Time Relaxed Monte Carlo Methods based on sampling from McKean graphs

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Abstract. A new Monte Carlo technique is proposed for sampling from the solution of the Boltzmann equation, which is based on sampling from the expansion of the solution in terms of McKean graphs. McKean graphs corresponding to particles "close" to equilibrium are replaced by sampling from a Maxwellian. Numerical tests performed on the space homogeneous Boltzmann equation show a good agreement with other techniques and better statistical properties than previously developed Recursive Time Relaxed Monte Carlo methods.

Keywords: Boltzmann equation, Monte Carlo methods, Time Relaxed methods, McKean graphs
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INTRODUCTION

Time Relaxed Monte Carlo methods (TRMC) have been developed with the aim of providing an efficient solution for the Boltzmann Equation (BE) of rarefied gas dynamics, even in regions of small Knudsen number. The idea behind the method is that if the Knudsen number is small, particles undergo many collisions, and most of them lose information of the initial condition and become distributed almost as a Maxwellian. The Time Relaxed approach provides a systematic way to identify which particle can be replaced by Maxwellian sampling. TRMC methods have been proposed in [7], where first and second order in time schemes are presented. Accurate comparison with other methods have been performed in [12] for the space homogeneous BE, and in [13] for the 1D Couette flow. In both papers, TRMC results have been compared to the Madjorant Frequency Scheme (MFS) [3]. In paper [8], 2D flow past an ellipse has been considered, and the numerical tests show the effectiveness of TRMC schemes for small Knudsen numbers.

A recursive version of TRMC, allowing arbitrary order of approximation in time (for the space homogeneous BE) has been presented in [9] by Pareschi and Wennberg. Several truncation criteria have been considered in [10]. In the same paper, an adaptive strategy is considered, which is based on the rate of change of high order moments during a time step. If the rate is too high, then the number of terms in the Wild sum expansion is increased. If it is too small, then at the next time step one will use a smaller number of terms.

In this paper we propose a different technique for sampling the Wild sum, and a different truncation criterion.

A detailed test on Pareshi-Wennberg recursive algorithm shows that it produces a biased average number of particles per level in the sampling from the Wild sum, while the new algorithm overcomes this drawback. We computed the coefficient of the new expansion, showing that in the basic algorithm (no replacement of particles by Maxwellian) the coefficients are all positive under a suitable stability condition on the ratio between time step Δt and Knudsen number K_n (positivity of the coefficient is essential to maintain the probabilistic interpretation of the expansion, and therefore to use such a sum as a sampling technique).

Test problems on the space homogeneous BE and on the one dimensional Couette flow are solved in [4].

WILD SUM AND MCKEAN GRAPHS

Let us consider the space homogeneous Boltzmann equation for Maxwell molecules, written in the form

$$\frac{\partial f}{\partial t} = P(f,f) - \mu f, \quad f(v,0) = f^0(v) \tag{1}$$

where $P(f,g)$ is the positive, symmetric, bilinear gain term, and μ is the (constant) coefficent of the loss term. The generalization to other collision kernels, such as, for example, hard spheres, will be described later.

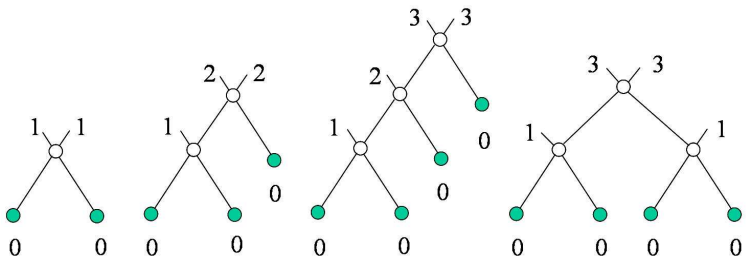

FIGURE 1. McKean graphs needed to sample from f_1, f_2, and f_3. There are two graphs corresponding to f_3

The solution of this equation at time t may be written as a series (Wild sum [15]), as

$$f(v,t) = (1-\tau)\sum_{k=0}^{\infty} \tau^k f_k(v) \tag{2}$$

where $\tau = 1-\exp(-\mu t)$ is the *relaxed time*, and the coefficients are recursively defined as

$$f_k(v) = \frac{1}{k}\sum_{\ell=0}^{k-1}\frac{1}{\mu}P(f_\ell, f_{k-\ell-1}), \quad f_0 \equiv f(v,t=0)$$

