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Stochastic interacting particle systems as a numerical tool

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Abstract. Stochastic particle methods for the numerical treatment of the nonlinear Boltzmann equation are considered. An approach to the problem of variance reduction is discussed, and results of some numerical experiments are presented.

Contents

1. Introduction

An important field of application of Monte Carlo methods is the numerical solution of nonlinear equations of high dimension. An example is the Boltzmann equation in rarefied gas dynamics. In the case of monatomic gases, this equation takes the form (cf. [6], [7])

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = \tag{1.1}$$
$$\int_{\mathcal{R}^3} dw \int_{S^2} de\, B(v,w,e) \left[f(t,x,v^*) f(t,x,w^*) - f(t,x,v) f(t,x,w) \right],$$

$$f(0,x,v) = f_0(x,v)\,, \tag{1.2}$$

where $t \geq 0$, $x \in D \subset \mathcal{R}^3$, $v \in \mathcal{R}^3$, and appropriate boundary conditions are assumed. The symbol ∇_x denotes the vector of the partial derivatives with respect to x, D is a bounded domain in three–dimensional Euclidean space $\mathcal{R}^3$, and $(.,.)$ is the scalar product. The symbols de and dw denote the uniform surface

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measure on the unit sphere $\mathcal{S}^2$ and the Lebesgue measure on $\mathcal{R}^3$, respectively. The function B is called the collision kernel. The objects v^* and w^* are defined as

$$v^* = v + e\,(e, w - v)\,, \quad w^* = w + e\,(e, v - w)\,, \tag{1.3}$$

where $v, w \in \mathcal{R}^3$, $e \in \mathcal{S}^2$. They are interpreted as the post–collision velocities of two particles with the pre–collision velocities v and w.

The function f describes the time evolution of the distribution of gas particles in the position and velocity space, thus depending on seven independent variables. In real world applications (like the reentry of a space shuttle into the atmosphere) Monte Carlo methods are the most common tools for the numerical solution of the Boltzmann equation (cf. [5], [18, Ch. 7]). They are based on the simulation of trajectories of stochastic interacting particle systems.

In Section 2 we give a rough description of the procedure for the direct simulation of a rarefied gas flow governed by Eq. (1.1). The stochastic components of this algorithm are determined by the parameters of the equation, namely the collision kernel B and the boundary conditions (if there is, e.g., diffuse reflection).

An important problem in Monte Carlo methods is the reduction of the statistical fluctuations. To this end, generalizations of the direct simulation method are of considerable interest. In Section 3 we discuss an approach to the variance reduction problem. This approach is based on a mechanism of random weight transfer during collisions giving some additional degrees of freedom. These free parameters are used to influence the variance of estimators for certain functionals of the solution f.

Section 4 contains some numerical results illustrating the effect of the new procedure.

2. Direct simulation schemes

A system of simulation particles

$$\big(x_i(t), v_i(t)\big)\,, \quad i = 1, \ldots, n\,, \quad t \geq 0\,, \tag{2.1}$$

is used to approximate the behaviour of the real gas described by the Boltzmann equation (1.1). Here $x_i(t) \in D$ and $v_i(t) \in \mathcal{R}^3$ denote the position and the velocity of the i–th particle, respectively. The number of particles in the system is n.

The time evolution of the particle system (2.1) is defined using a splitting technique. Namely, the simulation of the free flow of the particles and the simulation of their collisions are separated on a small time interval Δt. This means that on Δt, at a first step, the free flow is simulated disregarding the possible

collisions. Then, at a second step, the collisions are simulated neglecting the free flow.

During the free flow simulation step, the particles move according to their velocities, i.e.

$$x_i(t+\Delta t) = x_i(t) + \int_t^{t+\Delta t} v_i(s)\, ds\,.$$

The velocities do not change unless a particle hits the boundary. In this case, the corresponding velocity changes according to the boundary conditions.

During the collision simulation step, a partition

$$D = \cup_{l=1}^{l_c} D_l \tag{2.2}$$

of the spatial domain D into a finite number l_c of disjoint cells is used. There is no interaction between different cells. In each cell, collisions of the particles are simulated. A detailed description of the approach based on random weight transfer will be given in Section 3. The direct simulation procedure will be contained as a special case. Here we mention only the main idea, on which the elementary interaction (collision between two particles) is based.

