state distribution function

$$f_\infty(v) = \lim_{t\to\infty} f(t,v)\,,\ |v| \to \infty$$

for different values of parameter λ in the VHS-model (5). We assume that the function f_∞ is radially symmetric

$$f_\infty(v) = f_\infty(r)\,,\ r = |v|$$

and compute its histogram using uniform discretisation with respect to parameter r, i.e. discretisation of the whole velocity space in a system of concentric shells with increasing radius

$$r_k = k\,h_r\,,\ k = 1,\ldots,K\,,\ h_r = \frac{R}{K}\,. \tag{31}$$

In (31), $R > 0$ and $K \in \mathbb{N}$ are some additional parameters of the simulation. The histogram of the numerical steady state solution is then obtained counting the weight of the particles in the corresponding shells

$$\begin{aligned} f_1 &= g\,\#\Big\{v_j \ :\ |v_j| < r_1\Big\}\,, \\ f_k &= g\,\#\Big\{v_j \ :\ r_{k-1} \le |v_j| < r_k\Big\}\,,\ k = 2,\ldots,K\,, \qquad (32) \\ f_{K+1} &= g\,\#\Big\{v_j \ :\ R \le |v_j|\Big\}\,. \qquad (33) \end{aligned}$$

Example 6 *We use the Maxwell pseudo-molecules model ($\lambda = 0$ in (5)) and Maxwell distribution (27) as the initial condition and the following set of parameters in (1)*

$$\alpha = \frac{1}{10}\,,\ \beta = 30\,,\ \gamma = 16\,,\ C_0 = \frac{1}{4\,\pi}$$

and

$$R = 40\,,\ K = 128$$

in (31).

We use $n = 10^7$ particles and compute $N = 100$ independent ensembles on the time interval $[0.0, 2.5]$. The histograms for the initial Maxwell distribution (thick solid line) and for the final numerical distribution (thin solid line) are shown in **Figure 6**.

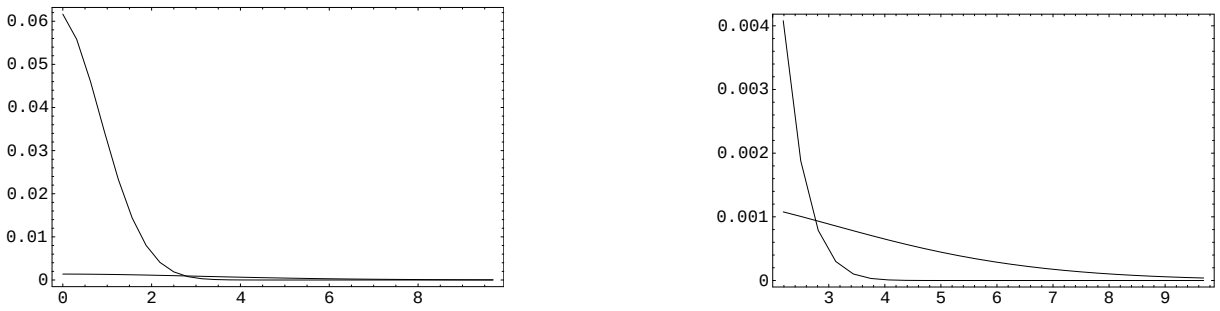

Figure 6. Initial and final histograms, Example 6

The left plot in **Figure 6** shows the histograms for $r \in [0, 10]$ while the right plot shows the "overpopulated tail" of the steady state distribution function for $r \in [2, 10]$. In order to obtain the exponent in (15) numerically we assume

$$f_k = c \exp\Big(- a\,(r_k - r_{k_0})^b \Big)\,,\ k \geq k_0$$

and plot the pairs (x_k, y_k)

$$x_k = \ln(r_k - r_{k_0})\,,\ y_k = \ln(\ln f_{k_0} - \ln f_k)\,,\ k = k_0 + 1, \ldots, K\,.$$

Thus we expect with $y_k = \ln a + b\, x_k$ almost linear plot which slope will show the exponent b in (34). The numerical results are shown in **Figure 7**.