Such representation has a natutal probabilistic interpretation, because $f_k(v)$ are non negative, and $\int f_k(v)\,dv = \int f^0(v)\,dv$, and $\sum_k \tau^k(1-\tau) = 1$, (we refer to the paper [11] in the same proceeding). Such interpretation is at the basis of the Time Relaxed Monte Carlo methods [7]. ppp The sampling process can be graphically represented by the so called McKean graph [5, 6], which represents the collision history corresponding to a given realization of a sample from the Wild sum. Particles sampled from $f_1(v) = P(f_0, f_0)/\mu$ are obtained by colliding two original particles. This process is represented by the first graph on the left in Figure 1. Such a graph has one node (unshaded circle) corresponding to one collision which generates two particles of level 1, and two leaves (shaded circles) corresponding to the original particles from level zero. There are two McKean graphs of level 2 corresponding to $P(f_0, f_1)$ and $P(f_1, f_0)$, but they present the same collisional history because of symmetry $P(f,g)$, hence can be considered as identical graphs, therefore we say that there is only one McKean graph of level two (second graph in Fig. 1).

There are two different graphs of level 3 (last two graphs in Fig. 1), corresponding to possible realization of the sampling from $f_3(v)$. The occurrence probability of these two graphs are, respectively, $2/3$ and $1/3$ (since the first one corresponds to $P(f_0, f_2)$ and to $P(f_2, f_0)$). In addition to two particles from level 3, these graphs produce other particles, namely 1 particle from level 1 and 1 particle from level 2 (left graph), or 2 particles from level 1 (right graph).

We shall denote by G^1, G^2, G^3_1, G^3_2, the McKean graphs of level one and two and the two McKean graphs of level three. It is possible to assign to each graph an integer vector containing the number of particles produced at each level. The vectors corresponding to the four McKean graphs in Fig. 1 will be denoted by

$$\mathbf{G}^1 = \begin{pmatrix} 2 \end{pmatrix}, \quad \mathbf{G}^2 = (1,2)^T, \quad \mathbf{G}^3_1 = (1,1,2)^T, \quad \mathbf{G}^3_2 = (2,0,2)^T.$$

Vector $\mathbf{G}^3$ is obtained as $\mathbf{G}^3 = (2\mathbf{G}^3_1 + \mathbf{G}^3_2)/3$, since $2/3$ and $1/3$ are the occurrence probabilities of graphs $\mathbf{G}^3_1$ and $\mathbf{G}^3_2$. The merging of two graphs of level ℓ and r forming a graph of level $k = \ell + r + 1$ may be represented as $G^k_i = (G^\ell_{i_\ell}, G^r_{i_r})$, where i, i_ℓ, i_r denote the particular graph of level, respectively, k, ℓ, r.

The vector corresponding to the average number of particles of graphs of level k in principle can be computed as

$$\mathbf{G}^k = \sum_{i=1}^{n_k} p^k_i \mathbf{G}^k_i$$

where n_k denotes the number of different graphs of level k, and p^k_i denotes the occurring probability of such graph.

A simpler formula for the generation of vectors $\mathbf{G}^k$ can be derived, as illustrated in [14].

Once the vectors $\mathbf{G}^k$ have been generated, they can be used to sample the Wild sum by sampling directly from the McKean graph. Suppose we have N particles at the initial time. Then the average number of particles that have

to be sampled from level k is $N(1-\tau)\tau^k$. This number can be obtained as follows. Let us define the coefficients $C_k, k = 1,\ldots,m$ to satisfy the linear system

$$\sum_{k=1}^{m} C_k g_\ell^k = N(1-\tau)\tau^\ell \tag{3}$$

where $(g_\ell^k, \ell = 1,\ldots,k)$ denote the components of vector $\mathbf{G}^k$. If all C_k are nonnegative, the particles from the Wild sum can be obtained by sampling from McKean graph G^k C_k times (on average). It means, that the realization of recursive construction of independent McKean graphs will lead to unbiased number of molecules for each level $k = 1,\ldots,\ell$.

Final time limitation. Although in theory the maximum number of levels in the McKean graph is unbounded, in practice it is bounded by the finite number N of particles. Since $m+1$ particles are needed in order to generate a McKean graph of order m, we have the limitation $m \leq N-1$, if we want that the McKean graph is obtained from the merging of independent subgraphs. If we want to sample from McKean graphs to produce an unbiased sampling from the truncated Wild sum, then we need nonnegative coefficients C_ℓ. Notice that the coefficients C_ℓ obtained from (3) depend on τ. For small values of τ all C_ℓ are nonnegative. As $\tau > \tau_1 = 2/3$, the coefficient C_1 becomes negative, therefore the probabilistic interpretation of Eq. (3) breaks down. Before we describe a technique which allows to go beyond this limitation, let us show that such procedure provides a sampling from the Wild sum which is less biased than the Pareschi-Wennberg algorithm presented in [9].

