Simulation of rarefied gas flows by Improved TRMC method

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Abstract. We present some recent numerical results on Time Relaxed Monte Carlo (TRMC) methods, which is a Monte Carlo technique for the numerical solution of the Boltzmann equation (BE). The Improved Time Relaxed Monte Carlo is based on the direct sampling from McKean graphs. Such approach is tested for the solution of spatially homogeneous and non-homogeneous classical problems. A comparison with the analytical BKW solution of the BE for Maxwellian molecules is performed. The effect of the time step size for ITRMC method and replacement of selected collisions by sampling from Maxwell distribution is investigated. The new scheme is tested by computing the numerical solution of one dimensional Couette flow, in a regime near the fluid dynamic limit. As the reference solution the time-proved majorant frequency scheme of the DSMC was used for Couette flow.

Keywords: Boltzmann equation, Time Relaxed methods, McKean graphs

INTRODUCTION

The present paper contains numerical results by improved TRMC method (ITRMC) while the theoretical bas of the method can be found in [1]. The main idea of ITRMC is sampling from McKean graphs G_ℓ with replacement of well balanced graphs by Maxwellians. We assume that a splitting scheme is used, with alternation of collision and convection steps, therefore we describe the method only for homogeneous BE.

Description of algorithm. Here we follow the notation in [1]. Before starting simulation, we perform the following preprocessing steps:

- Define TRMC parameter $\tau = 1-\exp(-\mu\Delta t)$ from estimate μ and define maximum level m (that depends on the number of particles N and τ), here Δt is time step.
- Perform selection of well-balanced graphs, calculate coefficients g_ℓ^k.
- Compute number of graphs C_ℓ on the level $\ell = 1,\dots,m$ from equations $\sum_{k=1}^m C_k g_\ell^k = N(1-\tau)\tau^\ell$.
- For levels $\ell \le \ell_0$ with negative coefficient C_ℓ, compute probability of reusage p_ℓ.

Correction of the method using *reusage teqnique* will lead to the change of number of molecules in levels, hence, the coefficients C_ℓ need to be corrected as described in [1] befor simulation. Then transition from time t_n to time t_{n+1} ($\Delta t = t_{n+1}-t_n$) can be presented as follows. Starting from maximum level $\ell = m,\dots,\ell_0+1$ we realize C_ℓ McKean graphs of level ℓ recursively, as follows

- select h uniformly in $[0,\ell-1]$
- if $h=0$ sample from the original distribution $f^n(v)$
- if $C_h > 0$ sample v' recursively from McKean graph of level h
- if $C_h < 0$ (i.e. $h \le \ell_0$) then use a stored particle at level h (if it exists) with probability p_h, otherwise generate a McKean graph of level h.
- if $\ell-h-1=0$ sample from the original distribution $f^n(v)$
- if $C_{\ell-h-1} > 0$ sample v'_* recursively from McKean graph of level $\ell-h-1$
- if $C_{\ell-h-1} < 0$ then use a stored particle at level $\ell-h-1$ (if it exists) with probability $p_{\ell-h-1}$, otherwise generate a McKean graph of level $\ell-h-1$.
- collide molecules $(v', v'*)$ obtaining (v, v_*), and store v_* in the list of molecules of level ℓ

