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A Direct Simulation Monte Carlo Scheme and Uniformly Distributed Sequences for Solving the Boltzmann Equation

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Abstract — Zusammenfassung

A Direct Simulation Monte Carlo Scheme and Uniformly Distributed Sequences for Solving the Boltzmann Equation. The Direct Simulation Monte Carlo (DSMC) scheme of Nanbu is considered for the solution of the Boltzmann equation in a simplified case. It is interpreted as a one-step method using particles combined with numerical quadratures after each step. A modified scheme in which the particles are ordered after each step is proposed. It is called the Low Discrepancy (LD) method. The error of the LD method is defined as the discrepancy of the set of particles relative to the exact solution. This error is estimated by means of other discrepancies, namely those of the sequences which perform the quadratures. The replacement of pseudo-random numbers used in the quadratures by uniformly distributed sequences is consequently suggested. Numerical comparisons are given between the DSMC scheme and the LD method that repeatedly uses the Hammersley sequence in the quadratures (LDH method).

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Ein direktes Monte-Carlo-Simulationsverfahren und gleichverteilte Folgen zur Lösung der Boltzmann-Gleichung. Es wird das direkte Monte-Carlo-Simulationsverfahren (DSMC) von Nanbu betrachtet, um die Boltzmann-Gleichung in einem vereinfachten Fall zu lösen. Das Verfahren wird als eine Einschrittmethode mit Teilchen interpretiert, die nach jedem Schritt mit Quadraturen kombiniert wird. Es wird ein modifiziertes Verfahren vorgeschlagen, in dem die Teilchen nach jedem Schritt angeordnet werden. Es heißt die niedrige Diskrepanz-Methode (LD). Der Fehler der LD-Methode wird als die Diskrepanz der Menge der Teilchen bezüglich der exakten Lösung definiert. Die Abschätzung der Fehler erfolgt dabei über die Diskrepanzen der Folgen, die die Quadraturen generieren. Es wird folglich vorgeschlagen, die Pseudozufallszahlen in den Quadraturen durch gleichverteilte Folgen zu ersetzen. Es werden numerische Vergleiche zwischen dem DSMC-Verfahren und der niedrigen Diskrepanz-Methode, die mehrmals die Folge von Hammersley benutzt (LDH-Methode), angegeben.

Introduction

In 1980 K. Nanbu [12] proposed a DSMC scheme for solving the Boltzmann equation for the spatially independant case which can be summarized as follows. The initial velocity distribution (in $\mathbb{R}^3$) f_0 is approximated by a sum of N Dirac measures:

$$f^{(0)} = \frac{1}{N} \sum_{1 \le i \le N} \delta(\underline{v} - \underline{v}_i^{(0)});$$

the time is discretized by steps of length Δt; the approximation

$$f^{(n)} = \frac{1}{N} \sum_{1 \le i \le N} \delta(\underline{v} - \underline{v}_i^{(n)})$$

of the velocity distribution at time $t^{(n)} = n\Delta t$ is obtained from $f^{(n-1)}$ in two phases. First an intermediary measure $g^{(n)}$ is defined by a direct one-step method. It is a linear combination of N Dirac masses and also of N^2 surface measures on spheres. Nanbu interprets the coefficients as collision probabilities, the points where the Dirac masses are concentrated as velocities of uncollided molecules and the spheres as sets of new velocities of colliding molecules. The approximation $f^{(n)}$ is then computed by using pseudo-random numbers which sample new discrete velocities according to the preceding collision probabilities and probability measures. The computing task of the original algorithm of Nanbu is proportional to N^2 (to N when a Maxwellian molecular model is used). In 1986 H. Babovsky [1] proposed a stochastic equivalent (subsequently called DSMC*) to the DSMC scheme that reduces the computing task to be always proportional to N. He has recently proved [2] that the DSMC (and DSMC*) scheme converges almost surely to the solution of the time-discretized Boltzmann equation. On the other hand, the numerical experiments of H. Ploss [16] have shown that the DSMC* scheme can compete with the Bird algorithm [3] which is almost always applied by engineers.

It turns out that the crucial tool for the numerical analysis of simulation schemes is the discrepancy. It was already used in 1973 by H. Neunzert and J. Wick [13] as a measure of the difference between the exact solution of an integro-differential equation and its simulated solution. For general information about uniform distribution of sequences and discrepancy, we refer to [9].

Here the analysis is restricted to the Boltzmann equation for an infinite, spatially homogeneous and isotropic gas (the velocity distribution is radially symmetric). A crude simplification of the Maxwellian molecular model is used: the differential cross section $\sigma(g)$ equals k/g, where g is the relative speed and k is some nonnegative constant.

The paper is organized as follows. In Section 1 we first derive a weak formulation of the simplified Boltzmann equation to which the analysis is restricted. A formulation of the DSMC scheme is then given: the intermediate step which leads from $g^{(n)}$ to $f^{(n)}$ is presented as a numerical quadrature of some function on $[0, 1)^4$, with the pseudo-random numbers as nodes. A modified scheme, subsequently called Low Discrepancy (LD) method, is proposed. In addition to the steps of the DSMC scheme, the $v_i^{(n)}$, $1 \le i \le N$, must be ordered according to their magnitude. In Section 2 we recall the definitions of discrepancy, *-discrepancy and uniformly distributed sequences. We then define the error of the LD method at time $t^{(n)}$ as the *-discrepancy of $V^{(n)} = \{v_i^{(n)} : 1 \le i \le N\}$ relative to the exact velocity density at time $t^{(n)}$. The numerical analysis of the LD scheme is achieved by combining a classical error analysis of a one-step method with an estimation of a quadrature error (the ordering of the $v_i^{(n)}$, $1 \le i \le N$, is crucial here). The error is estimated by means of the discrepancies of the sequences in $[0, 1)^4$ which perform the quadratures. This ensures the convergence when uniformly distributed sequences are used. In Section 3 we first

give the exact solution discovered by M. Krook and T. T. Wu [8]. The three schemes that are implemented are precisely presented. The DSMC and DSMC* schemes make use of linear congruential pseudo-random numbers; the LD method repeatedly uses the same Hammersley sequence for the quadratures (LDH method). In the case considered by Krook and Wu, the effective errors at a given time T are then computed by these three schemes. The errors of the DSMC and DSMC* schemes increase when N grows and is always a power of 2. Otherwise, the LDH method outperforms the others for large time steps but, in accordance with the theoretical predictions of Section 2, its error increases when Δt decreases.

