# Time Relaxed Monte Carlo Methods for the Boltzmann equation: an overview

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**Abstract.** Time Relaxed Monte Carlo methods (TRMC) have been developed with the goal of providing an efficient treatment of the Boltzmann equation in conditions of large variation of local Knudsen number. In this review the basic ideas behind TRMC are exposed, and modern developments and improvements are reviewed.

**Keywords:** Boltzmann equation, Monte Carlo methods, Time Relaxed methods
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## INTRODUCTION

In this talk we give a review of Time Relaxed Monte Carlo methods (TRMC) for the numerical solution of the Boltzmann equation of rarefied gas dynamics. TRMC schemes have been introduced with the purpose of providing efficient Monte Carlo methods for the numerical solution of the Boltzmann equation, even in regions of small Knudsen number, where the distribution of particles is very close the a local Maxwellian.

TRMC scheme, in its original form, is based on writing the solution of the space homogeneous Boltzmann equation using a Wild sum expansion, truncating the Wild series by a finite sum, and replacing all the high order terms by a Maxwellian [14].

Formally the scheme is justified by some property of the Wild sum coefficients. The replacement of particles with other sampled from Maxwellians is motivated by the objective of obtaining an efficient scheme even in situations in which standard Monte Carlo approach become particularly inefficient (for example when the Knudsen number is very small, and the particle distribution is near local thermodynamical equilibrium).

Several tests have been performed to validate TRMC schemes. In [14] results of fixed order (in time) TRMC methods are compared with results obtained by Nanbu-Babovsky method, for space homogeneous and one dimensional problems. In [16] computations are perormed of 2D flow around an ellipse. In both papers it is shown that for large Knudsen number the performance of the method is comparable to the Nanbu-Babovsky scheme, while for small Knudsen number TRMC schemes are able to obtain similar results at a much lower computational cost.

The original TRMC schemes, however, have some limitations, such as finite order of accuracy, and the fact that the particles replaced by a Maxwellian may not be close to equilibrium. A first attempt to extend the method to a scheme of infinite order in time has been performed by Pareschi and Wennberg [17], who constructed a scheme which recursively samples from the infinite Wild series. The truncation of the series can be performed at an arbitrarily high order. Their approach, however, does not take into account the collision history of the particles sampled from the different Wild sum coefficients.

This effect has been considered in a recent work by Pareschi, Trazzi and Wennberg [18], who use a recursive scheme which stops if the length of the collision history of a sampled particles (called the McKean graph [12, 13]) is too long, and replaces the particles by Maxwellian samples.

Recently, a new formulation of TRMC has been proposed by A.Shevyrin and G.Russo [21], which is based on rewriting the Wild sum expansion in terms of McKean graphs of given level $k$, each of which contributes to the formation of exactly $k+1$ particles which have undergone at least one collision. This new approach has the advantage that each McKean graph is exactly conservative, and therefore one can perform a simulation by sampling a certain number of independent McKean graphs. An account of the method is presented at this conference [21], and a more detailed description is given in [22].

## BASIC TRMC

Let us consider the Boltzmann equation in the form

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \frac{1}{\varepsilon} Q(f,f), \tag{1}$$

where $\varepsilon$ denotes the Knudsen number. The distribution function $f$ is represented by a collection of $N_{\text{tot}}$ particles each with its own velocity and position at a given time. We assume that a splitting scheme is used in the numerical solution of the equation: space is discretized in cells, and in the convection step (free flow) the particles move of constant velocity for a time step $\Delta t$. If they hit the boundary, suitable boundary conditions are applied. In the collision step, a space homogeneous equation is solved in each cell.

When the Knudsen number is very small, the distribution function approaches a local Maxwellian. In the limit $\varepsilon \to 0$, one could move the particles, during the convection step, and replace them by particles sampled from a Maxwellian with the same momentum and energy, during the collision step. Such a scheme, which can be considered a Monte Carlo implementation of a kinetic scheme for the numerical solution of the compressible Euler equation of gas dynamics, has been proposed by Pullin [19]. A more sophisticated version containing a similar idea has been recently proposed by Macrossan [9].

Here our goal is to construct a scheme that is able to solve the Boltzmann equation, and that will relax to Pullin's scheme in the limit of small Knudsen number.

From now on, we shall concentrate on the space homogeneous B.E.