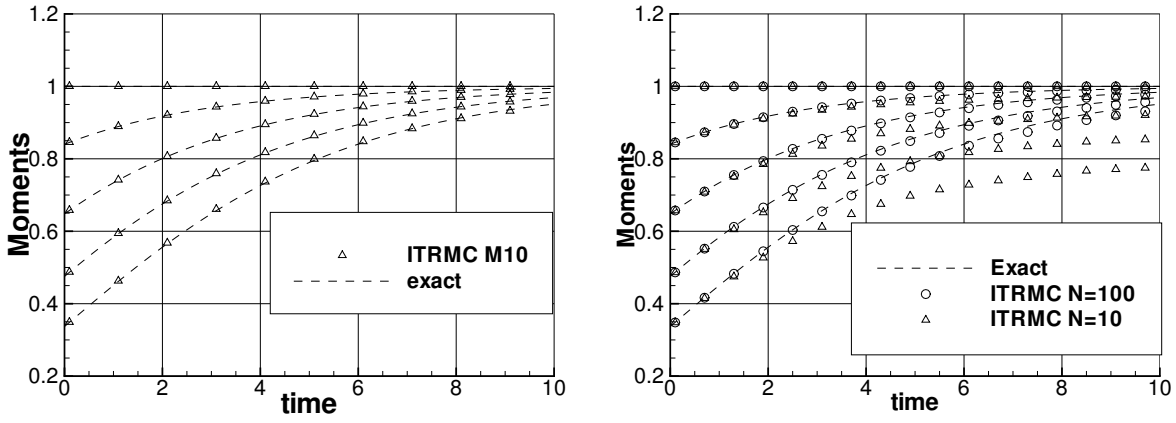

FIGURE 1. Lines from top to bottom: M_2, M_4, M_6, M_8 and M_{10}. Left: $N = 1000$. Right: $N = 100$ and $N = 10$. Time step $\Delta t = 0.1$.

COMPARISON WITH BKW-SOLUTION

For Maxwell molecules the exact solution for space homogeneous Boltzmann is available. This Bobylev-Krook-Wu (BKW) solution takes the expression [3], [4]

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

where $C = C(t) = 1 - \frac{2}{5}\exp(-t/6)$. The solution is defined for $t \geq 0$.

The analytic representation of the even moments $M_{2k} = \int_0^\infty v^{2k} f_r(v,t) dv$ of the radial distribution function $f_r(v,t) = 4\pi v^2 f(\mathbf{v},t)$ is

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

A comparison of the calculated even moments with BKW solution of the Boltzmann equation is shown in figure 1. Moments are normalized with the theoretical value of moments in $t \to \infty$: $M_{2k} = (2k+1)!!/2^k$. For large number of simulated molecules $N = 1000$ (left plot) there is excellent agreement between analytical values of even moments and calculated moments. Smaller number of molecules (case $N = 100$, circles on right plot of figure 1) allows to obtain solution of the Boltzmann equation only for time $t \lessapprox 5$. For $t > 5$ high order moment M_{10} differs from analytical result. ITRMC simulations with $N = 10$ allow to obtain correct result only for $t < 2$ because deviation from analytical solution become significant already for $t > 2$.

Effect of time step size

Since the decisive parameter for TRMC methods $\tau = 1 - \exp(-\mu\Delta t)$ depends on Δt, it is important to determine the validity of using large time steps. In the figure 2 we present the behavior of moments for different time steps. The simulations with $N = 100$ (left plot in Fig. 2) allow to use $\Delta t = 1$, while for $\Delta t = 2$ there is an observable deviation of the moment behavior from BKW solution. The usage of $\Delta t = 1$ for $N = 10$ (Fig. 2, right) leads to large deviation for M_{10} already after first time iteration (for $t = 1$). Consequently, the numerical solution for large Δt depends on the number of simulated molecules N: for small N TRMC method is more sensitive to the large time step. In practice, Δt can be slightly larger then $1/\mu$ (μ is collisional frequency).

We conclude that the finite number of particles is responsible for two different sources of approximation: the first is due to particle correlations, and persists even for small time steps; the second is due to the truncation of the Wild sum expansion; this effect vanishes as $\Delta t \to 0$.