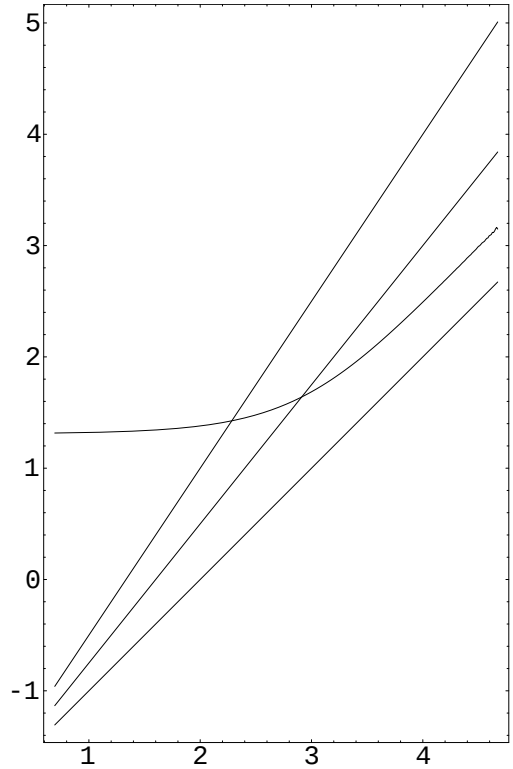

Figure 7. Logarithmic plot of the histogram, Example 6

In **Figure 7**, the thick solid line shows the course of the values y_k computed for $k_0 = 1$ while the thin straight lines $y = x - 2$, $y = 1.25x - 2$, $y = 1.5x - 2$ are drawn for

comparison of the slopes. Thus the asymptotic

$$f_\infty(v) \sim \exp(-a|v|)\,,\ |v| \to \infty$$

is clearly indicated. The unstable behaviour of the numerical curve for "large" r is due to usual difficulties by computing the "tails" of the distribution function using particles with constant weights.

Example 7 *We consider the hard spheres model ($\lambda = 1$ in (5)), Maxwell distribution (27) as the initial condition and the following set of parameters in (1)*

$$\alpha = \frac{1}{10}\,,\ \beta = 30\,,\ \gamma = 16\,,\ C_0 = \frac{1}{4\,\pi}$$

and

$$R = 16\,,\ K = 128$$

in (31).

We use again $n = 10^7$ particles and compute $N = 100$ independent ensembles on the time interval $[0.0, 0.25]$. The numerical results are shown in **Figure 8**.

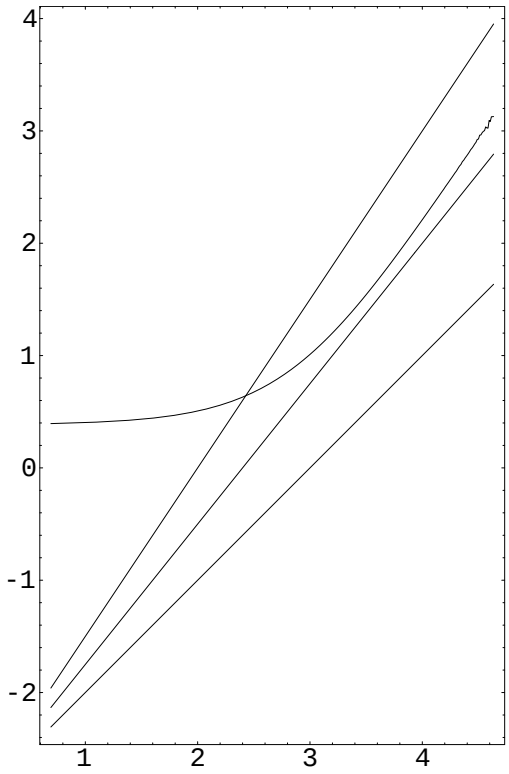

Figure 8. Logarithmic plot of the histogram, Example 7

In **Figure 8**, the thick solid line shows the course of the values y_k computed for $k_0 = 1$ while the thin straight lines $y = x - 3\,,\ y = 1.25x - 3\,, y = 1.5x - 3$ are drawn for comparison of the slopes. Thus the asymptotics

$$f_\infty(v) \sim \exp(-a|v|^{\frac{3}{2}})\,,\ |v| \to \infty$$

is clearly indicated.