## Wild sum expansion

We first consider Maxwellian molecules. More general kernels will be described later. The initial value problem for the space homogeneous B.E. for Maxwellian molecules can be written as

$$\frac{\partial f}{\partial t} = P(f,f) - \mu f \tag{2}$$

Here $P(f,f)$ is a positive, symmetric, bilinear operator, that represents a gain term, while $\mu$ (which is constant for Maxwellian molecules) is the coefficient of the loss term. Through a change of variables, it can be shown that the solution of (2) can be written in the form of a series, the so called *Wild sum* [23],

$$f(v,t) = (1-\tau) \sum_{k=0}^{\infty} \tau^k f_k(v), \tag{3}$$

where $\tau = 1 - \exp(-\mu t)$ is the *relaxed time*, and the coefficients $f_k(v)$ of the geometric series can be recursively computed as

$$f_k(v) = \frac{1}{k} \sum_{\ell=0}^{k-1} \frac{1}{\mu} P(f_\ell, f_{k-\ell-1}), \tag{4}$$

with $f_0(v) \equiv f(v, t=0)$.

The coefficients $f_k(v)$ have several interesting properties. For example they have the same mass, momentum and energy of $f_0$. This property relies on the definition of collision invariant, and on the bilinearity of $P$. In particular, $f_k(v)$ are nonnegative, because of the positivity of the operator $P$, and their integral in $v$ is equal to $\int f_0 \, dv$. If we normalize such integral to one, then $f_k$ may be interpreted as probability densities in $v$. Also, it can be shown that

$$\lim_{k \to \infty} f_k(v) = M(v),$$

where $M(v)$ is the Maxwellian with the same moments of $f_0$. This property suggests that a reasonable way to truncate the series would be to replace all remaining terms by a Maxwellian. This leads to the time-relaxed scheme of order $m$:

$$f^{n+1}(v) = (1-\tau) \sum_{k=0}^{m} \tau^k f_k(v) + \tau^{m+1} M(v) \tag{5}$$

where $\tau = 1 - \exp(-\mu\Delta t)$, $f_k$ are obtained from (4) with $f_0(v) = f^n(v)$, and $f^n(v)$ represents a numerical approximation of the solution at time $t^n$: $f^n(v) \approx f(v,t^n)$.

A generalization of such approximation may be written in the form

$$f^{n+1}(v) = \sum_{k=0}^{m} A_k(\tau) f_k(v) + A_{m+1}(\tau) M(v) \tag{6}$$

where the coefficients $A_k(\tau)$ satisfy suitable accuracy, conservation, and asymptotic preservation conditions [14]. In particular, $A_k$, $k = 0,\ldots,m+1$ are non negative and have unit sum, and $A_{m+1}(1) = 1$.

Note that the case $m = 0$ corresponds to the exact solution of the BGK approximation of the space homogeneous BE

$$\frac{\partial f}{\partial t} = \mu(M - f)$$

In a space non homogeneous problem, the time step $\Delta t$ of the collision step is determined on the basis of the so called CFL condition, which, roughly speaking, states that the fastest particles have to travel approximately one cell per time step. Once the convection time step $\Delta t$ has been chosen, in each cell one has to choose a suitable collision time step. If one uses a scheme which has no discertization in time, such as Bird's scheme [2] or Madjorant Frequency scheme [4], then the collision time step can be chosen equal to the convection time step. If the method has finite order in time, or if there are positivity restrictions on the time step, then the convection step is subdivided into a certain number of smaller collision time steps, determined by suitable accuracty and/or positivity conditions.

## TRMC methods

Monte Carlo methods follow from the probabilistic approximation of (6). Let us illustrate this with a first order scheme:

$$f^{n+1}(v) = A_0(\tau) f_0(v) + A_1(\tau) f_1(v) + A_2(\tau) M(v) \tag{7}$$

Because of their properties, the coefficients $A_k$ may be interpreted as probabilities, therefore, according to Eq. (7), in order to sample from $f^{n+1}(v)$, we

- sample from $f_0(v) = f^n(v)$ with probability $A_0$,
- sample from $f_1(v) = P(f_0, f_0)/\mu$ with probability $A_1$,
- sample from $M(v)$ with probability $A_2$.

If we have $N$ particles in our cell, Eq.(7) can be interpreted as follows. During time step $\Delta t$

- $NA_0$ particles remain unchanged
- $NA_1$ particles are obtained as the outcome of $NA_1/2$ collisions from original particles
- $NA_2$ particles are sampled from a Maxwellian with the same moments of $f_0$.

Note that the numbers $NA_k$ have to be suitably rounded to integers. The proper way to do it is described in [15].

