Time Relaxed Monte Carlo methods for the Boltzmann equation

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Abstract

A new family of Monte Carlo schemes is introduced for the numerical solution of the Boltzmann equation of rarefied gas dynamics. The schemes are inspired by the Wild sum expansion of the solution of the Boltzmann equation for Maxwellian molecules, and consist in a novel time discretization of the equation. In particular, high order terms in the expansion are replaced by the equilibrium Maxwellian distribution. The two main features of the schemes are high order accuracy in time and asymptotic preservation. The first property allows to recover accurate solutions with time steps larger than those required by Direct Simulation Monte Carlo, while the latter guarantees that for vanishing Knudsen number, the numerical solution relaxes to the local Maxwellian. Conservation of mass, momentum and energy are preserved by the scheme. Numerical results on several space homogeneous problems show the improvement of the new schemes over standard DSMC. Applications to a one-dimensional shock wave problem are also presented.

1 Introduction

When a gas is near thermodynamical equilibrium, a detailed kinetic description is unnecessary, and the evolution of the moments can be described by Euler or Navier-Stokes equations. From a computational point of view, these equations are much less expensive than the full Boltzmann equation.

Far from thermodynamic equilibrium, the equation of gas dynamics do not give a satisfactory description of the physical system, and the full kinetic description is necessary.

The departure from local thermodynamic equilibrium can be measured by the so called Knudsen number, which is the ratio between the collisional mean free path of the molecules and the characteristic length of variation of macroscopic variables. When the Knudsen number is small, then the distribution function is close to the local Maxwellian. Collisions occur at a fast rate, and a kinetic treatment of the system is very expensive, because of the large ratio of time scales between macroscopic and microscopic effects. One may say that the system is numerically *stiff* [8]. Because of the stiffness, standard explicit schemes for the numerical solution of the Boltzmann equation become extremely expensive in this case.

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If the Knudsen number is uniformly small in the region one is interested in, then one should use a gas dynamic description of the system. There are several circumstances, however, where the Knudsen number varies over several orders of magnitude. In such cases a standard kinetic treatment would be too expensive, and a pure gas dynamic approach inappropriate. Domain decomposition methods have been proposed for this problem, in which the computational domain is divided into an *aerodynamic region* in which the system is treated by gas dynamic equations (Euler or Navier-Stokes), and a *Boltzmann region*, where a kinetic treatment is used. Suitably boundary conditions make the two regions coupled together [3]. Such schemes can be very effective in treating large scale problems, but they are quite complicated to implement, and they require a great care by the user.

In some recently developed Monte Carlo methods a different approach is taken, with the goal of constructing simple and efficient numerical methods for the solution of the Boltzmann equation in regions with a large variation in the mean free path [13, 12].

These algorithms are based on a suitable time discretization of the Boltzmann equation, first introduced in [7], which has the following properties: for large Knudsen number it is a time discretization of the Boltzmann equation of a given order, and when the Knudsen number vanishes, the numerical solution tends to the local Maxwellian. We will call this last property *asymptotic preservation*. In addition the time discretization preserves mass, momentum and energy.

Although the paper deals mainly with the space homogeneous case, the real motivation for the development of these Monte Carlo methods is their use for spatially dependent problems. In that case, standard splitting can be used, and the evolution of the system is obtained by alternating a collision step, which is space homogeneous in each space cell, and a convection step, which describes the free flow of the molecules. In the limit of very small Knudsen number, the collision step replaces the distribution function by a local Maxwellian with the same moments. A Monte Carlo method based on such time discretization will behave as a sort of stochastic kinetic scheme for the underlying Euler equations of gas dynamics. Such limit scheme was introduced by Pullin [15].

The plan of the paper is the following. In the next section we give a short introduction on the Boltzmann equation and some of its relevant properties. In Section 3 we introduce the Time Relaxed discretizations, starting from the Wild sum expansion, and making use of some of its properties. Section 4 is devoted to the derivation of Monte Carlo Methods based on TR discretization (TRMC). The section starts with a review of DSMC, in particular of the Nanbu-Babovsky scheme, which is revisited, and reinterpred in a new light. A detailed description is given of TRMC algorithms. In the last section we show some numerical tests performed with the new schemes. In particular, it is shown that it is possible to obtain the same accuracy of the Nanbu-Babovsky scheme, with a lower computational cost. We conclude the paper with a plan of future extensions and improvements.

2 Time discretizations of the Boltzmann equation

2.1 The Boltzmann equation

We consider the Boltzmann equation [5]

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

supplemented with the initial condition

$$f(x,v,t=0) = f_0(x,v), \tag{2}$$

where $f = f(x,v,t)$ is a non negative function describing the time evolution of the distribution of particles which move with velocity v in the position x at time $t > 0$. The parameter $\varepsilon > 0$ is the Knudsen number and is proportional to the mean free path between collisions. The bilinear collision operator $Q(f,f)$ describes the binary collisions of the particles and is given by

$$Q(f,f)(v) = \int_{I\!R^3} \int_{S^2} \sigma(|v - v_1|, \omega)[f(v')f(v'_*) - f(v)f(v_*)]\, d\omega\, dv_*. \tag{3}$$