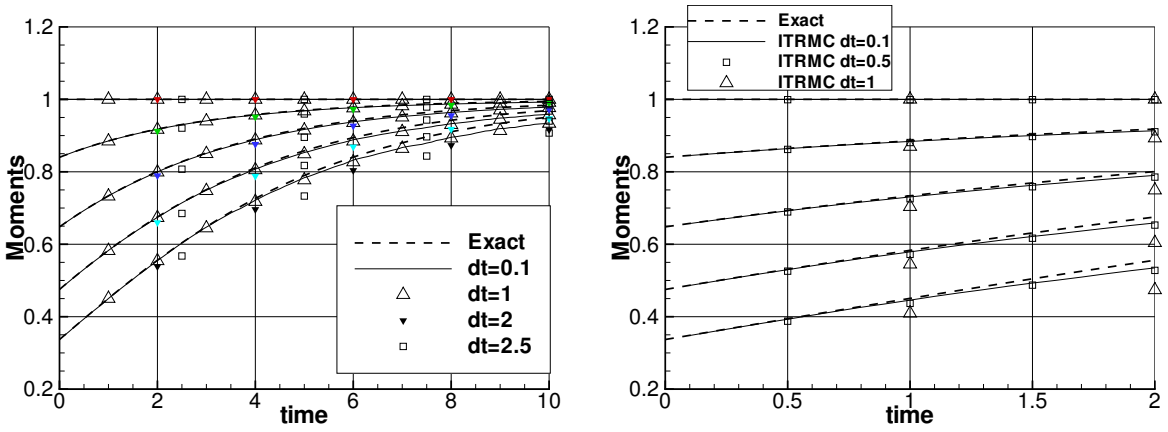

FIGURE 2. Left: Cases with $N = 100$. Right: Cases with $N = 10$.

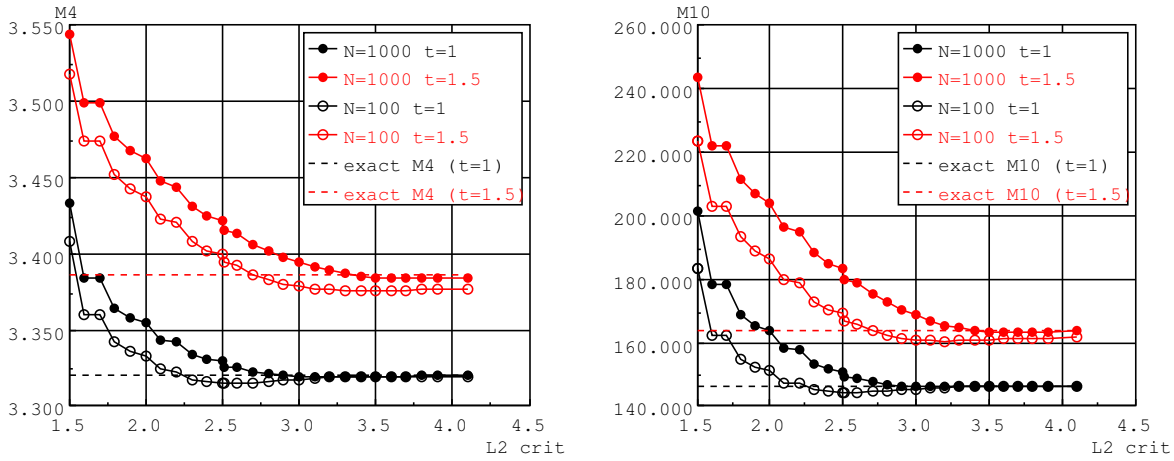

FIGURE 3. M_4 and M_{10} versus L_{2crit}

Redistribution by Maxwell distr. function

If a particle has a long collision history (this depends on some effective length of the corresponding McKean graph that generates the particle), then the particles is sampled from a Maxwellian. We study the effect of the error introduced by this approximation. For a McKean graph constructed by sub-graphs **A** and **B**, this parameter is recursively defined as $L_2 = 1 + (L_2(A) + L_2(B))/2$ [1]. The condition for replacement of a particle obtained by a graph by a particle sampled from Maxwellian is $L_2 \geq L_{2crit}$. The smaller L_{2crit} the more replacements are performed.

For four cases of particle number and final time t, the evolution of the moments of distribution function M_4 and M_{10} for different value L_{2crit} is considered. The solution was obtained using single step $\Delta t = t$. Here we used $\mu = 1$. The moments values for case of large L_{2crit} (all collisions are performed) are presented in the following table:

time	N	ITRMC M_4	MFS M_4	Exact M_4	ITRMC M_{10}	MFS M_{10}	Exact M_{10}
1	1000	3.3200	3.3199	3.3201	146.34	146.31	146.36
1	100	3.3198	3.3194		146.34	146.13	
1.5	1000	3.3847	3.3857	3.3861	163.64	163.80	163.93
1.5	100	3.3771	3.3848		161.66	163.47	

Results of the computations with varying L_{2crit} are presented in figure 3. It could be seen from the behavior of M_4 and M_{10} on L_{2crit} that

- the effect of replacement of collisions with redistribution is small for arbitrary large L_{2crit}, while for small L_{2crit} the deviation becomes more pronounced;
- smaller number of particles $N = 100$ allows to perform calculations with smaller parameter L_{2crit} (large fraction of redistributed molecules instead of collisions);
- large time step $\Delta t = 1.5$ requires more accurate choice of parameter L_{2crit} in comparison with smaller $\Delta t = 1$.