A *naive* implementation of the method may loose strict conservation of momentum and energy, when sampling from $f_1(v)$ of from $M$. In order to make the selection from $f_1(v)$ exactly conservative, instead of sampling $NA_1$ particles, we sample $NA_1/2$ collision pairs, randomly selected among the possible $N(N-1)/2$ pairs. Strict conservation then follows from the conservation properties of binary collisions.

The sampling from $M$ can be performed as follows. We randomly select $NA_2$ particles, compute their moments, and sample $NA_2$ particles from a Maxwellian with such computed moments. This procedure, however, will give conservation only on average. In order to have exact conservation of the moments one could adjust the moments of the sample by an affine transformation on the sampled velocity, or, better, use a technique for random sampling from a Maxwellian with given moments of sampled particles. We use the latter technique, due to Pullin [20].

Second order TRMC methods can be constructed in a similar way. In this case the sampling from

$$f_2(v) = \frac{1}{\mu} P(f_0, f_1)$$

is obtained by sampling particles sampled from the original distribution $f_0$ and colliding them with particles sampled from $f_1$, i.e. with particles obtained as the outcome of a collision between particles sampled from $f_0$. Fixed order in time TRMC can be constructed in a similar way.

## Generalization to other collision kernels

With a slight modification, TRMC schemes can be used for other collision kernels, for example for the hard sphere molecules. The modification is the same used in standard Monte Carlo methods, when the pairs are chosen uniformly, dummy collisions are performed, and rejection is used to decide whether a dummy collision is a real collision.

Consider a Boltzmann equation for a general kernel

$$\frac{\partial f}{\partial t} = Q_+(f,f) - \tilde{\mu}(v) f(v),$$

where the coefficient of the loss term, now, depends on the velocity.

If we denote by $\mu \geq \tilde{\mu}(v)$ a bound on such coefficient, we can write the equation as

$$\frac{\partial f}{\partial t} = P(f,f) - \mu f,$$

where $P(f,g) = Q_+(f,g) + \frac{1}{2}(\mu - \tilde{\mu}(v))(f+g)$ is a positive, symmetric, bilinear operator. Sampling from $f_1(v) = P(f_0,f_0)/\mu$ means to perform a dummy collision. If the collision is accepted, then it is a real collision i.e. we are sampling from $Q_+$, while if it is rejected then the particles will remain unchanged, i.e. we are sampling from $f_0$. Note that this approach can be used even if the function $\tilde{\mu}(v)$ is unbounded. In the case of hard spheres, for example, the only thing which is needed in order to perform the rejection, is a bound on the relative cross section between all pairs of particle: $\sigma_{ij} = k|v_i - v_j|$, which can be obtained, for example, by

$$|\sigma_{ij}| \leq \Sigma = 2k \max_j |\bar{v} - v_j|, \quad \bar{v} = \frac{1}{N}\sum_{j=1}^{N} v_j$$

Then the parameter $\mu$ is given by $\mu = 4\pi\Sigma\rho$, where $\rho$ is the mass density.

# NUMERICAL RESULTS AND COMPARISON WITH OTHER METHODS

Here we report some numerical results obtained by TRMC schemes on test problems. We write the Boltzmann equation as

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \frac{1}{\varepsilon} Q(f,f)$$

and we are interested in the performance of the method for very small values of $\varepsilon$.

## Validation tests

TRMC schemes have been compared with several other numerical methods for the B.E. Comparison with Nanbu-Babovsky scheme [10] [11] is reported in [14] for space-homogeneous problems, and for shock profile computation, and in [16] for 2D flow past an ellipse.

It is shown that for very small values of $\varepsilon$, TRMC schemes provide a numerical solution comparable to the one obtained by Nanbu-Babovsky scheme, at a much lower computational cost.

We report here the results of the flow past an ellipse performed by the NB scheme and TRMC schemes of order 1 and 2 [16]. As an example we show the contour plot of the density, for Mach $Ma = 5$, for $\varepsilon = 0.001$, obtained with NB and TRMC2 scheme.

It is evident that the two results are comparable. For TRMC schemes the collision time step has been chosen 1/5 of the free flow time step, while for the NB scheme the collision time step has to satisfy a positivity condition that becomes more and more stringent as the Knudsen number decreases. Several tests are performed, using $Ma = 5, 10, 20$, and $\varepsilon = 0.1, 0.01, 0.001$. The total number of "collisions" per convection time step is reported in Figure (2).