Two indices i and j as well as an element e of the unit sphere $\mathcal{S}^2$ are chosen randomly. Two new velocities

$$v_i^* = v_i + e\,(e, v_j - v_i)\,, \quad v_j^* = v_j + e\,(e, v_i - v_j) \tag{2.3}$$

are calculated (cf. (1.3)) for the particles with the indices i and j. This procedure is continued until a certain time counting mechanism reaches Δt. Then, again the free flow is simulated, and so on.

The basic idea of particle methods for the numerical solution of the Boltzmann equation (cf. [9], [16]) is to approximate the measures

$$\lambda(t, dx, dv) = f(t, x, v)\, dx\, dv\,, \tag{2.4}$$

where f is the solution of Eq. (1.1), by a sequence of point measures defined by a particle system (2.1). One considers measures of the form

$$\mu^{(n)}(t, dx, dv) = \frac{1}{n}\sum_{i=1}^{n} \delta_{(x_i(t), v_i(t))}(dx, dv)\,, \quad t \geq 0\,, \tag{2.5}$$

where δ denotes the Dirac measure. The solution of Eq. (1.1) is approximated in the sense that

$$\lim_{n\to\infty} \int_D \int_{\mathcal{R}^3} \varphi(x,v)\, \mu^{(n)}(t, dx, dv) = \int_D \int_{\mathcal{R}^3} \varphi(x,v)\, \hat{\lambda}(t, dx, dv)\,, \tag{2.6}$$

for appropriate test functions φ, where $\hat{\lambda}$ is a deterministic measure–valued function close to λ defined in (2.4).

The particle method roughly described above was introduced on the basis of physical intuition by G. A. Bird in 1963 and called direct simulation Monte Carlo (DSMC) method (cf. [5]). In 1980 Nanbu [14] derived a stochastic simulation procedure starting from an approximation to the Boltzmann equation. A modification of this procedure comparable in efficiency with Bird's method was proposed in [1]. Stochastic algorithms based on the theory of interacting random processes were derived in [3], [10], [13]. In [8] an algorithm based on branching processes was presented.

In recent years considerable progress has been achieved in the mathematical foundation of particle methods for the Boltzmann equation. We refer to [2], [15], [23], [17] concerning convergence results (as the number of particles in the system tends to infinity). Stochastic particle methods for nonlinear equations are related to Markov systems of (many) interacting particles. So the classical DSMC method is closely connected with the n–particle "master" process described by the Kac–Leontovich equation (cf. [11], [12]). As $n \to \infty$, the empirical measures (2.5) converge in the sense of (2.6) to the solution of an approximate Boltzmann equation. We describe the limiting equation, which has been obtained for Bird's DSMC method in [23] and which holds also for the stochastic weighted particle method presented in this paper.

Consider a time discretization

$$t_k = k\,\Delta t\,, \quad k = 0, 1, \dots\,, \quad \Delta t > 0\,. \tag{2.7}$$

Let the functions

$$f^{(1,k)}(t,x,v)\,, \quad f^{(2,k)}(t,x,v)\,, \quad t \in [t_k, t_{k+1}]\,, \quad x \in D\,, \quad v \in \mathcal{R}^3\,,$$

where $k = 0, 1, \dots$, be defined as the solutions to the following system of equations,

$$\frac{\partial}{\partial t} f^{(1,k)}(t,x,v) + (v, \nabla_x)\, f^{(1,k)}(t,x,v) = 0\,, \tag{2.8}$$

with the initial conditions

$$f^{(1,k)}(t_k,x,v) = f^{(2,k-1)}(t_k,x,v)\,, \quad \text{for} \quad k = 1, 2, \dots\,, \tag{2.9}$$

and

$$f^{(1,k)}(t_k,x,v) = f_0(x,v)\,, \quad \text{for} \quad k = 0\,, \tag{2.10}$$

and

$$\frac{\partial}{\partial t} f^{(2,k)}(t,x,v) = \int_D dy \int_{\mathcal{R}^3} dw \int_{S^2} de\, h(x,y)\, B(v,w,e) \times \tag{2.11}$$
$$\left[f^{(2,k)}(t,x,v^*)\, f^{(2,k)}(t,y,w^*) - f^{(2,k)}(t,x,v)\, f^{(2,k)}(t,y,w)\right],$$