Note, that there is a value of parameter L_{2crit} for which all moments are approximately equal to exact values even for $N = 100$. It means that the distribution function becomes closer to the exact one.

COUETTE FLOW

In this part of the paper applicability of ITRMC method to spatially non-uniform gas flows studied in the case of plane Couette flow between two parallel plates.

This problem was considered in the following statement. Two plates are kept in temperature $T_w = 300$ K. Distance between plates is 1 m. Left plate is stationary ($V_1 = 0$) and the other one moves in its own plane with velocity $V_2 = 1766$ m/s. The x-axis is directed perpendicular to walls, and the y-axis is in the direction of the motion. The space between plates is filled with monoatomic gas of average density $n_0 = 1.3442 \cdot 10^{20} m^{-3}$. Mass of gas molecule is $m = 6.64 \cdot 10^{-26}$ kg which corresopnds to Argon. For simulation of collisions between molecules, the approxmation of Maxwellian molecules was used, the effective diameter for $T_{ref} = 300$ K is $d_{ref} = 4.0679 \cdot 10^{-10}$ m (the collisional frequency can be estimated as $\mu = 4 d_{ref}^2 n \sqrt{2kT_{ref}/m} = 3.8513 \cdot 10^4$ s^{-1}). When stationary flow was reached, the usual estimation of the macro-parameters in samping cells was performed.

The dimensionless parameters for the problem are the Knudsen number Kn and the ratio S of wall velocity to temperature velocity of molecules. For the given parameters, the Knudsen number calculated at temperature 300 K and density n_0 were $\mathrm{Kn}_{T=300K,n_0} = 0.01$ and velocity ratio $\mathrm{S} = V_2/\sqrt{2kT_w/m} = 5$.

The collisional cells size was varied through computational domain from $\Delta x = 0.002$ m near walls (where the temperature is low and hence density is higher then in center) to $\Delta x = 0.005$ m in the central area.

The reference solution was obtained using Majorant Frequency Scheme (MFS) of DSMC method, which in the limit of infinite number of simulated molecules can be treated as numerical solution of Boltzmann equation [2]. ITRMC result is compared with MFS for Couette flow and then the effect of redistribution by Maxwellians studied for different critical values of the parameter L_2.

Simulation of Couette flow was perfomed by ITRMC method and MFS. In both simulations time step size was $\Delta t = 10^{-6}$ s corresponding to $\tau = 6.785 \times 10^{-2}$, and the number of simulated molecules was $N = 5000$. Notice that with such parameters MFS scheme produces very accurate solutions [2].

The velocity and temerature profiles are presented in the figure 4. The temerature value at the center is equal 841 K (right plot on figure 4). This strong heating of the gas is caused by high velocity of the right wall (figure 4, left). As shown in both plots MFS and ITRMC produce similar profiles. The heat flux S_x is function of higher order moment of the distribution function. The functions of high-order moments are more sensitive to parameters of the simulations, however the S_x-profile obtained by ITRMC is almost similar to the reference one, obtained by MFS (see figure 5, left). In Couette flow in transitional and free-molecular regimes there is a component of heat-flux, parallel to the plates. This component is not described in the framework of Navier-Stokes equations. As follows from the profile of parallel component S_y in figure 5 (right) the value of S_x is about three times larger then S_y component, wich means that the flow with used parameters is in strong non-equilibrium.

Hence, in the example of Couette flow it is shown that the ITRMC method can produce results close to the solution of the Boltzmann equation for spatially non-homogeneous case. However, the sensitivity of the solution to the calculational parameters showld be studied. ITRMC method in comparison with traditional DSMC method like MFS has not only parameters such as N, Δt and Δx, but also the parameter of the truncation of L_{crit}. The dependence of deviation of solution on L_{crit} showld be studied additionally.