1. The DSMC Scheme and the LD Method

We consider an infinite spatially homogeneous gas whose differential cross section is inversely proportional to the relative speed. We suppose that the velocity distribution is radially symmetric. From the Boltzmann equation which describes the evolution of this gas we derive a weak formulation which is suited to a numerical treatment. For the mathematical analysis of the Boltzmann equation we refer to [4].

Let $k>0$ and f_0 be a function $\mathbb{R}_+ \to \mathbb{R}_+$ such that

$$\int_{\mathbb{R}_+} v^2 f_0(v)\,dv = 1. \tag{1.1}$$

Let $T>0$ and f be a regular function $\mathbb{R}_+ \times [0, T] \to \mathbb{R}_+$ which verifies the Boltzmann equation

$$\begin{aligned} \frac{\partial f}{\partial t}(|\underline{v}|,t) = \frac{k}{\pi} \int_{\mathbb{R}^3 \times S^2_{\underline{v},\underline{w}}} & [f(|\underline{v}'|,t) f(|\underline{w}'|,t) \\ & - f(|\underline{v}|,t) f(|\underline{w}|,t)] \frac{\underline{n}\cdot(\underline{v}-\underline{w})}{|\underline{v}-\underline{w}|}\,d\underline{w}\,d\underline{n},\ \underline{v}\in\mathbb{R}^3,\ t\in(0,T) \end{aligned} \tag{1.2}$$

where

$$S^2_{\underline{v},\underline{w}} = \{\underline{n}\in S^2 : \underline{n}\cdot(\underline{v}-\underline{w})>0\},$$

$$\underline{v}' = \underline{v} - \underline{n}\cdot(\underline{v}-\underline{w})\,\underline{n},\ \underline{w}' = \underline{w} + \underline{n}\cdot(\underline{v}-\underline{w})\,\underline{n}$$

with the initial condition

$$f(|\underline{v}|,0) = f_0(|\underline{v}|),\ \underline{v}\in\mathbb{R}^3. \tag{1.3}$$

The integral on the right-hand side of (1.2) a priori depends on $\underline{v}$: we establish that it only depends on $|\underline{v}|$.

If $B(\mathbb{R}_+)$ is the *space of all bounded measurable functions everywhere defined on* $\mathbb{R}_+$, f also satisfies

$$\begin{aligned} \frac{d}{dt}\int_{\mathbb{R}_+} \phi(v) v^2 f(v,t)\,dv = \frac{k}{4\pi^2} \int_{\mathbb{R}^6 \times S^2_{\underline{v},\underline{w}}} & \phi(|\underline{v}|)[f(|\underline{v}'|,t) f(|\underline{w}'|,t) \\ & - f(|\underline{v}|,t) f(|\underline{w}|,t)] \frac{\underline{n}\cdot(\underline{v}-\underline{w})}{|\underline{v}-\underline{w}|}\,d\underline{v}\,d\underline{w}\,d\underline{n},\ \phi\in B(\mathbb{R}_+). \end{aligned} \tag{1.4}$$

For $\underline{n} \in S^2$ the application

$$T_{\underline{n}} : (\underline{v}, \underline{w}) \in \mathbb{R}^6 \to (\underline{v}', \underline{w}') \in \mathbb{R}^6$$

is linear and its determinant equals -1. The change of variables defined by $T_{\underline{n}}$ in the first part of the right-hand side of (1.4) leads to

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}_+} \phi(v) v^2 f(v,t)\, dv = \frac{k}{4\pi^2} \int_{\mathbb{R}^6 \times S^2_{\underline{v},\underline{w}}} [\phi(|\underline{v}'|) - \phi(|\underline{v}|)] \\ \cdot f(|\underline{v}|, t) f(|\underline{w}|, t) \frac{\underline{n} \cdot (\underline{v} - \underline{w})}{|\underline{v} - \underline{w}|}\, d\underline{v}\, d\underline{w}\, d\underline{n}, \quad \phi \in B(\mathbb{R}_+). \end{aligned} \tag{1.5}$$

For $(\underline{v}, \underline{w}) \in \mathbb{R}^6$ with $\underline{v} \neq \underline{w}$, the application

$$T_{\underline{v},\underline{w}} : \underline{n} \in S^2_{\underline{v},\underline{w}} \to \underline{v} = \frac{1}{|\underline{v} - \underline{w}|} [\underline{v} - \underline{w} - 2\, \underline{n} \cdot (\underline{v} - \underline{w})\, \underline{n}] \in S^2$$

is a C^1-diffeomorphism. The change of variables defined by $T_{\underline{v},\underline{w}}$ in the integral term of (1.5) leads to

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}_+} \phi(v) v^2 f(v,t)\, dv = \frac{k}{(4\pi)^2} \int_{\mathbb{R}^6 \times S^2} [\phi(|\underline{v}'|) - \phi(|\underline{v}|)] \\ \cdot f(|\underline{v}|, t) f(|\underline{w}|, t)\, d\underline{v}\, d\underline{w}\, d\underline{v}, \quad \phi \in B(\mathbb{R}_+), \end{aligned} \tag{1.6}$$

where

$$v' = \frac{1}{2} (\underline{v} + \underline{w} + |\underline{v} - \underline{w}|\, \underline{v}).$$

Let us denote $I = [0, 1)$. The right-hand side of (1.6) is expressed by using the variables

$$v = |\underline{v}|, \quad w = |\underline{w}|, \quad a = \frac{1}{2} + \frac{(\underline{v} + \underline{w}) \cdot \underline{v}}{2 |\underline{v} + \underline{w}|}, \quad b = \frac{1}{2} + \frac{\underline{v} \cdot \underline{w}}{2 |\underline{v}|\, |\underline{w}|}.$$

For $(a, b, w, v) \in I^2 \times \mathbb{R}_+^2$ let

$$[a, b; w, v] = [v^2 + w^2 + ((v^2 + w^2)^2 - 4(2b - 1)^2 v^2 w^2)^{1/2} (2a - 1)]^{1/2} / 2^{1/2}.$$

We then obtain the convenient weak formulation

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}_+} \phi(v) v^2 f(v,t)\, dv = 4k\pi \int_{\mathbb{R}_+^2 \times I^2} [\phi(v') - \phi(v)] \\ \cdot v^2 f(v,t) w^2 f(w,t)\, dv\, dw\, da\, db, \quad \phi \in B(\mathbb{R}_+), \end{aligned} \tag{1.7}$$

where $v' = [a, b; w, v]$.