with the initial condition

$$f^{(2,k)}(t_k, x, v) = f^{(1,k)}(t_{k+1}, x, v)\,. \tag{2.12}$$

The function

$$h(x,y) = \sum_{l=1}^{l_c} \frac{1}{|D_l|} \P_{D_l}(x)\, \P_{D_l}(y) \tag{2.13}$$

is a mollifying kernel depending on the partition (2.2), where $|D_l|$ denotes the Lebesgue measure of the cell D_l, and $\P$ denotes the indicator function. Then (cf. (2.6))

$$\hat{\lambda}(t_k, dx, dv) = f^{(2,k-1)}(t_k, x, v)\, dx\, dv\,, \quad k \geq 1\,. \tag{2.14}$$

The various approximations involved in the algorithm are clearly displayed in the limiting equations (2.8) and (2.11). The splitting of the free flow simulation and the collision simulation leads to a corresponding splitting of the Boltzmann equation (1.1) based on the time discretization (2.7). The introduction of the cell structure (2.2) during the collision simulation step is represented by the mollifier (2.13) in the limiting equation (2.11). The transition from an approximate equation of the type (2.8)–(2.12) to the Boltzmann equation (1.1) has been studied in [2] in connection with Nanbu's simulation scheme.

3. The variance reduction problem

The convergence results mentioned in the previous section provide a mathematical justification of direct simulation Monte Carlo methods for the Boltzmann equation (1.1). However, from a numerical point of view, the improvement of the convergence behaviour of the particle methods remains a challenging task. For stochastic particle methods, this task is mainly related to the problem of variance reduction, i.e. the reduction of the random fluctuations around the deterministic limit.

The problem of variance reduction is far from being trivial, especially in the case of nonlinear equations. In the context of the DSMC method, we refer to the discussion in [4]. Low discrepancy sequences were used in [16] to replace random numbers in some parts of the algorithm called finite pointset method. Weighted particles in connection with this method were considered in [22].

In this section we discuss another approach to the variance reduction problem for the nonlinear Boltzmann equation (cf. [20] and references therein). The main idea is to introduce a generalized interaction mechanism, which is based on a partial weight transfer during the interaction. This mechanism provides

certain degrees of freedom, which are used for the purpose of variance reduction. The algorithm contains the standard DSMC method as a special case, and an analogous convergence theorem is valid (cf. [24]).

We introduce a system of particles

$$\left(x_i^{(n)}(t), v_i^{(n)}(t), g_i^{(n)}(t)\right), \quad i = 1, \ldots, m^{(n)}(t), \quad t \geq 0, \tag{3.1}$$

where $x_i^{(n)}(t) \in D$, $v_i^{(n)}(t) \in \mathcal{R}^3$, and $m^{(n)}(t)$ is the number of particles. The quantities $g_i^{(n)}(t) \in [0, \frac{1}{n}]$ are interpreted as artificial weights of the particles. The parameter $n = m^{(n)}(0)$ is the number of particles at time zero, thus governing the approximation of the initial function f_0 in (1.2).

The numerical method consists in the simulation of the particle system (3.1), and in the approximation of the measures (2.4) by the corresponding empirical measures

$$\mu^{(n)}(t, dx, dv) = \sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\, \delta_{(x_i^{(n)}(t), v_i^{(n)}(t))}(dx, dv), \quad t \geq 0, \tag{3.2}$$

where δ denotes the Dirac measure. This means that functionals of the solution of Eq. (1.1) (e.g., density, momentum, energy), that are of the form

$$\int_D dx \int_{\mathcal{R}^3} dv\, \varphi(x, v)\, f(t, x, v), \tag{3.3}$$

where φ is an appropriate test function, are approximated by the term

$$\sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\, \varphi(x_i^{(n)}(t), v_i^{(n)}(t)). \tag{3.4}$$

Note that the empirical measures (3.2) take the form (2.5) in the special case

$$g_i^{(n)}(t) = \frac{1}{n}, \quad m^{(n)}(t) = n, \quad \forall t \geq 0. \tag{3.5}$$

We describe the collision simulation for the subsystem of those particles situated in one of the spatial cells (cf. (2.2)). The rest of the algorithm is analogous to that described in Section 2. The stochastic evolution of the system is determined by an intensity function q and a weight transfer function G.

