Comparison between Time Relaxed Monte Carlo Method and Majorant Frequency Scheme methods for the space homogeneous Boltzmann equation

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Abstract. Recently a new class of schemes, called Time Relaxed Monte Carlo (TRMC) has been introduced for the numerical solution of the Boltzmann equation of gas dynamics. The motivation is to propose a systematic framework to derive Monte Carlo methods effective near the fluid dynamic regime. Before the methods can be accepted as alternative tools to other methods, they have to show that they are able to reproduce results obtainable by well established reliable methods. In this paper a detailed comparison is performed between TRMC methods and the Majorant Frequency Scheme in the case of the space-homogeneous Boltzmann equation. In particular, the effect of finite number of particles is considered.

INTRODUCTION

Monte Carlo methods are very commonly used in the numerical solution of the Boltzmann equation of gas dynamics. The reasons of their popularity are the efficiency of the method (the computational cost per time step is essentially proportional to the number of particles, while deterministic methods are usually much more expensive) and the ability to effectively treat situations very far from thermodynamical equilibrium (in a particle method the particles fill the proper region of phase space, without useless memory allocation for a virtually zero distribution function). Furthermore they can be used with complicated geometries with a much less effort than the one required by deterministic schemes, and they are very flexible and can be easily extended to treat very complicated physical situation.

Probably the two main drawbacks of Monte Carlo methods are the statistical noise, that requires a CPU-time consuming time average if one needs accurate solution, and their difficulty to deal with situations near the fluid dynamic regime. In the latter case, in fact, the macroscopic quantities change on a macroscopic time scale, while the collision occur on a collisional time scale, which may be considerably lower. As a result, the particles spend most of their time performing a large number of collisions whose main effect is to drive them close to local equilibrium. In this respect we may say that the system presents some kind of stiffness.

Recently, a new class of Monte Carlo methods, called Time Relaxed Monte Carlo (TRMC) [2], for the simulation of the Boltzmann equation have been introduced, with the purpose of providing a systematic tool for the numerical approximation of the Boltzmann equation on a wide range of Knudsen number. The methods are based on a suitable series representation of the solution of the Boltzmann equation [3] containing only positive terms. Numerical schemes are obtained by a probabilistic interpretation of the sum. Schemes with finite order of accuracy in time are obtained by truncating the infinite sum, and using a Maxwellian for the reminder. Schemes of infinite order in time are obtained by taking into account, recursively, all infinite terms of the sum (TRMC-R) [4].

The purpose of this work is to perform a detailed test on these new schemes by comparing their results with those obtained by the Majorant Frequency Schemes (MFS) [5], which is considered a reliable and efficient Monte Carlo technique for the Boltzmann equation.

The plan of the paper is the following. In the next section we give a brief description of the Majorant Frequency Scheme. In Section 3 we illustrate the essence of TRMC methods. The section on numerical results will contain two test problems, one for Maxwell molecules, where we can use the Bobylev-Krook-Wu (BKW) solution [6], [7], and hard sphere molecules. The main goal is to study the effect of finite number of particles with both schemes.
MAJORANT FREQUENCY SCHEMES

The DSMC method is traditionally considered as a method of computer simulation of the behavior of a great number of model gas molecules. Each simulated particle is then regarded as representing an appropriate number $F_n$ of real molecules. The state of each model particle is characterized by its coordinate $r$ and velocity $v$. The evolution of a system of $N$ model particles can be represented as a jump-like motion of a point $(\vec{R}, \vec{V}) = \{r_1, v_1, ..., r_N, v_N\}$ in the $6N$-dimensional phase space. The DSMC method can be then treated as computer simulation of the $6N$-dimensional random jump-like process. For such a simulation, we represent the trajectory of the random process from the initial point $(t_0, \vec{R}_0, \vec{V}_0)$, as a transition in time between subsequent collisions (free motion) from the state $(t_0, \vec{R}_0, \vec{V}_0)$ to the state $(t_1, \vec{R}_1, \vec{V}_1)$, and the changes in particle velocities after collisions, i.e. the transition from the state $(t_1, \vec{R}_1, \vec{V}_1)$ to $(t_1, \vec{R}_1, \vec{V}_1)$. For a spatially-uniform rarefied gas flow case, there is no dependence on spatial coordinates $\vec{R}$, and a simulation of the process can be performed only in a $3N$-dimensional space of velocities $\{\vec{V}\}$.