It is evident that the gain in computational time becomes more evident when the Knudsen number is decreased.

A detailed comparison with he well-established Madjorant Frequency Scheme (MFS) [4] is performed in [6] for the space homogeneous problem, and in [7] for one dimensional Couette flow.

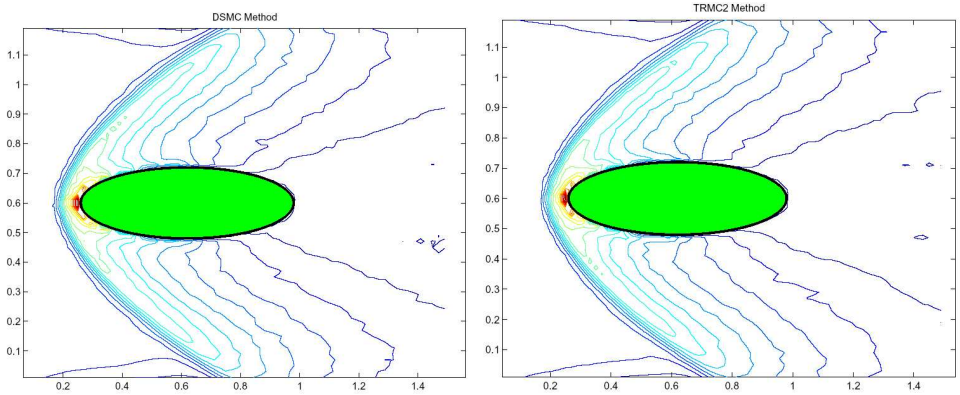


**FIGURE 1.** Density contour plot obtained by NB scheme (left) and TRMC2 (right) for Mach $Ma = 5$ and $\varepsilon = 0.001$ [from [16]]

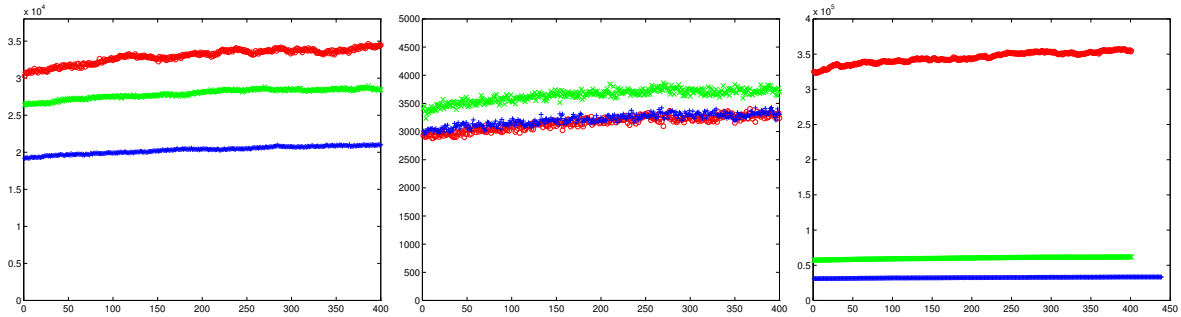

**FIGURE 2.** 2D flow: Number of "Collisions". From left to right $\varepsilon = 0.1, 0.01, 0.001$; NB ($\circ$), TRMC1 ($+$), TRMC2 ($\times$).

A comparison between TRMC and various other methods for the solution of the B.E. in the case of a shock arising from Argon reflecting on a wall is presented in [8]. In this paper the purpose was to compare different numerical tools (including molecular dynamics) with the results of an actual experiment.

The overall results of the comparison is that TRMC schemes provide similar results of other methods, at a comparable cost, when the Knudsen number is not too small, and at lower cost when the Knudsen number is decreased.

The correct choice of time step is in its own an interesting problem. Roughly speaking, in TR schemes the collision time step is chosen large (say equal to the convection time step) in regions of very large or very small Knudsen number, while in intermediate regions it is chosen a fraction of the convection time step. A discussion on the choice of the time step for TR time discretization applied to a deterministic scheme for the solution of the Boltzmann equation is presented in [3].

## RECURSVIVE AND ADAPTIVE TRMC

The Wild sum has itself a probabilistic interpretation, and can be used directly to construct a Monte Carlo method. Such a method would be based on sampling from the exact solution of the space-homogeneous problem, and therefore it would have no time discretization error (for the collision step, of course).