Given a state

$$z = \left((x_1, v_1, g_1), \ldots, (x_m, v_m, g_m)\right), \tag{3.6}$$

the system waits a random time having an exponential distribution with the parameter

$$\pi(z) = \frac{1}{2} \sum_{1 \leq i \neq j \leq m} \int_{S^2} q(z, i, j, e)\, de.$$

The probability of a pair with the indices i, j to collide is proportional to

$$\int_{S^2} q(z, i, j, e)\, de\,. \tag{3.7}$$

Given the indices i, j, the distribution of the direction parameter $e \in S^2$ is proportional to

$$q(z, i, j, e)\,.$$

Two new velocities

$$v_i^* = v_i + e\,(e, v_j - v_i)\,, \quad v_j^* = v_j + e\,(e, v_i - v_j)$$

are calculated as in (2.3).

Instead of replacing the pre–collision velocities v_i, v_j of the two particles by the post–collision velocities v_i^*, v_j^*, we replace the pair of particles (x_i, v_i, g_i), (x_j, v_j, g_j) by a group of four particles

$$(x_i, v_i, g_i - G)\,, \quad (x_j, v_j, g_j - G)\,, \quad (x_i, v_i^*, G)\,, \quad (x_j, v_j^*, G)\,, \tag{3.8}$$

where G is a function depending on the state z of the system and on the parameters i, j, e. Thus, each of the particles taking part in the collision gives a part of its weight to an particle with the post–collision velocity.

The relationship between the intensity function q and the weight transfer function G on the one side and the Boltzmann equation on the other side is given by the equality

$$q(z, i, j, e)\, G(z, i, j, e) = h(x_i, x_j)\, B(v_i, v_j, e)\, g_i\, g_j\,, \tag{3.9}$$

where the state z of the system has the form (3.6), B is the collision kernel of Eq. (1.1), and h is the mollifying kernel defined in (2.13).

Note that for the choice

$$G(z, i, j, e) = g_i = g_j = \frac{1}{n}$$

there is complete weight transfer (cf. (3.8)). Thus, (3.5) holds, condition (3.9) takes the form

$$q(z, i, j, e) = \frac{1}{n}\, h(x_i, x_j)\, B(v_i, v_j, e)\,,$$

and Bird's DSMC method comes out as a special case.

4. Numerical examples

Some preliminary numerical tests of the variance reduction procedure have been performed for the equation

$$\frac{\partial}{\partial t} f(t,v) = \int_0^1 \Big[f(t,v-w) f(t,w) - f(t,v) f(t,w) \Big] dw \,, \tag{4.1}$$

where $t > 0$, $0 \le v \le 1$, with the initial condition

$$f(0,v) = f_0(v) \,. \tag{4.2}$$

The solution f is assumed to be $1-$periodic in v, i.e.

$$f(t,v) = f(t,1+v) \,, \quad t \ge 0 \,, \quad v \in \mathcal{R} \,.$$

Eq. (4.1)-(4.2) is a model kinetic equation, which is nonlinear, but has a very simple collision mechanism. The simplicity of this equation allows us to check all steps of the numerical algorithm very carefully. In [19] Eq. (4.1) is studied in detail.