The so-called "master" kinetic equations (MKE) [8], [9], [10] describe the behavior of an $N$-particle gas model with binary collisions. These linear MKE transform to the nonlinear Boltzmann equation as $N \to \infty$ and molecular chaos conditions are satisfied (see, e.g., [11]). It is natural to utilize directly these equations for constructing numerical schemes of the DSMC method.

Using a function $w$ – denoting the probability density of the transition of a pair of particles from $(v_i', v_j')$ to $(v_i, v_j)$, Kac’s MKE in a spatially-uniform rarefied gas flow case is written as

$$\frac{\partial}{\partial t} f_N(t, \vec{V}) + v(\vec{V}) f_N(t, \vec{V}) = \frac{n}{N} \sum_{i<j} \int f_N(t, \vec{V}'_{ij}) w(v_i', v_j' \to v_i, v_j) dv'_i dv'_j,$$

where the sum over $i < j$ means summation over $N(N-1)/2$ collision pairs, $v(\vec{V})$ is the total collision frequency

$$v(\vec{V}) = \frac{n}{N} \sum_{i<j} \sigma_i(g_{ij}) g_{ij} < \infty$$

and $g$ is the relative collision velocity, $\sigma_i(g_{ij})$ is the total collision cross-section. By introducing the majorant collision frequency [5]

$$v_m = \frac{N(N-1)}{2} \frac{[g\sigma_i(g)]_{\text{max}}}{[g\sigma_i(g)]_{\text{max}}} \geq v(\vec{V}),$$

summation over $N(N-1)/2$ collision pairs can be avoided, and MKE can be transformed to be suitable for constructing a random process that describes the behavior of the $N$-particle gas model with computational time linearly depending on the number of modeling molecules $N$.

For a spatially-uniform case the time of the next collision $t_1$ has the probability density distribution $v_m \exp\{-v_m(t_1 - t_0)\}$. For the transition $(t_1, \vec{V}_0) \to (t_1, \vec{V}_1)$, a collisional pair $(i, j)$ is uniformly chosen from $N(N-1)/2$ pairs. A real collision occurs with the probability $P = \frac{\epsilon_i \sigma_i(g_i)}{[g\sigma_i(g)]_{\text{max}}}$, and with the probability $(1 - P)$ the velocities will not change, i.e. a fictitious collision occurs.

Note that presented MFS scheme is time-accurate (does not use time discretization). A more detailed description of the derivation of the MFS schemes can be found in [12].

TIME RELAXED MONTE CARLO METHODS

Time Relaxed schemes are based on a formal expansion of the solution of the Boltzmann equation, and on its subsequent probabilistic interpretation.

Consider the differential system

$$\frac{\partial f}{\partial t} = \frac{1}{\epsilon} \left[P(f, f) - \mu f\right]$$

with initial condition $f(v, 0) = f_0(v)$, $\mu > 0$ is a constant and $P$ a positive bilinear operator. With the identification $P = Q_+$ and $\mu = \nu$, such equation may represent the Boltzmann equation for Maxwell molecules.

It is possible to show that the function $f$ satisfies the following formal expansion [3]

$$f(v,t) = (1 - \tau) \sum_{k=0}^{\infty} \tau^k f_k(v), \quad f_{k+1}(v) = \frac{1}{k+1} \sum_{i=0}^{k} \frac{1}{\mu} P(f_{i+1}, f_{k-i}),$$

(1)
where \( \tau = (1 - \exp(-\mu \Delta t / \epsilon)) \) is the so-called relaxed time. The functions \( f_k \) satisfy several nice properties, such as preservation of invariants. Furthermore, if the sequence \( \{f^{(k)}\}_{k \geq 0} \) is convergent, then its limit \( M \) is also the asymptotic equilibrium of \( f(v, t) \), i.e. \( \lim_{t \to \infty} f(v, t) = \lim_{k \to \infty} f_k(v) = M(v) \).

Usually one is interested in more general Boltzmann collision integral, which in general takes the form

\[
Q(f, f) = \int_{\mathbb{R}^3} \int_{S^2} \sigma(|v - v_1|, \omega)(f(v')f(v'_1) - f(v)f(v_1)) d\omega dv_1
\]

where \( \sigma \) is the differential cross section. If we approximate the differential cross section by a bounded one \( \sigma_B(|v - v_1|, \omega) \leq B \), then the BE can always be written in the above form, where \( \mu = 4\pi \rho B \) is a positive constant s.t.

\[
\mu \geq L_B[f](v) \equiv \int_{\mathbb{R}^3} \int_{S^2} \sigma_B(|v - v_1|, \omega)f(v_1) d\omega dv_1
\]

and \( P(f, f) = Q_B^\ast (f,f) + (\mu - L_B[f])f \).