Starting from equation (1.7) we present the DSMC scheme and the alternative DSMC* scheme. By modifying the DSMC scheme we define a new method. As this method is expected to lead to small discrepancies, that is, to small errors (see Section 2), we call it Low Discrepancy method.

We denote by $\delta(v-v_0)$ the Dirac measure located at the point $v_0 \in \mathbb{R}$. For two nonnegative integers M and N, define

(i) a time step $\Delta t = T/M$, assuming $q = 4k\pi\Delta t < 1$,

(ii) a sequence $V^{(0)} = \{v_i^{(0)} : 1 \le i \le N\}$, such that

$$f^{(0)} = \frac{1}{N} \sum_{1 \le i \le N} \delta(v - v_i^{(0)})$$

approximates (in a sense that will be subsequently specified) the initial velocity density $v^2 f_0(v)$. For $1 \le n \le M$,

$$V^{(n)} = \{v_i^{(n)} : 1 \le i \le N\} \subset \mathbb{R}_+$$

and

$$f^{(n)} = \frac{1}{N} \sum_{1 \le i \le N} \delta(v - v_i^{(n)})$$

are generated as follows.

(i) A Radon measure $g^{(n)}$ on $\mathbb{R}_+$ is defined by

$$\begin{aligned} \int_{\mathbb{R}_+} \phi(v)\, g^{(n)}(dv) &= \int_{\mathbb{R}_+} \phi(v)\, f^{(n-1)}(dv) \\ + q \int_{\mathbb{R}_+^2 \times I^2} &[\phi(v') - \phi(v)]\, f^{(n-1)}(dv)\, f^{(n-1)}(dw)\, da\, db, \quad \phi \in B(\mathbb{R}_+), \end{aligned} \tag{1.8}$$

or equivalently,

$$\begin{aligned} \int_{\mathbb{R}_+} \phi(v)\, g^{(n)}(dv) &= \frac{1}{N}\Big[(1-q) \sum_{1 \le i \le N} \phi(v_i^{(n-1)}) \\ + \frac{q}{N} \sum_{1 \le i \le N} \sum_{1 \le j \le N} \int_{I^2} &\phi([a, b; v_j^{(n-1)}, v_i^{(n-1)}])\, da\, db\Big], \quad \phi \in B(\mathbb{R}_+). \end{aligned} \tag{1.8'}$$

(ii) For $1 \le i \le N$, $1 \le j \le N$, let

$\chi_{j,i}$ be the characteristic function of

$$\left[q\frac{j-1}{N}, q\frac{j}{N}\right) \times \left[\frac{i-1}{N}, \frac{i}{N}\right),$$

χ_i be the characteristic function of

$$[q, 1) \times \left[\frac{i-1}{N}, \frac{i}{N}\right).$$

If $K^{(n)}\phi$ is defined on I^4 by

$$\begin{aligned} K^{(n)}\phi(a, b, c, d) &= \sum_{1 \le i \le N} \phi(v_i^{(n-1)})\, \chi_i(c, d) \\ + \sum_{1 \le i \le N} \sum_{1 \le j \le N} &\phi([a, b; v_j^{(n-1)}, v_i^{(n-1)}])\, \chi_{j,i}(c, d) \end{aligned}$$

then

$$\int_{\mathbb{R}_+} \phi(v)\, g^{(n)}(dv) = \int_{I^4} K^{(n)}\phi(z)\, dz.$$

Let us choose a sequence in I^4,

$$Z^{(n)}=\{z_{(n-1)N+l}=(a_{(n-1)N+l},\, b_{(n-1)N+l},\, c_{(n-1)N+l},\, d_{(n-1)N+l}) : 1\le l\le N\}$$

such that:

Any subset $I^3\times\left[\frac{i-1}{N},\frac{i}{N}\right)$, $1\le i\le N$, *contains one term of* $Z^{(n)}$. (1.9)

Then $f^{(n)}$ is defined by

$$\int_{\mathbb{R}_+}\phi(v)\,f^{(n)}(dv)=\frac{1}{N}\sum_{1\le l\le N}K^{(n)}\,\phi(z_{(n-1)N+l}). \tag{1.10}$$

According to property (1.9) the possibility of a collision for a given molecule i within the time interval $(t^{(n-1)},t^{(n)}]$ is once considered. If

$$\chi_{j,i}(c_{(n-1)N+l},\, d_{(n-1)N+l})=1,$$

then molecule i collides with molecule j and its new velocity $v_i^{(n)}$ equals

$$[a_{(n-1)N+l},\, b_{(n-1)N+l};\, v_j^{(n-1)},\, v_i^{(n-1)}].$$

If

$$\chi_i(c_{(n-1)N+l},\, d_{(n-1)N+l})=1,$$

then molecule i does not collide and $v_i^{(n)}=v_i^{(n-1)}$.

A formulation of the DSMC* scheme is obtained as follows:

$\chi_{j,i}$ is replaced by χ_{ji}^*, the characteristic function of

$$\left[\frac{j-q}{N},\frac{j}{N}\right)\times\left[\frac{i-1}{N},\frac{i}{N}\right);$$

χ_i is replaced by

$$\chi_i^*=\chi_i'-\sum_{1\le j\le N}\chi_{j,i}^*,$$

where χ_i' is the characteristic function of

$$I\times\left[\frac{i-1}{N},\frac{i}{N}\right).$$

The LD method is defined by modifying the DSMC scheme as follows:

Each sequence $V^{(n)}$, $0\le n\le M$, *is ordered such that if* $i\le i'$, *then* $v_i^{(n)}\le v_{i'}^{(n)}$.

This additional requirement permits us to estimate the errors of the LD method by means of the discrepancies of the $Z^{(n)}$.