level	N_{req}	IRTRMC	PW
0	73.576	73.570	73.803
1	46.509	46.505	46.510
2	29.399	29.389	29.403
3	18.584	18.586	18.578
4	11.747	11.748	11.745
5	7.426	7.432	7.427
6	4.694	4.688	4.697
7	2.967	2.974	2.953
8	1.876	1.879	1.825
9	1.186	1.183	1.020
10	⋮	⋮	⋮

TABLE 1. Number of obtained molecules in each level. Case $t = 1$, $N = 200$. Calculations by IRTRMC, and original RTRMC method (PW), both obtained by averaging over 5×10^4 runs

For $\mu t = 1$ the recursive algorithm that samples from McKean graphs gives an average number of particles per level which is in better agreement with the exact one (see Table 1). However, one can show that the use of direct sampling from independent McKean graphs for $\mu t = 1.5$ leads to an expected number of particles at level one much larger that the exact one, because in this case $C_1 < 0$.

IMPROVED RTRMC

We present here a modification of the technique based on sampling from McKean graphs, which can be used to produce unbiased sampling from the Wild sum. Let us consider the equation for the coefficients (3). Let us suppose that for some value of k, say $k < k_c(\tau)$, the coefficients C_k are negative. This means that even if we do not sample from G^k, $k < k_c$, there will be an excess of particles at such levels. This excess of particles can be eliminated by re-using a particle generated at a level k, with some probability p_k. Re-using probabilities can be chosen in such a way that the expected number of particles generated at each level k is the correct one. These probabilities are obtained as follows. Let us denote by I_ℓ the number of events that alter the number of particles at level ℓ, and let us denote by X_{I_ℓ} the number of molecules on level ℓ after I_ℓ events. With the original procedure, each time we realize a sub graph at level ℓ, the number I_ℓ is increased by one (because the other particle is used to generate a graph of level higher that ℓ). The expectation value of this number can therefore be written as

$$< I_\ell >= \sum_{k\geq\ell} C_k g_\ell^k. \tag{4}$$

If $p_\ell = 0$, then $X_{I_\ell} = I_\ell$. If $p_\ell \neq 0$, then the evolution of X_I follows the conditions

$$X_I = \begin{cases} 1 & \text{if } X_{I-1} = 0 \\ X_{I-1}-1 & \text{with probability } p_\ell \quad (\text{provided } X_{I-1} \neq 0) \\ X_{I-1}+1 & \text{with probability } 1-p_\ell \quad (\text{provided } X_{I-1} \neq 0) \end{cases}$$

The average number of generation events I_ℓ is given by [14]

$$< I_\ell >= \frac{1}{2} N \tau^\ell (1-\tau) - \sum_{k=\ell+1}^{k_c} C_k g_\ell^k.$$

The expected number $< X_{I_\ell} >$ of particles at level ℓ can be computed as a function of the probability p_ℓ [14].

Here we use the simple analytical approximation

$$< X_{I_\ell} > \approx 1 - I_\ell p_\ell + I_\ell (1-p_\ell).$$

By imposing $< X_{I_\ell} >= N(1-\tau)\tau^\ell$ and making use of the expression for I_ℓ we determine the probability p_ℓ that has to be used in the simulation.

Figure 2 shows the dependence of $< X_I > /I$ as a function of p, for various values of I, and $p \in [0, 0.5]$. The picture shows that for moderate values of p_ℓ, and for large values of I_ℓ the analytical approximation is quite good.

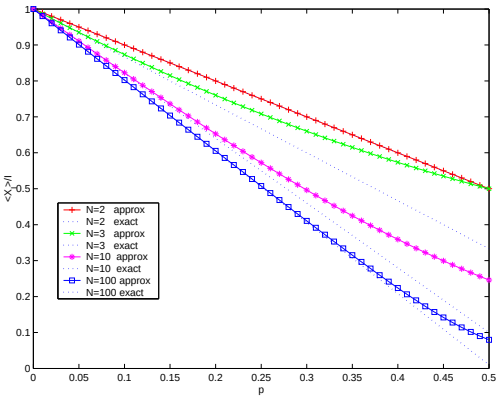

FIGURE 2. Average number of generated particles per generating event, as a function of the reusage probability