As was shown for the homogeneous case (figure 2), redistribution by Maxwell distribution in case of comparatively large Δt with suitable parameter L_{2crit} in principle can lead to an accurate numerical solution, just as in the case without redistribution. To check this we perform calculations with the same parameters (τ and L_{2crit} values) as was established for the homogeneous case. Comparison of most sensitive profiles for cases $L_{2crit} = 2$ and $L_{2crit} = 2.7$, $\Delta t = 10^{-5}$ s and

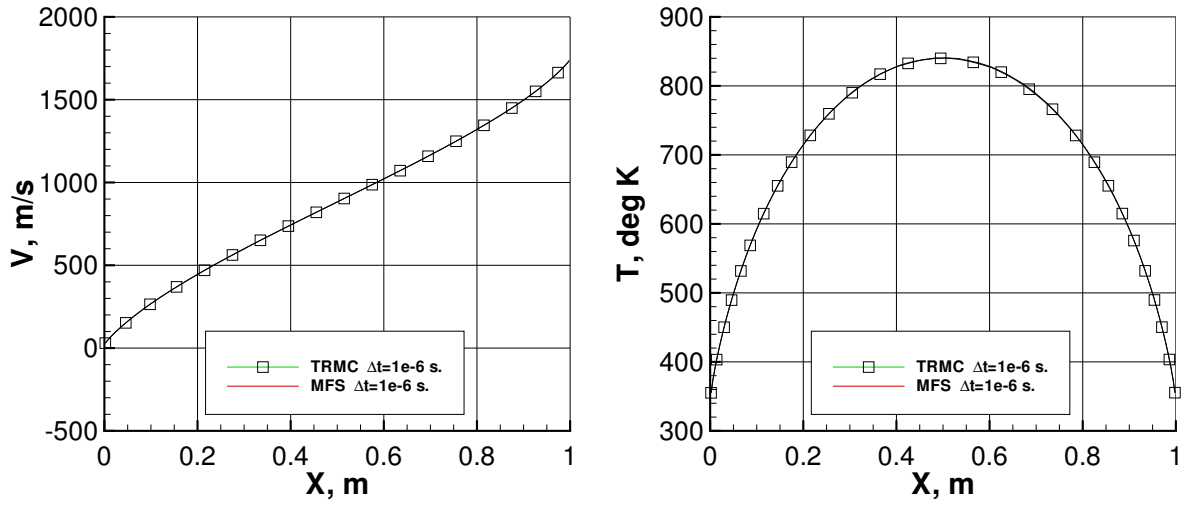

FIGURE 4. Velocity and temperature profiles for MFS and ITRMC methods.

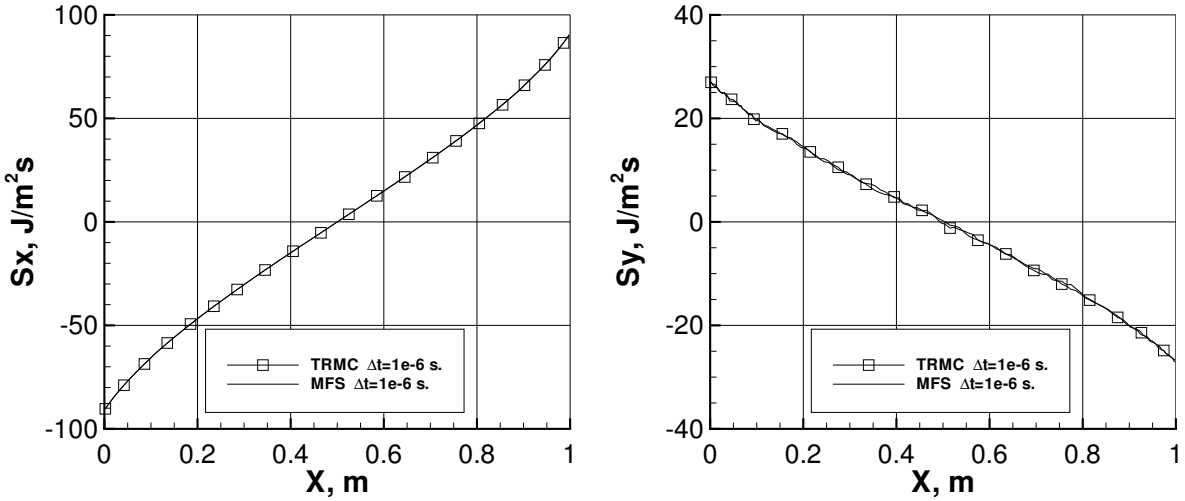

FIGURE 5. Heat flux and parallel heat flux profiles for MFS and ITRMC methods.