2. Error Estimates for the LD Method

We first recall the definition of the discrepancy of a sequence. It measures how well this sequence is uniformly distributed. We then define the error at time $t^{(n)}$ of the LD method as the discrepancy of $V^{(n)}$ relative to $v^2 f(v, t^{(n)})$. It measures how well $V^{(n)}$ is uniformly distributed with density $v^2 f(v, t^{(n)})$.

Let s be some nonnegative integer.

A *subinterval* J of I^s is a subset of I^s of the form

$$\prod_{1 \le l \le s} [a_l, b_l);$$

its measure is

$$|J| = \prod_{1 \le l \le s} |b_l - a_l|.$$

Let $\tilde{I}$ denote the family of all subintervals of I^s and $\tilde{I}^*$ the family of all subintervals of the form

$$\prod_{1 \le l \le s} [0, c_l).$$

If $X = \{x_i : 1 \le i \le N\}$ is a sequence of I^s, the *discrepancy* $D_N(X)$ of X is defined by

$$D_N(X) = \operatorname{Sup}_{J \in \tilde{I}} \left| \frac{\operatorname{Card}(\{i : x_i \in J\})}{N} - |J| \right|;$$

the **-discrepancy* $D_N^*(X)$ of X is defined by

$$D_N^*(X) = \operatorname{Sup}_{J \in \tilde{I}^*} \left| \frac{\operatorname{Card}(\{i : x_i \in J\})}{N} - |J| \right|.$$

An infinite sequence $X = \{x_i : i \ge 1\}$ is *uniformly distributed* if

$$\lim_{N \to \infty} D_N(\{x_i : 1 \le i \le N\}) = 0$$

(or equivalently $\lim_{N \to \infty} D_N^*(\{x_i : 1 \le i \le N\}) = 0$).

Throughout the paper $t^{(n)} = n \Delta t$ and, for $r > 0$, ϕ_r is the characteristic function of $[0, r)$. Let

$$d_N^{(n)}(r) = \frac{1}{N} \sum_{1 \le i \le N} \phi_r(v_i^{(n)}) - \int_{\mathbb{R}_+} \phi_r(v)\, v^2 f(v, t^{(n)})\, dv, \tag{2.1}$$

$$D_N^*(V^{(n)}, f) = \operatorname{Sup}_{r > 0} |d_N^{(n)}(r)|. \tag{2.2}$$

According to the definition of E. Hlawka and R. Mück [6], $D_N^*(V^{(n)}, f)$ is the *-discrepancy of $V^{(n)}$ relative to $v^2 f(v, t^{(n)})$. It is the error that we estimate. For this purpose we need some additional error terms:

$$\begin{aligned} e_N^{(n)}(r) = & \int_{\mathbb{R}_+^2 \times I^2} [\phi_r(v') - \phi_r(v)]\, f^{(n)}(dv)\, f^{(n)}(dw)\, da\, db \\ & - \int_{\mathbb{R}_+^2 \times I^2} [\phi_r(v') - \phi_r(v)]\, v^2 f(v, t^{(n)})\, w^2 f(w, t^{(n)})\, dv\, dw\, da\, db, \end{aligned} \tag{2.3}$$

where $v' = [a, b; w, v]$;

$$\varepsilon^{(n)}(r) = \int_{[t^{(n)}, t^{(n+1)}] \times \mathbb{R}_+} \phi_r(v) \left[\frac{\partial f}{\partial t}(v, t^{(n)}) - \frac{\partial f}{\partial t}(v, t) \right] v^2 \, dv \, dt; \tag{2.4}$$

$$\delta_N^{(n)}(r) = \frac{1}{N} \sum_{1 \le l \le N} K^{(n+1)} \phi_r(z_{nN+l}) - \int_{I^4} K^{(n+1)} \phi_r(z) \, dz. \tag{2.5}$$

A relation between $d_N^{(n)}(r)$ and $d_N^{(n-1)}(r)$, $e_N^{(n-1)}(r)$, $\varepsilon^{(n-1)}(r)$, $\delta_N^{(n-1)}(r)$ is derived by a classical error analysis of a one-step method. We first estimate the error terms $e_N^{(n)}(r)$ and $\varepsilon^{(n)}(r)$. In order to estimate $\delta_N^{(n)}(r)$ we need to bound the difference between the exact measure of a set and its quasi-Monte Carlo approximation: this is achieved by an analysis of H. Niederreiter and J. M. Wills [15]. The final error estimation is obtained by gathering the previous ones.

Theorem 1: *The error term* (2.3) *can be estimated by*

$$|e_N^{(n)}(r)| \le 3 D_N^*(V^{(n)}, f). \tag{2.6}$$

Proof: Since $\forall t \in [0, T]$, $\int_{\mathbb{R}_+} v^2 f(v, t) \, dv = 1$ we get

$$e_N^{(n)}(r) = \frac{1}{N} \sum_{1 \le j \le N} \int_{I^2} d_N(a, b; v_j^{(n)}) \, da \, db + \int_{\mathbb{R}_+^2 \times I^2} d_N(a, b; v) v^2 f(v, t^{(n)}) \, dv \, da \, db - d_N^{(n)}(r),$$

where

$$d_N(a, b; v) = \frac{1}{N} \sum_{1 \le j \le N} \phi_r([a, b; v_j^{(n)}, v]) - \int_{\mathbb{R}_+} \phi_r([a, b; w, v]) w^2 f(w, t^{(n)}) \, dw.$$

Estimation (2.6) is obtained by noticing that, for $(a, b, v) \in I^2 \times \mathbb{R}_+$ and $r > 0$, the application $w \in \mathbb{R}_+ \to \phi_r([a, b; w, v])$ is the characteristic function of an interval $[0, s(a, b, v))$ where $s(a, b, v) \in \bar{\mathbb{R}}_+$. □

One gets immediately by integration by parts:

Theorem 2: *If f is twice continuously differentiable with respect to t, the error term* (2.4) *can be estimated by*

$$|\varepsilon^{(n)}(r)| \le \Delta t \int_{[t^{(n)}, t^{(n+1)}] \times \mathbb{R}_+} \left| \frac{\partial^2 f}{\partial t^2}(v, t) \right| v^2 \, dv \, dt. \tag{2.7}$$