A *naive* implementation of the method is obtained as follows:

- sample an integer $k$ according to a geometric distribution $(1-\tau)\tau^k$
- sample from $f_k(v)$

The latter is obtained from the recursive definition of $f_k(v)$:

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if k = 0
    sample from f_0(v)
else
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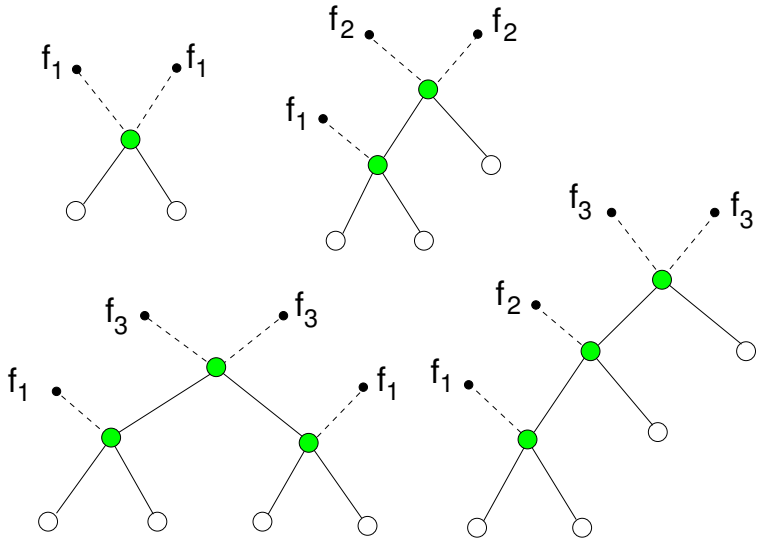


**FIGURE 3.** McKean graphs needed to sample from $f_1$, $f_2$, and $f_3$. There are two equivalent graphs corresponding to $f_2$. The one shown is the one corresponding to $(G_1, G_0)$, the other is symmetric, and corresponds to $(G_0, G_1)$. Similarly, there are three graphs generating $f_3$, nalemy $(G_1, G_1)$ (lower left), $(G_2, G_0)$ (lower right), and $(G_0, G_2)$, which is equivalent to $(G_2, G_0)$, therefore we say that there are two graphs generating $f_3$, occurring with probability, respectively, 1/3 and 2/3

∘ select an integer $\ell$ uniformly in $[0, \dots, k-1]$
sample $v'$ from $f_\ell(v)$
sample $v'_*$ from $f_{k-\ell-1}$
perform collision between $v'$ and $v'_*$, and take $v$ as one of the output particles.
`end if`

Such a method, however, is not exactly conservative, and it is very inefficient. A better implementation is obtained by sampling pairs. Given $N$ particles, compute an integer $N_k$ of pairs needed at level $k$. $N_k$ is a random integer whose expectation value $< N_k >$ equals $\bar{N}_k \equiv N(1-\tau)\tau^k/2$.

Let $m$ be the maximum integer for which $N_k > 0$. The quantity $2N_{m+1} = N - 2\sum_{k=0}^{m} N_k$ will determine the number of particles that need to be sampled from a Maxwellian. We do not discuss here the technical points involved in performing such sampling.

Once the number $N_k$, $k = 1, \dots, m+1$ are computed, then one recursively samples pairs of particles from $f_k$, starting from $k = m$, and decreasing $k$ up to $k = 1$. Finally one samples $2N_{m+1}$ particles from Maxwellian, if $N_{m+1} > 0$.

When generating a particle from level $k$, several other particles are generated. The collision history obtained to generate a pair at a given level is clearly represented by a McKean graph of level $k$. For example, Figure 3 represents all the McKean graphs of level 1, 2, and 3, needed for generating particles of level 1, 2, and 3.

So, if we want to generate a particle pair from level 3, we shall perform exactly three collisions, and we shall generate some additional particles at level 1 (and maybe at level 2, if the collision history corresponds to the lower right graph. 3.

In practice, when sampling from a level $k$, one actually samples from a random McKean graph of level $k$, obtaining in addition to the two particles from level $k$, $k-1$ particles at lower levels.

Such particles can be stored in a list, and then used when particles from lower levels are needed. An algorithm based on this idea has been proposed by Pareschi and Wennberg [17]. Such algorithm has however the drawback that the expected number of particles generated in this way is slightly biased.