case $\Delta t = 10^{-5}$ s without redistribution are presented in the figure 6. It can been seen from figure, that there is only a small difference between cases $\Delta t = 10^{-6}$ and $\Delta t = 10^{-5}$ for both temperature and heat flux profiles.

For Couette flow, shear stress components P_{xx} and P_{xy} are constant over area. Calculation of P_{xx} and P_{xy} was made on the wall by summation of incident and reflected molecules momentum $m\mathbf{v}$. The values of P_{xx} and P_{xy} are presented in the following table:

Method	$\Delta t \cdot 10^6$,s	redistr.	P_{xx},kg/ms^2	P_{xy}	redistributed, %
MFS	1	–	1.2493	-0.10758	–
ITRMC	1	no	1.2493	-0.10758	0
ITRMC	10	no	1.2519	-0.11141	0
ITRMC	10	$L_{2crit} = 2.7$	1.2516	-0.11083	0.35
ITRMC	10	$L_{2crit} = 2$	1.2496	-0.11053	6.22

The fraction of replaced collisions is presented in the last column. The values of P_{xx} and P_{xy} for the case $\Delta t = 10^{-5}$ s

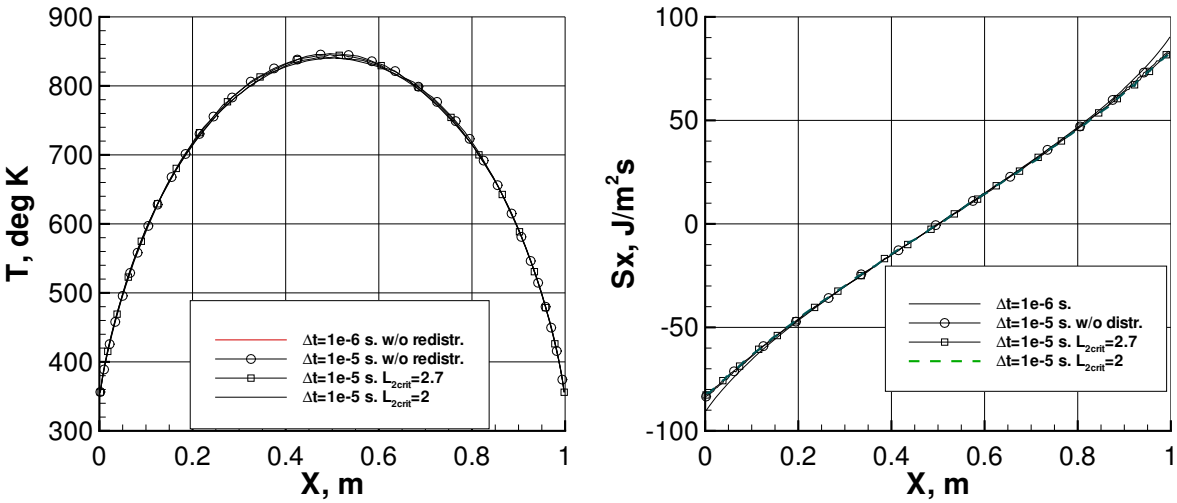

FIGURE 6. Calculations with redistribution.

and $L_{2crit} = 2.7$ are closer to the solution of the Boltzmann equation (MFS result) then without replacement by redistribution. It points to existence of the optimal value for L_{2crit} parameter for Couette flow.

CONCLUSION

The proposed ITRMC method for modeling of the rarefied gas flows in case of small time step produces results very close to the solution of the Boltzmann equation for homogeneous case as well as for spatially one-dimensional flow. The new approach has the potential of providing more efficient codes. The efficiency of the proposed method has still to be verified.

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