In order to estimate $\delta_N^{(n)}(r)$ we need some new notations. For $0 \le n \le M$ let

$$i^{(n)}(r) = \sum_{1 \le i \le N} \phi_r(v_i^{(n)});$$

since the $v_i^{(n)}$, $1 \le i \le N$ are ordered according to their magnitude, we have

$$\{i : 1 \le i \le N, \, v_i^{(n)} < r\} = [1, i^{(n)}(r)]. \tag{2.8}$$

For $(b, v, w) \in [0,1] \times \mathbb{R}_+^2$ we define

$$\tilde{g}_{w,v}(b) = \min\left[\mathrm{Max}\left(\frac{2r^2 - v^2 - w^2}{2[(v^2+w^2)^2 - 4(2b-1)^2 v^2 w^2]^{1/2}} + \frac{1}{2}, 0\right), 1\right],$$

if $v \neq w$ or $v = w \neq 0$ and $b \neq 0, 1$; otherwise

$$\tilde{g}_{v,v}(0) = \tilde{g}_{v,v}(1) = \phi_r(v),\ \tilde{g}_{0,0}(b) = 1.$$

The function $\tilde{g}_{w,v}$ is continuous and satisfies

$$v \leq v'\ w \leq w' \Rightarrow \forall b \in [0,1]\ \tilde{g}_{w,v}(b) \geq \tilde{g}_{w',v'}(b), \tag{2.9}$$

$$[a, b; w, v] < r \Leftrightarrow a < \tilde{g}_{w,v}(b). \tag{2.10}$$

For $1 \leq i \leq N$, $1 \leq j \leq N$, let $g_{ji}^{(n)} = \tilde{g}_{v_j^{(n)}, v_i^{(n)}}$.

We denote by

$$J_N^{(n)}(r) = I^2 \times [q, 1) \times \left[0, \frac{i^{(n)}(r)}{N}\right),$$

$$E_N^{(n)}(r) = \bigcup_{1 \leq i \leq N} \bigcup_{1 \leq j \leq N} A_{ji}^{(n)} \times C_{ji}, \tag{2.11}$$

where

$$A_{ji}^{(n)} = \{(a, b) \in I^2 : a < g_{ji}^{(n)}(b)\},$$

$$C_{ji} = \left[q\frac{(j-1)}{N}, q\frac{j}{N}\right) \times \left[\frac{i-1}{N}, \frac{i}{N}\right).$$

We deduce from (2.8) and (2.10) that $K^{(n+1)}\phi_r$ is the characteristic function of $J_N^{(n)}(r) \cup E_N^{(n)}(r)$. Consequently, the error term (2.5) is expressed as follows:

$$\begin{aligned}\delta_N^{(n)}(r) = &\frac{1}{N}\mathrm{Card}\,(J_N^{(n)}(r) \cap Z^{(n+1)}) - |J_N^{(n)}(r)| \\ &+ \frac{1}{N}\mathrm{Card}\,(E_N^{(n)}(r) \cap Z^{(n+1)}) - |E_N^{(n)}(r)|.\end{aligned} \tag{2.12}$$

The first difference on the right-hand side of (2.12) is bounded by $D_N(Z^{(n+1)})$. In order to estimate the second difference we need the following result of Niederreiter-Wills [15]:

Let E be measurable subset of I^s. For $\varepsilon > 0$ let

$$E_\varepsilon = \{z \in I^s : \exists z' \in E,\ \| z - z' \| < \varepsilon\},$$

$$E_{-\varepsilon} = \{z \in I^s : \forall z' \in I^s \backslash E,\ \| z - z' \| \geq \varepsilon\},$$

where $\| \cdot \|$ is the Euclidean norm in $\mathbb{R}^s$. Then,

$$\text{if } \exists K > 1\ \forall \varepsilon > 0,\ \mathrm{Max}\,(|E_\varepsilon \backslash E|, |E \backslash E_{-\varepsilon}|) \leq K\varepsilon \tag{2.13}$$

then, for every sequence $X = \{x_i : 1 \leq i \leq N\}$ in I^s

$$\left|\frac{1}{N}\mathrm{Card}\,(E \cap X) - |E|\right| \leq (4Ks^{1/2} + 2K + 1)\, D_N(X)^{1/s}. \tag{2.14}$$

Lemma: *For all* $\varepsilon>0$ *the set* (2.11) *satisfies*

$$\mathrm{Max}\left(|E_N^{(n)}(r)_\varepsilon\backslash E_N^{(n)}(r)|, |E_N^{(n)}(r)\backslash E_N^{(n)}(r)_{-\varepsilon}|\right)\leq 5\varepsilon. \tag{2.15}$$

Proof: Let $\varepsilon>0$ and define

$$S_\varepsilon=\{z=(a,b,c,d)\in I^4 : c<\varepsilon \text{ or } d<\varepsilon\}.$$

For $1\leq i\leq N$, $1\leq j\leq N$, we set

$$T_\varepsilon C_{ji}=\left[q\frac{j-1}{N}+\varepsilon, q\frac{j}{N}+\varepsilon\right)\times\left[\frac{i-1}{N}+\varepsilon, \frac{i}{N}+\varepsilon\right)\cap I^2.$$

If

$$T_\varepsilon=\bigcup_{1\leq i\leq N}\ \bigcup_{1\leq j\leq N} A_{ji\varepsilon}^{(n)}\times T_\varepsilon C_{ji},$$

we first prove

$$E_N^{(n)}(r)_\varepsilon\subset S_\varepsilon\cup T_\varepsilon. \tag{2.16}$$

Let $z=(a,b,c,d)\in E_N^{(n)}(r)_\varepsilon$. Then

$$\exists (i',j')\ \exists z'\in A_{j'i'}^{(n)}\times C_{j'i'}$$

such that $\|z-z'\|<\varepsilon$. Either $z\in S_\varepsilon$ or

$$\exists (i,j),\ 1\leq i\leq i',\ 1\leq j\leq j',\ (c,d)\in T_\varepsilon C_{ji}.$$