A different algorithm has been proposed by Russo and Shevyrin, and presented to this conference [21]. The method is based on sampling McKean graphs. Let us denote by $G^k$ a vector whose elements represent the average number of particles produced by a randomly generated McKean graph of degree $k$ (the components of $G^k$, denoted $g_i^k$, $i = 1, \dots, k$, are nonnegative numbers, with $\sum_{i=1}^{k} g_i^k = k+1$), then one could try to sample from the geometric distribution $(1-\tau)\tau^k$

by representing such distribution as a linear combination of McKean graphs:

$$\sum_{\ell} C_\ell g_k^\ell = (1-\tau)\tau^k \tag{8}$$

If the coefficients $C_\ell$ are non negative, then one can use the probabilistic interpretation of (8) and sample from the McKean graph $G^k$ with probability proportional to $C_k$. In this case there is no need to use particles generated at a given level in order to produce particles at other levels.

In [21] it is shown that such an approach gives an unbiased sample for the exact solution. However, the coefficients $C_k$ obtained by solving Eq.(8) are nonnegative only for $\tau \leq 2/3$, which gives a limitation on the time step which is not very different from the limitation imposed by the positivity requirement of Nanbu-Babovsky scheme.

In order to overcome this limitation, an improvement is proposed in [21], which makes use of existing particles in the generation of new particles with a given probability. Such improvement allows to reach larger values of the time step, still providing an unbiased distribution of particles.

## The truncation problem

In regions of small Knudsen number, the convection time step is much larger than mean collision time, resulting in a large value of $\mu\Delta t$, and therefore a value of $\tau$ very close to 1. In such case, the geometric distribution decays very slowly, and it is likely to sample from $f_k$ with a large value of $k$, which requires $k$ collisions. It is therefore desirable to replace $f_k$ by Maxwellian, if $k$ is large enough.

Now, even if $f_k \to M$ as $k \to \infty$, such convergence is rather slow. The reason is that for a given level $k$, there are McKean graphs that produce particles closer to equilibrium and other which produce particles far from equilibrium. Consider, for example, the two graphs of level seven shown in Figure 3 of paper [21] in the same proceedings. The graph on the left is well balanced, and all particles involved in the production of the two particles of level 7 underwent three collisions, while in the case of the right the collision that generated the two particles of level 7 involved one particle which never collided before. We therefore expect that while it may be a reasonable approximation to assume that the particles generated by the graph on the left lost memory of their initial condition, and therefore their distribution may be close to a Maxwellian, this assumption is much riskier in the case of the graph on the right. When checking whether a particle is close to equilibrium, one should therefore take into account the whole collision history, rather than just the level of the McKean graph. Several attempts have been made in trying to decide what particles can be replaced by Maxwellian distribution. One of the first papers that discusses this problem is [1]. One technique consists in defining an effective length of the McKean graph, which takes into account how strongly the graphs is unbalanced. Possible indicators are defined recursively 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 $\ell$ and $r$. Then three different indicators $L_1, L_2, L_3$ are recursively defined as

$$L_1(G_i^k) = 1 + \min(L_1(G_{i_\ell}^\ell), L_1(G_{i_r}^r)) \tag{9}$$

$$L_2(G_i^k) = 1 + \text{mean}(L_2(G_{i_\ell}^\ell), L_2(G_{i_r}^r)) \tag{10}$$

$$L_3(G_i^k) = 1 + \text{hmean}(L_3(G_{i_\ell}^\ell), L_3(G_{i_r}^r)) \tag{11}$$

and, for all definitions, $L_j(G^0) = 0$, $j = 1, \ldots, 3$. Here $\text{mean}(x,y) = (x+y)/2$ is the arithmetic mean, and $\text{hmean}(x,y) = 2xy/(x+y)$ is the harmonic mean. Carvalho, Carlen and Gabetta in [1] propose the use of $L_1$, while Pareschi, Trazzi and Wennberg in [14] propose the use of $L_2$. In paper [21] we propose the use of indicator $L_3$, which appears to be more natural to incorporate replacement of certain subgraphs by Maxwellians.

In [18] the authors propose an algorithm which is based on a recursive call for the sampling of $f_k$. First the effective length ($L_1$ or $L_2$) of the sampled McKean graph is computed. If the length is less than a prescribed critical value, then all predicted collisions corresponding to the generated graph are actually performed, otherwise, the two particles from $f_k$ are marked as being sampled from a Maxwellian. At the end of the loop on $k$, the marked particles are sampled from Maxwellian.

A different technique, which combines sampling from McKean graph with sampling from Maxwellians is presented in [21] in this conference.

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