Example 8 *We consider now the variable hard spheres model with* $\lambda = 0.5$ *in (5), the same Maxwell distribution (27) as the initial condition and the following set of parameters in (1)*

$$\alpha = \frac{1}{10}\,,\ \beta = 30\,,\ \gamma = 16\,,\ C_0 = \frac{1}{4\,\pi}$$

and

$$R = 24\,,\ K = 128$$

in (31).

We use again $n = 10^7$ particles and compute $N = 100$ independent ensembles on the time interval $[0.0, 0.5]$. The numerical results are shown in **Figure 9**.

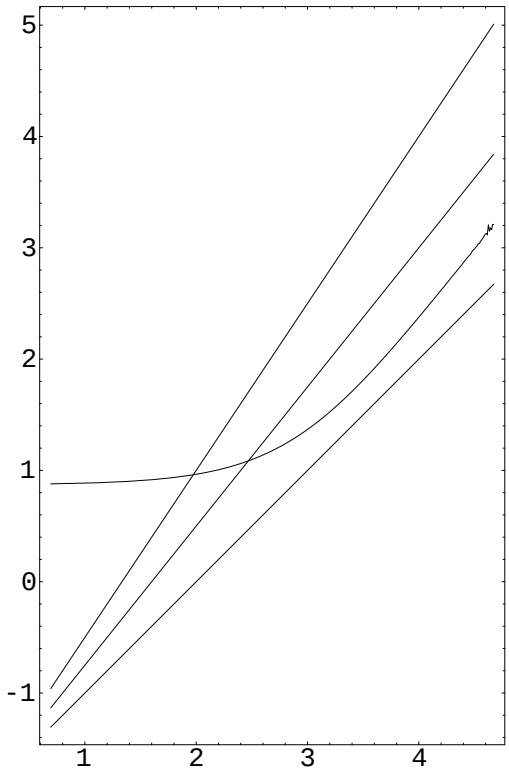

Figure 9. Logarithmic plot of the histogram, Example 8

Figure 9 shows the course of the values y_k computed for $k_0 = 1$ and the thin straight lines $y = x - 2\,,\ y = 1.25x - 2\,, y = 1.5x - 2$ for comparison of the slopes. Thus the asymptotics

$$f_\infty(v) \sim \exp(-a|v|^{1+\frac{\lambda}{2}})\,,\ |v| \to \infty$$

(cf. (16)) is clearly indicated.

Conclusions

In the present paper we develop a new stochastic numerical method for the uniformly heated inelastic Boltzmann equation. This method is a particle method where particles

are continuously subjected to a Gaussian white noise forcing and obtain the kinetic energy executing individual Brownian motion between the inelastic collisions which dissipate the kinetic energy. The numerical results obtained for spatially homogeneous problems are carefully tested using known analytical curves for the time relaxation of the temperature for the Maxwell pseudo-molecules. Furthermore, we investigate the "tails" of steady state distribution functions computed for different values of parameter λ in the VHS model (5). The asymptotic behaviour of the tails can be seen clearly. However the investigation of the "tails" leads to the modelling of very rare events and probably weighted particles schemes, like SWPM proposed in [24],[25],[26] for the classical, elastic Boltzmann equation are more efficient for such calculations.

Acknowledgement

The first author has been supported by NSF under grant DMS-0204568. Support from the Institute for Computational and Engineering Sciences at The University of Texas at Austin is also gratefully acknowledged.

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