Since the $v_i^{(n)}$ are ordered, we deduce from (2.9) that $(a',b')\in A_{ji}^{(n)}$. Therefore $(a,b)\in A_{ji\varepsilon}^{(n)}$ and the inclusion (2.16) holds. Consequently,

$$|E_N^{(n)}(r)_\varepsilon\backslash E_N^{(n)}(r)|\leq |S_\varepsilon|+|T_\varepsilon|-|E_N^{(n)}(r)|.$$

The inequality

$$|E_N^{(n)}(r)_\varepsilon\backslash E_N^{(n)}(r)|\leq 5\varepsilon$$

follows then by noticing

$$|A_{ji\varepsilon}^{(n)}\backslash A_{ji}^{(n)}|\leq 2(\varepsilon+\varepsilon^2).$$

The inequality

$$|E_N^{(n)}(r)\backslash E_N^{(n)}(r)_{-\varepsilon}|\leq 5\varepsilon$$

is similarly established. □

Inequality (2.15) leads to estimation (2.14). This, in turn, combined with identity (2.12) leads to:

Theorem 3: *The error term* (2.5) *can be estimated by*

$$|\delta_N^{(n)}(r)|\leq 52\, D_N(Z^{(n+1)})^{1/4}. \tag{2.17}$$

An estimation of the error of the LD method is then obtained by gathering inequalities (2.6), (2.7) and (2.17). As an additional regularity requirement on f, let us assume that it is twice continuously differentiable with respect to t and that

$$v^2\frac{\partial^2 f}{\partial t^2}(v,t)\in L^1\left(\mathbb{R}_+\times(0,T)\right).$$

Theorem 4: *If the discrepancies of all the $Z^{(n)}$ are bounded by some D_N, then*

$$\begin{aligned} D_N^*(V^{(n)}, f) &\le \exp(12k\pi t^{(n)})\, D_N^*(V^{(0)}, f) \\ &+ \Delta t \int_{[0,t^{(n)}]\times\mathbb{R}_+} \exp[12k\pi(t^{(n)}-t)] \left|\frac{\partial^2 f}{\partial t^2}(v,t)\right| v^2\, dv\, dt \\ &+ \frac{13}{3k\pi}\exp(12k\pi t^{(n)})\,\frac{D_N^{1/4}}{\Delta t},\quad 1\le n\le M. \end{aligned} \tag{2.18}$$

Proof: The Boltzmann equation (1.7) together with equalities (1.8) and (1.10) leads to

$$d_N^{(n)}(r) = d_N^{(n-1)}(r) + q\, e_N^{(n-1)}(r) + \varepsilon^{(n-1)}(r) + \delta_N^{(n-1)}(r).$$

The result of the theorem is achieved by combining estimations (2.6), (2.7) and (2.17) with the standard error analysis of a one-step method. □

The third term on the right-hand side of (2.18) has an unpleasant Δt in the denominator. But the computational experiments show that, for fixed N, $D_N^*(V^{(M)}, f)$ does not grow to infinity when Δt tends towards 0. The following theorem provides us with another estimation.

Theorem 5: *If all the sequences $Z^{(n)}$ equal*

$$Z^* = \{(a_l, b_l, c_l, d_l): 1\le l\le N\} \subset (0,1)^4 \cup \{0\}$$

then, for

$$\Delta t \le \frac{1}{4k\pi}\min\{c_l: 1\le l\le N, c_l>0\},$$

$$\begin{aligned} D_N^*(V^{(n)}, f) &\le \exp(12k\pi t^{(n)})\, D_N^*(V^{(0)}, f) \\ &+ \Delta t \int_{[0,t^{(n)}]\times\mathbb{R}_+} \exp[12k\pi(t^{(n)}-t)] \left|\frac{\partial^2 f}{\partial t^2}(v,t)\right| v^2\, dv\, dt \\ &+ \frac{1}{3}\exp(12k\pi t^{(n)}). \end{aligned} \tag{2.19}$$

Proof: The error term (2.5) can be expressed as follows:

$$\begin{aligned} \delta_N^{(n)}(r) &= -\frac{1}{N}\sum_{1\le l\le N}\sum_{1\le i\le N}\phi_r(v_i^{(n)})\,\chi_{[0,q)}(c_l)\,\chi_{[i-1/N,\,i/N)}(d_l) \\ &+ \frac{1}{N}\sum_{1\le l\le N}\sum_{1\le i\le N}\sum_{1\le j\le N}\phi_r([a_l, b_l; v_j^{(n)}, v_i^{(n)}])\,\chi_{j,i}(c_l, d_l) \\ &+ q\frac{i^{(n)}(r)}{N} - \frac{q}{N^2}\sum_{1\le i\le N}\sum_{1\le j\le N}|A_{ji}^{(n)}|, \end{aligned} \tag{2.20}$$

where χ_J denotes the characteristic function of J. When

$$q < \min\{c_l: 1\le l\le N, c_l>0\},$$

the right-hand side of (2.20) equals

$$q\left(\frac{i^{(n)}(r)}{N}-\frac{1}{N^2}\sum_{1\le i\le N}\sum_{1\le j\le N}|A_{ji}^{(n)}|\right).$$

Estimation (2.19) is then obtained with the same techniques that are used in Theorem 4. □

The estimate (2.18) provides us with some hints for the optimization of the LD method: the error is kept to a minimum if the $Z^{(n)}$ have small discrepancies. In the next section we test the simplest choice: all the $Z^{(n)}$ equal Z^*, a sequence of very low discrepancy introduced by J. M. Hammersley [5] (which fulfills the assumption of Theorem 5).

3. Computational Experiments

In 1977 M. Krook and T. T. Wu [8] have reported the discovery of an exact solution of the Boltzmann equation, in the simplified case to which the present analysis is restricted, for the following initial velocity distribution

$$f_0(v)=\frac{20\pi}{9}\left(\frac{5}{6\pi}\right)^{3/2}v^2\exp\left(-\frac{5}{6}v^2\right). \tag{3.1}$$

Then, for $k=3/2\pi$,

$$f(v,t)=\frac{4}{(2\pi)^{1/2}H(t)^{5/2}}\left(5H(t)-3+\frac{1-H(t)}{H(t)}v^2\right)\exp\left(-\frac{v^2}{2H(t)}\right) \tag{3.2}$$

where

$$H(t)=1-\frac{2}{5}\exp(-t).$$

We take $T=1.5$ which almost corresponds to an equilibrium state. We compute the effective error $D_N^*(V^{(M)},f)$ when f_0 and f are given by (3.1) and (3.2), $k=3/2\pi$ and by using three schemes: DSMC, DSMC* and LDH. Let us first specify the choices of $V^{(0)}$ and $Z^{(n)}$ (verifying hypothesis (1.9)) for each scheme.