From the previous representation, the following class of numerical schemes is obtained

\[
f^{n+1}(v) = (1 - \tau) \sum_{k=0}^m \tau^k f^n_k(v) + \tau^{m+1} M(v),
\]

where \( f^n \approx f(n\Delta t) \), \( \Delta t \) is a small time interval, and \( \tau = 1 - e^{-\mu \Delta t / \epsilon} \).

Such methods preserve the moments, and are asymptotically preserving, i.e. in the limit \( \epsilon \to 0 \) the function is projected into a Maxwellian. Time accuracy depends on the level of truncation \( m \). A generalization of the above schemes (generalized TRMC) can be written as

\[
f^{n+1}(v) = \sum_{k=0}^m A_k f^n_k(v) + A_{m+1} M(v), \quad (2)
\]

where the weights \( A_k = A_k(\tau) \) are nonnegative function satisfying some conservation consistency, and asymptotic preservation property. A more detailed description can be found in [2].

TRMC schemes are a direct consequence of the probabilistic interpretation of the truncated expansion (2). As an example we illustrate the first order TR method. Form \( m = 1 \) the generalized TR schemes give

\[
f^{n+1} = A_0 f^n + A_1 f_1 + A_2 M
\]

Since \( A_k, k = 0, 1, 2 \), are nonnegative numbers that sum to 1, they are probabilities. Furthermore, \( f_1 = P(f^n, f^n) / \mu \) is also a probability density. The probabilistic interpretation of the above equation is the following. A particle extracted from \( f^n \)

- does not collide with probability \( A_0 \), (i.e. it is sampled from \( f^n \))
- collides with another particle extracted from \( f^n \) with probability \( A_1 \) (i.e. it is sampled from the function \( f_1 \))
- is replaced by a particle sampled from a Maxwellian with probability \( A_2 \).

**Remark.** In this formulation the probabilistic interpretation holds uniformly in \( \mu \Delta t \), at variance with schemes based on a different time discretization of the equation, which require \( \mu \Delta t < c \), for some suitable \( c > 0 \). Furthermore, as \( \mu \Delta t \to \infty \), the distribution at time \( n + 1 \) is sampled from a Maxwellian.

Similarly, second and high order TRMC can be constructed. In all our numerical tests to avoid the use of very small time step we use TRMC3 (i.e. \( m = 3 \)). As we shall see, for the third order scheme the results for \( \Delta t = 0.1 \) and \( \Delta t = 0.05 \) are comparable for number of particles not too large.

**NUMERICAL RESULTS**

We consider two test cases, one with Maxwell molecules, and one with hard sphere molecules. In both tests we compare the time evolution of high order moments. In all calculations the number of particles times the number of runs that has been used to collect statistics is equal to \( 4 \times 10^6 \).
FIGURE 1. Maxwell molecules. Normalized even moments $M_4, M_6, M_8, M_{10}$ (top to bottom) vs time. The continuous line represents the exact BKW solution.

Maxwell molecules

The test with Maxwell molecules is important, because in this case an exact solution is available. This is known as the BKW solution \([6, 7]\), and takes the expression

$$f(v, t) = \frac{1}{(\pi C)^{3/2}} \frac{1}{2C} \left( 5C - 3 + \frac{2(1 - C)|v|^2}{C} \right) \exp\left(-|v|^2/C\right),$$  \hspace{1cm} (3)

where $C = C(t) = 1 - \exp(-(t+t_0)/6)$, with $t_0 = 6\log(5/2)$. This solution is defined for all $t \geq 0$.

Considering that the distribution is radially symmetric, and denoting by $v = |v|$, we define a radial distribution function $f_r(v) = 4\pi v^2 f(v, t)$. The even moments of the distribution function can be expressed in terms of the radial distribution as $M_{2k} = \int_0^\infty v^{2k} f_r(v, t) \, dv$ \hspace{1cm} (4)

and admit an analytic representation as

$$M_{2k}(t) = \frac{(2k+1)!!}{2^k} C^k (k - (k - 1)C),$$

where $\forall n > 0, n!! = n(n-2)(n-4)\ldots n_0$, $n_0 = 1$ if $n$ is odd, and $n_0 = 2$ if $n$ is even.