Furthermore, we introduce the function

$$F_\varepsilon(t) = \int_{1-\varepsilon}^1 f(t,v)\, dv \,, \quad \varepsilon > 0 \,, \tag{4.3}$$

which takes the explicit form

$$F_\varepsilon(t) = 2\varepsilon + \frac{2\Big((1-e^{2t}) \sin(2\pi\varepsilon) - 4e^{2t}(1-\cos(2\pi\varepsilon)) \Big)}{\pi \left(1 - 2e^{2t} + 17 e^{4t} \right)} \tag{4.4}$$

in the case

$$f_0(u) = 2 + \sin(2\pi u) \,.$$

The basic ideas are the following. First, if a particle reaches the interesting region $[1-\varepsilon, 1]$ then a part of it will always remain there, because in this case we will choose the weight transfer function (cf. (3.8))

$$G = \frac{1}{1+\kappa_1} \min(g_i, g_j) \,, \quad \kappa_1 > 0 \,.$$

Second, with the help of another parameter κ_2 we will prefer collisions with post-collision velocities from the region $[1-\varepsilon, 1]$ in order to "encourage" the particles to enter this region.

Rigorously, the weight transfer function is defined as

$$G = \frac{1}{1+\gamma} \min(g_i, g_j) \,,$$

where

$$\gamma = \begin{cases} \kappa_1\,, & \text{if} \quad v_i \in [1-\varepsilon,1] \quad \text{or} \quad v_j \in [1-\varepsilon,1]\,, \\ \kappa_2\,, & \text{if} \quad v_i, v_j \notin [1-\varepsilon,1] \quad \text{and} \quad \tilde{v}_i, \tilde{v}_j \in [1-\varepsilon,1]\,, \\ 0\ , & \text{otherwise.} \end{cases} \tag{4.5}$$

The values $\tilde{v}_i$ and $\tilde{v}_j$ of the post-collision velocities are defined by the following collision transformation of velocities

$$\tilde{v}_i = \tilde{v}_j = v_i + v_j - [v_i + v_j]\,,$$

where $[x]$ denotes the integer part of the value x. The function q is proportional to $1+\gamma$. This follows from the corresponding analogue of the basic relationship (3.9). Therefore, the probability (3.7) of pairs with $\tilde{v}_i, \tilde{v}_j \in [1-\varepsilon,1]$ to collide increases with κ_2.

The functional (4.3) is approximated by the random variables (cf. (3.3), (3.4))

$$\xi^{(n)}(t) = \sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\, ¶_{[1-\varepsilon,1]}(v_i^{(n)}(t))\,, \tag{4.6}$$

where ¶ denotes the indicator function.

In order to estimate the fluctuations of the random variables (4.6), a number N of independent ensembles of particles is generated. The corresponding values of the random variables are denoted by $\xi_1^{(n)}(t), \ldots, \xi_N^{(n)}(t)$. Then the empirical mean

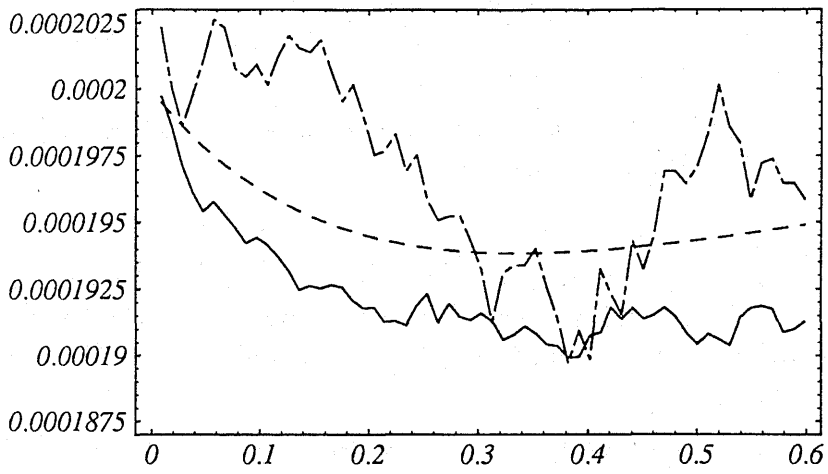
$$\frac{1}{N} \sum_{j=1}^{N} \xi_j^{(n)}(t) \tag{4.7}$$

converges as $N \to \infty$ to the expectation of the random variable (4.6). The statistical fluctuations around this deterministic limit are characterized by the quantity $\sqrt{\frac{\mathcal{D}^{(n)}(t)}{N}}$, where $\mathcal{D}^{(n)}(t)$ denotes the variance, i.e. the mean square deviation of the random variable (4.6) from its expectation. The order of convergence of the fluctuations is $\frac{1}{\sqrt{N}}$. However, the actual size of the fluctuations depends strongly on the value of $\mathcal{D}^{(n)}(t)$.