The DSMC and DSMC* schemes make use of pseudo-random numbers for defining $V^{(0)}$ as well as for defining the $Z^{(n)}$. These pseudo-random numbers are generated by a linear congruential method (for an account of pseudo-random number generation we refer to [14]):

Let $m\ge 3$ and r be integers, let y_0 be an integer with $0\le y_0<m$ and let λ be an integer co-prime to m with $2\le\lambda<m$ and

$$(\lambda-1)y_0+r\not\equiv 0 \pmod m.$$

A sequence $\{y_i : i\ge 0\}$ of integers with $0\le y_i<m$ is generated by the recursion

$$y_{i+1}\equiv\lambda y_i+r \pmod m,\ i\ge 0. \tag{3.3}$$

A sequence $X=\{x_i : i\ge 0\}$ of pseudo-random numbers is then defined by

$$x_i=y_i/m,\ i\ge 0. \tag{3.4}$$

We have used the program RANU2 which is implemented on the computer SIEMENS/FUJITSU VP100 of the University of Kaiserslautern. It takes $m=2^{31}$, $r=1234567891$, $y_0=0$ and $\lambda=32771$. The sequence $V^{(0)}$ is defined as follows. We associate to the initial condition f_0 the application

$$F_0 : v \in \mathbb{R}_+ \to \int_{[0,v]} u^2 f_0(u)\, du.$$

It is differentiable and its inverse function Φ_0 is also differentiable. We then set

$$v_i^{(0)} = \Phi_0(x_i), \quad 1 \le i \le N \tag{3.5}$$

(where $X=\{x_i : i \ge 0\}$ is defined by (3.3)−(3.4)).

The sequence $Z^{(n)}$ is defined as follows:

$$z_{(n-1)N+l} = \left(x_{(n-1)N+l}, x_{(n-1)N+l+1}, x_{(n-1)N+l+2}, \frac{l-1}{N} \right), \quad 1 \le l \le N$$

(where X is defined by (3.3)−(3.4)).

The last component never appears in the computations: it just means that the others are valid for particle l.

The LDH method makes use of sequences of low discrepancy for defining $V^{(0)}$ as well as for defining the $Z^{(n)}$.

We first want to minimize $D_N^*(V^{(0)}, f)$ which appears on the right-hand side of estimation (2.18). If $V^{(0)}$ is defined by (3.5), for some $X=\{x_i : 1 \le i \le N\}$, it is easily shown that $D_N^*(V^{(0)}, f) = D_N^*(X)$. Consequently we take $X = \left\{ \frac{2i-1}{2N} : 1 \le i \le N \right\}$: it is proved in the book of Kuipers-Niederreiter [9] that this sequence has the smallest *-discrepancy, namely $\frac{1}{2N}$.

On the other hand, all the $Z^{(n)}$ equal $Z^*=\{z_i^* : 1 \le i \le N\}$, i.e. the Hammersley sequence [5] in dimension 4:

$$z_i^* = \left(\phi_2(i-1),\ \phi_3(i-1),\ \phi_5(i-1),\ \frac{i-1}{N} \right),$$

where ϕ_l is defined as follows.

To any integer k let us associate its expansion in basis l:

$$k = \sum_{j \ge 0} a_j^{(l)}(k)\, l^j, \text{ where } 0 \le a_j^{(l)} \le l-1;$$

then

$$\phi_l(k) = \sum_{j \ge 0} a_j^{(l)}(k)\, l^{-j-1}.$$

The estimates of L. K. Hua and Y. Wang [7] lead to

$$D_N(Z^*) \le \frac{480}{N} \frac{\log 2N}{\log 2} \frac{\log 3N}{\log 3} \frac{\log 5N}{\log 5}, \text{ if } N \ge 5.$$

A convenient algorithm for vector computer generation of the Hammersley sequence is available in [10].

First experiment

N is always a power of 2. The values of $D_N^*(V^{(M)}, f)$ for the three schemes are listed in Tables 1, 2 and 3 respectively. The DSMC and DSMC* schemes exhibit some unpleasant features. For the DSMC scheme, when $M=4096$, the error first decreases and thereafter increases when N grows. For the DSMC* scheme and for small M the error decreases then increases and becomes constant when N grows; for $M \geq 1024$ it just increases and becomes constant. We believe that this peculiarity is related to the way the pseudo-random numbers are generated. Some interference may occur between the $m=2^{31}$ of the linear congruential method (3.2) and the number $N=2^v$ of particles. In addition, the DSMC scheme generally outperforms the DSMC* scheme. On the other hand, for all M, the error of the LDH method decreases when N grows (with an exception for $M=4096$). But, for a given N, the error of the method increases when M grows: this behaviour reflects estimation (2.18). In addition, for small M (16 or 64), the LDH method outperforms the others. Moreover, it attains the best accuracy ($1.25\,E-3$).