Truncation of McKean graphs. A crucial point in the effective use of TRMC methods is the capability of replacing particles which are near equilibrium by Maxwellians. As was shown in [2], it is possible to introduce an indicator how close the given set of collisions represented by given McKean graph to Maxwell distribution function. Notice that the level of a graph is bad indicator to check whether particles are close to equilibrium, in particular the collision of the molecule from initial distribution with molecule that was thermalized results to the velocity of both molecules can be far from thermalization (see Figure 3). They introduce L_1-indicator instead of level number (see [2] for details), while indicator L_2 was inroduced by Pareschi et al in [10]. Here we propose indicator L_3, which appears to be more natural to incorporate replacement of certain subgraphs by Maxwellians. We perform numerical test of these indicators in order to compare the correspondance wich indicator is best suited for accuracy of the replacement. Three indicators can be introduced as follows. Let us denote by $G_i^k = (G_{i_\ell}^\ell, G_{i_r}^r)$, $k = \ell + r + 1$, a particular graph of level k, generated by two sub graphs of level respectively ℓ and r. Then the indicators are recursively defined as

$$L_1(G_i^k) = 1 + \min(L_1(G_{i_\ell}^\ell), L_1(G_{i_r}^r)), \quad (5)$$

$$L_2(G_i^k) = 1 + \mathrm{mean}(L_2(G_{i_\ell}^\ell), L_2(G_{i_r}^r)), \quad (6)$$

$$L_3(G_i^k) = 1 + \mathrm{hmean}(L_3(G_{i_\ell}^\ell), L_3(G_{i_r}^r)), \quad (7)$$

and, for all definitions, $L_{1,2,3}(G0) = 0$. Here $\mathrm{mean}(x,y) = (x+y)/2$ is the arithmetic mean, and $\mathrm{hmean}(x,y) = 2xy/(x+y)$ is the harmonic mean.

The error introduced by substitution of collisions with Maxwellians the indicators was peformed using following procedure. The functional

$$\sqrt{\int_{-\infty}^{+\infty} \left(M(v) - f_{k,i}(v)\right) 2dv}. \quad (8)$$

was numerically estimated for large set of McKean graphs G_i^k where $f_{k,i}(v)$ the density function of the velocity of particales generated by McKean graph G_i^k.

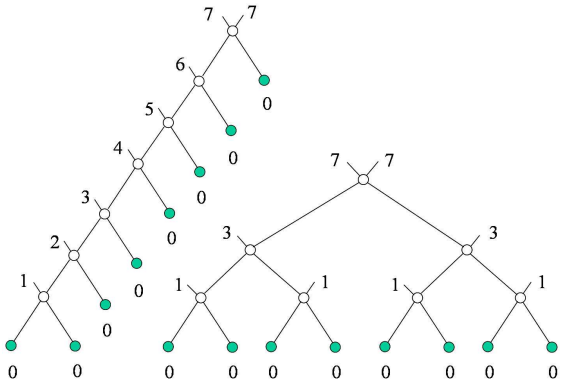

FIGURE 3. Two McKean graphs of level 7. The right one is well balanced, and the particles of level 7 generated are much closer to equilibrium than those generated by the graph on the left.

In order to check the relative quality of such indicators, we execute the following test. For McKean graph G_i^k of level k the function $f_{k,i}(v)$ numerically calculated. For this purpose $k+1$ velocities are generated uniformly from $(-1,1)$.

$$f(v) = \begin{cases} \frac{1}{2} & \text{if } -1 \le v \le 1 \\ 0 & \text{if } v \le -1 \text{ or } 1 \le v \end{cases}$$

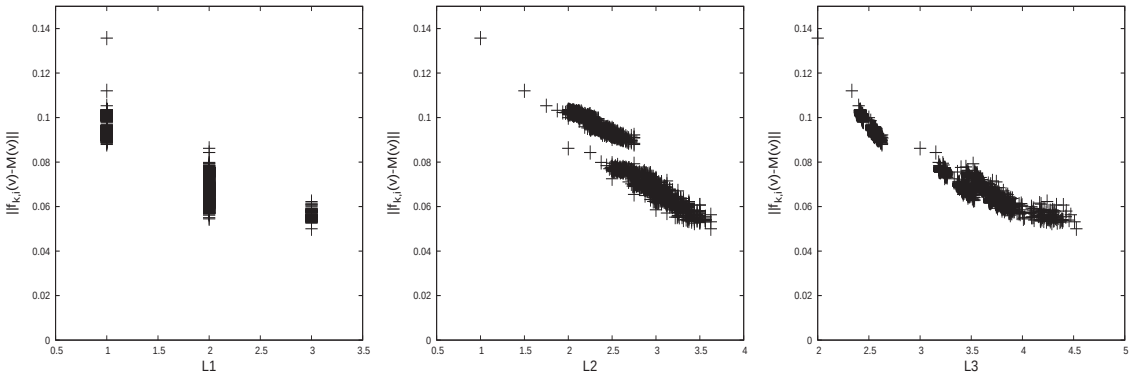

FIGURE 4. Scattered plot of the distance of the Maxwellian vs the indicators L_1, L_2, and L_3.