The moments can be computed from the particle approximation of the distribution function in a straightforward way. By collecting particles in spherical bins centered at the origin, one can compute an histogram, and compare it with the exact solution. In order to avoid approximations introduced by the space discretization, the histogram is compared with the exact cell average of the distribution function. If we divide the interval $[0, V_m]$ into $N_b$ bins of size $\Delta v$, then, for the BKW solution, the average can be computed as

$$\bar{f}_j = \frac{1}{\Delta v} \int_{v_{j-1}}^{v_j} f(v) \, dv = \frac{1}{\Delta v} (F(v_j) - F(v_{j-1})),$$

with

$$F(v) = \text{erf}(v/\sqrt{C}) - \frac{2v}{\sqrt{\pi C}} \left( 1 + \frac{1-C}{C^2} v^2 \right) \exp(-v^2/C).$$

Since we are interested mainly in the effect of finite number of particles, we shall take a large number of runs, so that statistical noise will be reduced, and the effect of finite time step and of finite number of particles will be evident. If the time step is sufficiently small, then the dominant effect is the finite number of particles. In Figure 1 we show the time dependence of the even order moments as a function of time. The continuous line represents the exact solution, while the marks represent numerical solutions obtained by different Monte Carlo methods.

Notice that for large number of particles MFS and TRMC3 give very similar results. On the other hand, for very small number of particles the behavior is slightly different. Notice, however, that the asymptotic value of the moments
for the two methods is quite close. In order to see the effect of the finite number of particles, we plot the difference between the exact and the computed values of moments $M_8$ and $M_{10}$. The results are reported in Figure 2.

The plot of the error seems to indicate a similar behavior of the error as a function of the number of particles. In all the calculations performed with TRMC3, the time step has been taken $\Delta t = 0.1$. The time discretization error of TRMC is observed in the computation performed with $N=1000$ particles. In such case MFS is more accurate. Clearly the difference in accuracy vanishes if a smaller time step is used.

**Hard spheres**

For Hard Sphere molecules we compute the evolution of the moments for different values of the number of particles $N$. We performed computations with $N = 10, 100, 1000, 10000$ using MFS and TRMC3. The result of the computation is illustrated in Figure 3. The initial condition is the same used for the Maxwell molecules. The time step for TRMC3 method is $\Delta t = 0.1$.

It is evident from the figures that MFS and TRMC3 method give similar results, and both schemes show that performing the computation with a limited number of particles produce the wrong time evolution of the moments.

The numerical results of TRMC3 depend on the time step. In Figure 4 (left) the time evolution of the moments is computed by using 1000 particles and TRMC3 with different time steps, namely $\Delta t = 0.1, 0.2, 0.5$. It is evident that while the calculations with $\Delta t = 0.1$ agree with the results of MFS method, larger time steps produce a sensible error.

Finally, in Figure 4 (right) we report the numerical results obtained with a variant of the TRMC3 method in which no Maxwellian term is added, i.e.

$$ f^{n+1} = A_0 f^n + A_1 f_1 + A_2 f_2 + (A_3 + A_4) f_3 $$

(5)
Hard spheres − No Maxwellian relaxation − Moments vs time

\[ \Delta t = 0.1, 0.2, 0.5 \]

MFS

TRMC3 \[ \Delta t = 0.1 \]

TRMC3 \[ \Delta t = 0.2 \]

TRMC3 \[ \Delta t = 0.5 \]

FIGURE 4. Hard sphere. Normalized even moments \( M_4, M_6, M_8, M_{10} \) (top to bottom) vs time. \( N = 10000 \) particles. Results for TRMC3 with \( \Delta t = 0.1, 0.2, 0.5 \) (left) and results for TRMC3 without Maxwellian term with \( \Delta t = 0.1 \) (right).

The results are very similar to the one obtained with the standard TRMC3 method, and the agreement with MFS is even better. Such scheme, however, is less attractive for space non-homogeneous calculations, since it does not preserve the correct fluid dynamic limit as the Knudsen number vanishes.

CONCLUSIONS

The comparison of the two methods, Majorant Frequency Scheme, and Time Relaxed Monte Carlo methods, has been performed using a large number of ensemble averages and the exact solution (for the Maxwell molecules). This allows a detailed quantitative comparison of the two approaches, and a careful study of the effect of finite number of particles. The comparison shows that both schemes give similar results when computing with a limited number of particles. Presented MFS scheme is time-accurate, and the numerical solution for any time moment can be obtained without time-descretization error. TRMC schemes presented in the paper, however, have a finite order of accuracy in time, and they require time discretization. The agreement between the two approaches is therefore good when the time step is small enough that the error introduced by time discretization is not the dominant one.

REFERENCES