Table 1. *Errors $D_N^*(V^{(M)}, f)$ for the DSMC scheme*

M \ N	256	1024	4096	16384	65536	262144
16	1.15 E−1	7.23 E−2	4.15 E−2	3.16 E−2	4.01 E−2	3.23 E−2
64	1.00 E−1	2.55 E−2	2.63 E−2	2.01 E−2	1.62 E−2	1.16 E−2
256	9.12 E−2	1.99 E−2	4.28 E−2	1.68 E−2	7.38 E−3	6.85 E−3
1024	5.67 E−2	1.41 E−2	1.33 E−2	1.95 E−2	7.29 E−3	7.63 E−3
4096	8.31 E−2	5.53 E−2	1.75 E−2	7.04 E−3	1.35 E−2	7.86 E−2

Table 2. *Errors $D_N^*(V^{(M)}, f)$ for the DSMC* scheme*

M \ N	256	1024	4096	16384	65536	262144
16	5.51 E−2	5.77 E−2	6.41 E−2	3.45 E−2	5.71 E−2	5.27 E−2
64	5.87 E−2	2.47 E−2	1.48 E−2	5.25 E−2	8.42 E−2	8.40 E−2
256	5.60 E−2	4.31 E−2	3.24 E−2	8.68 E−2	9.11 E−2	9.08 E−2
1024	2.96 E−2	2.93 E−2	6.54 E−2	9.42 E−2	9.30 E−2	9.21 E−2
4096	4.87 E−2	7.45 E−2	9.70 E−2	9.57 E−2	9.33 E−2	9.26 E−2

Table 3. *Errors $D_N^*(V^{(M)}, f)$ for the LDH method*

M \ N	256	1024	4096	16384	65536	262144
16	9.88 E−2	2.17 E−2	6.77 E−3	3.67 E−3	2.20 E−3	1.25 E−3
64	9.79 E−2	8.29 E−2	1.98 E−2	6.64 E−3	4.71 E−3	1.47 E−3
256	5.33 E−1	2.30 E−1	4.71 E−2	1.64 E−2	9.63 E−3	3.05 E−3
1024	3.96 E−1	3.06 E−1	3.05 E−1	6.05 E−2	4.64 E−2	8.30 E−3
4096	5.12 E−1	8.71 E−1	5.82 E−1	2.69 E−1	5.60 E−2	2.76 E−2

Second experiment

Here, N is always a power of 3. The values of $D_N^*(V^{(M)}, f)$ for the three schemes are listed in Tables 4, 5 and 6. The behaviour of the DSMC and DSMC* schemes is quite different from their behaviour in the first experiment. It happens that, for a given M, the error for N equal to a power of 2 completely differs from the error for N equal to a power of 3 of the same magnitude. But, in the present experiment, for a fixed M, the errors of the DSMC and DSMC* schemes decrease when N grows. This decrease is however irregular and it often appears that the error for a calculation with N particles is smaller than the error for a calculation with $3N$ particles: it cannot be assured that the accuracy increases when more particles are used. In addition, in this experiment, the differences in the performances of the DSMC and DSMC* schemes are small. On the other hand, for all M, the error of the LDH method regularly decreases when N grows (with an exception for $M=4096$). As in the preceding experience, for a given N, the error increases when M grows. However, for small M (16 or 64), the LDH method outperforms the others. Once again it attains the best accuracy ($1.60\,E-3$).

Table 4. *Errors $D_N^*(V^{(M)}, f)$ for the DSMC scheme*

M \ N	243	729	2187	6561	19683	59049	177147
16	5.79 E−2	8.85 E−2	4.59 E−2	5.03 E−2	4.56 E−2	3.80 E−2	3.23 E−2
64	1.07 E−1	7.32 E−2	2.15 E−2	3.40 E−2	2.46 E−2	1.20 E−2	1.26 E−2
256	4.47 E−2	1.94 E−2	2.04 E−2	9.67 E−3	8.99 E−3	5.16 E−3	2.01 E−3
1024	4.75 E−2	6.38 E−2	3.29 E−2	2.17 E−2	6.09 E−3	5.31 E−3	8.28 E−3
4096	3.72 E−2	4.78 E−2	4.55 E−2	3.39 E−2	1.72 E−2	4.63 E−3	1.99 E−3

Table 5. *Errors $D_N^*(V^{(M)}, f)$ for the DSMC* scheme*

M \ N	243	729	2187	6561	19683	59049	177147
16	1.17 E−1	6.65 E−2	7.67 E−2	4.33 E−2	1.65 E−2	2.94 E−2	3.20 E−2
64	6.88 E−2	7.68 E−2	5.36 E−2	1.29 E−2	5.97 E−3	1.36 E−2	8.29 E−3
256	4.12 E−2	1.17 E−1	4.48 E−2	1.17 E−2	1.24 E−2	7.58 E−3	2.78 E−3
1024	7.12 E−2	3.48 E−2	1.57 E−2	1.28 E−2	3.92 E−3	1.06 E−2	7.13 E−3
4096	1.47 E−1	4.99 E−2	2.06 E−2	2.07 E−2	1.14 E−2	5.49 E−3	7.36 E−3

Table 6. *Errors $D_N^*(V^{(M)}, f)$ for the LDH method*

M \ N	243	729	2187	6561	19683	59049	177147
16	6.36 E−2	3.51 E−2	1.57 E−2	9.27 E−3	4.41 E−3	2.74 E−3	1.60 E−3
64	1.88 E−1	6.12 E−2	5.74 E−2	1.76 E−2	1.08 E−2	4.21 E−3	1.76 E−3
256	4.04 E−1	2.70 E−1	6.80 E−2	6.87 E−2	2.06 E−2	7.83 E−3	3.82 E−3
1024	8.97 E−1	4.01 E−1	2.80 E−1	1.93 E−1	5.15 E−2	2.44 E−2	1.58 E−2
4096	4.86 E−1	3.82 E−1	8.44 E−1	1.14 E−1	1.26 E−1	8.58 E−2	3.00 E−2

Conclusion

The first estimations of the errors generated by a simulation method for solving the Boltzmann equation are given in this paper. The accuracy of these estimations is assessed through computation of effective errors in an example where an exact solution is known. The physically interesting macroscopic quantities such as mass velocity, momentum flow and energy flow are expressed by integrals involving the velocity distribution. Consequently, they can be approximated with a given accuracy by using the LD method. First, an arbitrarily low discrepancy $D_N^*(V^{(M)}, f)$ is assured as follows: a small time-step is selected (to minimize the second term of the right-hand side of (2.18)) and then a sufficiently large number of particles N is choosen (to minimize the first and third terms of the bound). Secondly, the differences between the exact macroscopic quantities and the computed ones are estimated by combining the Koksma-Hlawka inequality [9] and the previous estimation of $D_N^*(V^{(M)}, f)$. In addition, it is shown that the LD method is more reliable than the DSMC and DSMC* schemes which can diverge for ill-fated N (here a power of 2). The LD method already outperforms the DSMC and DSMC* schemes for large time steps. The improvement of the convergence properties of the LD method with respect to the time step is attempted in [11].

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