In order to illustrate the essential variance reduction, which can be achieved by the algorithm based on the function γ defined in (4.5), we choose $\varepsilon = 0.0001$, the time interval $[0, 0.6]$, and the parameters $\kappa_1 = 1$ and $\kappa_2 = 100$. In the following figures, the solid lines correspond to the γ-algorithm and the dashed-dotted lines correspond to the standard DSMC algorithm. The dashed lines represent the exact solution (4.4).

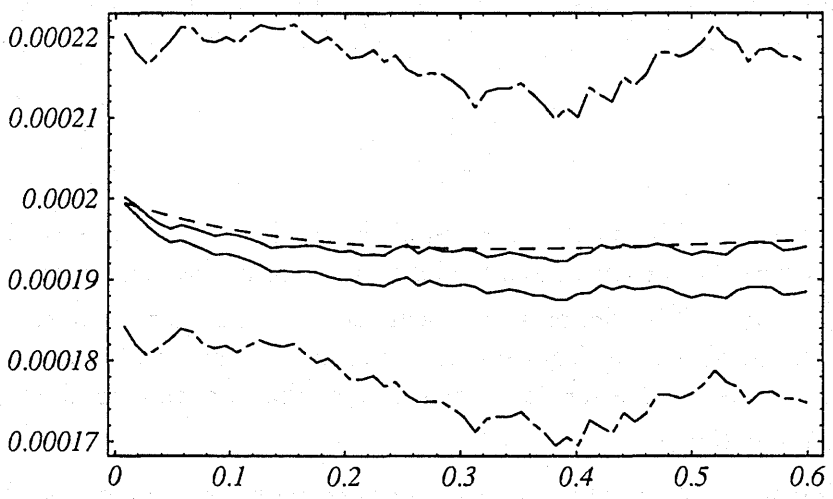
First we consider $n = 100$ and $N = 100000$. Figures 1 and 2 show the curves for the empirical mean values (cf. (4.7)) and the confidence intervals (with a confidence level of 0.99), respectively.

Figure 1



Empirical mean values for n=100 and N=100000

Figure 2

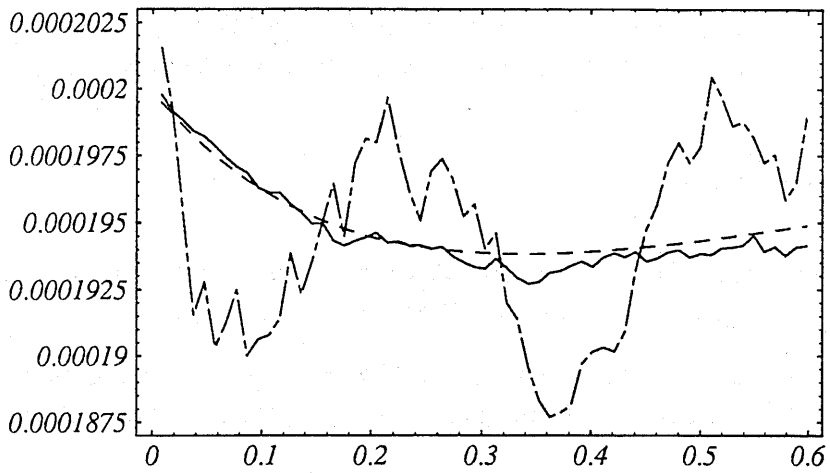


Confidence intervals for n=100 and N=100000

The small fluctuations of the γ–algorithm allow us to conclude that there is still a systematic error, i.e. a deviation of the expectation of the random variable (4.6) from the exact solution, since the number of particles n is not large enough.