The collisions between the particles are performed according the sequence given by graph G_i^k. After collisions, two velocities corresponding to the graph G_i^k were used to approximate $f_{k,i}(v)$ by a histogram, and the estimation of error, Eq.(8), was calculated. In our tests we chose the model of collisions like in Kac's one-dimensional model of Bolzmann equation:

$$v_1' = v_1\cos\theta - v_2\sin\theta, v_2' = v_1\sin\theta + v_2\cos\theta.$$

This model reproduced Maxwellian distribution for stationary case.

We sample from a set of N particles, uniformly distributed in velocity in the interval [-1,1]. Then we consider all possible distribution corresponding to sampling from all McKean graphs of level $k \leq 12$.

The results of the calculation are summarized in Figure 4, where we report the scattered plot of the values of the distance from Maxwellian and the values of the indicators, for the distribution functions corresponding to all McKean graphs up to level 12. It is evident that L_2 and L_3 show a better correlation with the distance from a Maxwellian than L_1. Furthermore, their almost continuous values make them more suitable as indicators.

Once an indicator is chosen, then one has to choose a threshold, L_{crit}: if $L < L_{\text{crit}}$ the McKean graph is used as it is, if $L > L_{\text{crit}}$ then the McKean graph is replaced by sampling from a Maxwellian.

EXTENSION TO HARD SPHERE MOLECULES

Most of the methods that are described here can be used for the numerical solution of the Boltzmann equation with other collision kernels. Let us describe the modifications needed to treat the case of hard sphere.

At a given time step, a bound Σ on the relative cross section is computed by standard technique, the parameter μ is set to $\mu = 4\pi\Sigma\rho$, where $\rho = \int f\,dv$. Then the procedure is the same as the one described for Maxwell molecules, except that *dummy collisions* are used in place of effective collisions (see [7] for the treatment of hard sphere molecules in TRMC).

Dummy collisions are performed on a randomly selected pair, and then they are converted into real collision with a probability that is equal to the ratio between the relative cross section between the selected particle and the bound Σ (rejection technique).

The problem with this approach is that it is more difficult to state if a particle may be replaced by a Maxwellian, because in addition to taking into account the balance of McKean graphs, one has to consider how many dummy collisions were effective collisions during the collision history corresponding to a given McKean graph.

Here we do not treat this problem, which is considered with some detail in [14]

It is possible to compute an effective length of a McKean graph, which takes into account not only the structure of the graph, but also the real collision history of a particle. Let us attach to each particle a label L which is a measure of the effective collision history associated to the particle. When two particles (v', L') and (v_*', L_*') collide by a dummy collision and generate the particles (v, L) and (v_*, L_*), then there are two possibilities

- if the particles effectively collided, then v and v_* will be the outcome of the collision, and $L = L_* = 1 +$ amean(L', L_*'), where amean denotes either min, mean or hmean, according to whether we use indicator L_1, L_2, or L_3.

- if the particles did not collide, then the velocities as well as the indicators remain unchanged, i.e. $(v,L) = (v',L')$ and $(v_*,L_*) = (v'_*,L'_*)$.

The drawback of this approach is that the indicator can be computed only after the rejection is applied, and one already decided whether a dummy collision is a real collision or not. This is not very useful in speeding up the calculations. However, one could empirically compute the correlation between the effective lengths of the graphs, computed as if all dummy collisions were effective collisions (as in the case of Maxwell molecules), and the effective lengths that takes into account the rejection. Such correlation can then be used to correct the critical value of the effective length, L_{crit}, by a suitable factor, which takes into account the effect of the rejection. This analysis is performed in [14].

CONCLUSIONS

In this paper we propose a new technique which can be used to sample the exact solution of the Boltzmann equation written in the form of a Wild sum, by sampling from independent McKean graphs. A technique is presented which allows the use of large time steps. The new method is able to perform sampling from the Wild sum which are less biased than previously developed recursive algorithms. A new indicator is presented for deciding when a given McKean graph can be replaced by a Maxwellian. An algorithm based on the ideas presented in this paper is described in a companion paper presented at this conference [4]. In the same paper, numerical tests of the method algorithm on space homogeneous Boltzmann equation and on one dimensional Couette flow are presented.

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