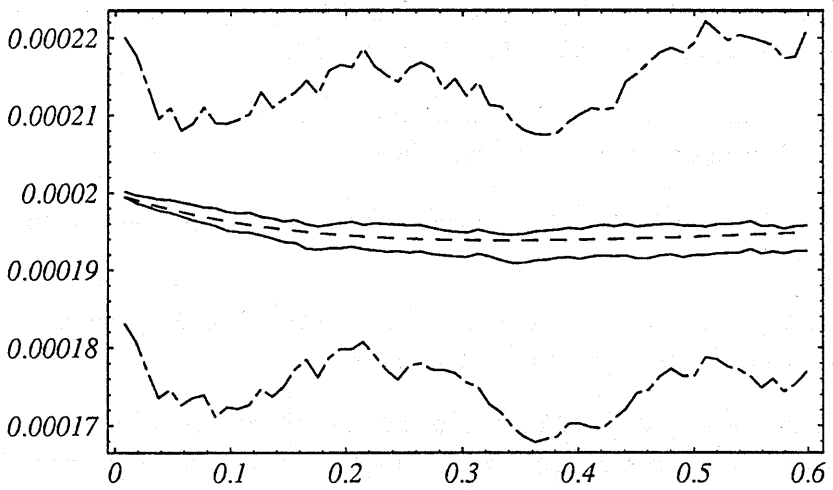
Next we consider $n = 100000$ and $N = 100$ in order to eliminate the systematic error. Figures 3 and 4 show the corresponding curves for the empirical mean values and the confidence intervals, respectively.

Figure 3



Empirical mean values for n=100000 and N=100

Figure 4



Confidence intervals for n=100000 and N=100

More extensive numerical tests will appear in [21].

5. Comments

The preliminary numerical tests for the model equation (4.1) show a variance reduction that is quite promising. Tests are in progress for the three–dimensional

relaxation problem related to the spatially homogeneous Boltzmann equation. A major difficulty to be tackled is the artificial blow-up in the system of simulation particles due to the partial weight transfer (cf. (3.8)). Here reduction methods based on a reasonable clustering in the velocity space seem to be useful.

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251. Michael Schwarz: Phase transitions of shape memory alloys in soft and hard loading devices.

252. Gottfried Bruckner, Masahiro Yamamoto: On the determination of point sources by boundary observations: uniqueness, stability and reconstruction.

253. Anton Bovier, Véronique Gayrard: Hopfield models as generalized random mean field models.

254. Matthias Löwe: On the storage capacity of the Hopfield model.

255. Grigori N. Milstein: Random walk for elliptic equations and boundary layer.

256. Lutz Recke, Daniela Peterhof: Abstract forced symmetry breaking.

257. Lutz Recke, Daniela Peterhof: Forced frequency locking in $\mathbf{S}^1$–equivariant differential equations.

258. Udo Krause: Idealkristalle als Abelsche Varietäten.

259. Nikolaus Bubner, Jürgen Sprekels: Optimal control of martensitic phase transitions in a deformation–driven experiment on shape memory alloys.

260. Christof Külske: Metastates in disordered mean field models: random field and Hopfield models.

261. Donald A. Dawson, Klaus Fleischmann: Longtime behavior of a branching process controlled by branching catalysts.

262. Tino Michael, Jürgen Borchardt: Convergence criteria for waveform iteration methods applied to partitioned DAE systems in chemical process simulation.

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268. Jörg Schmeling, Serge E. Troubetzkoy: Dimension and invertibility of hyperbolic endomorphisms with singularities.

269. Erwin Bolthausen, Dmitry Ioffe: Harmonic crystal on the wall: a microscopic approach.

270. Nikolai N. Nefedov, Klaus R. Schneider: Delayed exchange of stabilities in singularly perturbed systems.

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272. Priscilla E. Greenwood, Jiaming Sun: On criticality for competing influences of boundary and external field in the Ising model.

273. Michael S. Ermakov: On distinguishability of two nonparametric sets of hypothesis.

274. Henri Schurz: Preservation of probabilistic laws through Euler methods for Ornstein–Uhlenbeck process.

275. Lev B. Ryashko, Henri Schurz: Mean square stability analysis of some linear stochastic systems.

276. Nikolaus Bubner, Jan Sokołowski, Jürgen Sprekels: Optimal boundary control problems for shape memory alloys under state constraints for stress and temperature.

277. Alison M. Etheridge, Klaus Fleischmann: Persistence of a two–dimensional super–Brownian motion in a catalytic medium.