In the above expression, ω is a unit vector of the sphere S^2, so that $d\omega$ is an element of area of the surface of the unit sphere S^2 in $I\!R^3$. Moreover (v', v'_*) represent the post-collisional velocities associated with the pre-collisional velocities (v, v_*) and the collision parameter ω; i.e.,

$$v' = \frac{1}{2}(v + v_* + |v - v_*|\omega), \quad v'_* = \frac{1}{2}(v + v_* - |v - v_*|\omega). \tag{4}$$

The kernel σ is a nonnegative function which characterizes the details of the binary interactions. In the case of inverse k-th power forces between particles the kernel has the form

$$\sigma(|v - v_*|, \theta) = b_\alpha(\theta)|v - v_*|^\alpha, \tag{5}$$

where $\alpha = (k-5)/(k-1)$. For numerical purposes, a widely used model is the Variable Hard Sphere(VHS) model [2], corresponding to take $b_\alpha(\theta) = C_\alpha$ where C_α is a positive constant. The case $\alpha = 0$ is referred to as the Maxwellian gas, whereas the case $\alpha = 1$ yields the Hard Sphere gas.

2.2 Fluid-dynamical limit

During the evolution process, the collision operator preserves mass, momentum and energy, i.e.,

$$\int_{I\!R^3} Q(f,f)\phi(v)\, dv = 0, \quad \phi(v) = 1, v, v^2, \tag{6}$$

and in addition it satisfies Boltzmann's well-known H-theorem

$$\int_{I\!R^3} Q(f,f) \log(f) dv \leq 0. \tag{7}$$

From a physical point of view, Boltzmann's H-theorem implies that any equilibrium distribution function, i.e. any function f for which $Q(f,f)=0$, has the form of a locally Maxwellian distribution

$$M(\rho,u,T)(v)=\frac{\rho}{(2\pi T)^{3/2}}\exp\left(-\frac{|u-v|^2}{2T}\right), \tag{8}$$

where ρ, u, T are the density, mean velocity and temperature of the gas defined by

$$\rho=\int_{\mathbf{R}^3} f\,dv, \qquad u=\frac{1}{\rho}\int_{\mathbf{R}^3} vf\,dv, \qquad T=\frac{1}{3\rho}\int_{\mathbf{R}^3}[v-u]^2 f\,dv. \tag{9}$$

As $\varepsilon\to 0$ the distribution function approaches the local Maxwellian (8). In this case the higher order moments of the distribution f can be computed as function of ρ, u, and T, by using (8) and we obtain to the leading order the closed system of compressible Euler equations of gas dynamics

$$\begin{aligned}
&\frac{\partial\rho}{\partial t}+\nabla_x\cdot(\rho u)=0\\
&\frac{\partial\rho u}{\partial t}+\nabla_x\cdot(\rho u\otimes u)+\nabla_x p=0\\
&\frac{\partial E}{\partial t}+\nabla_x\cdot(Eu+pu)=0
\end{aligned} \tag{10}$$

$$p=\rho T, \quad E=\frac{3}{2}\rho T+\frac{1}{2}\rho u^2. \tag{11}$$

2.3 Time discretizations

The time integration of the Boltzmann equation represents a challenging problem, since the nonlinear collision operator becomes highly stiff near the fluid regime ($\varepsilon\ll 1$). An additional limitation is given by the high computational cost required for evaluating the five-fold collisional integral. The starting point is the usual first order splitting in time of Eq. (1), which consist in solving separately a purely convective step (i.e. $Q\equiv 0$ in (1)) and a collision step characterized by a space homogeneous Boltzmann equation (i.e. $\nabla_x f\equiv 0$ in (1)). Clearly, after this splitting almost all the main difficulties are contained in the collision step. For this reason in the sequel we will fix our attention on the time discretization of the homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t}=\frac{1}{\varepsilon}Q(f,f). \tag{12}$$

Let us consider the simple forward Euler scheme

$$f^{n+1}=f^n+\frac{\Delta t}{\varepsilon}Q(f^n,f^n), \tag{13}$$

which has been widely used in simulation. It leads to a stability condition which requires the time step Δt to be of order ε. Thus for small values of ε the scheme is unusable for practical purposes.

On the other hand, the use of fully implicit schemes for (12), like the backward Euler method

$$f^{n+1} = f^n + \frac{\Delta t}{\varepsilon} Q(f^{n+1}, f^{n+1}), \tag{14}$$

requires the solution of a large nonlinear system of algebraic equations and this makes the method prohibitively expensive.

Alternatively, semi-implicit discretizations have been proposed [17] based on taking only the function $f(v)$ implicitly in (3) whereas $f(v')$, $f(v'_*)$ and $f(v_*)$ are evaluated explicitly. This gives raise to unconditionally stable schemes that have the same cost of an explicit scheme. Unfortunately these schemes do not possess the correct fluid limit as $\varepsilon \to 0$ and in addition, except for Maxwell molecules, the numerical solution does not preserve the conserved quantities.

High order extensions of the previous schemes can be developed. At present, however, the practical interest of high order schemes is strongly reduced by the high computational cost required by multiple evaluations of the five-fold integral (3).

In the next sections, following the approach presented in [7], we will show how it is possible to construct unconditionally stable schemes for the space homogeneous equation that are accurate for a wide range of Knudsen numbers, while avoiding the solution of nonlinear algebraic equations.

3 The Time Relaxed (TR) schemes

As proposed in [7], a general idea for deriving robust numerical schemes, that is schemes that are unconditionally stable and preserve the asymptotics of the fluid dynamic limit, for a nonlinear equation like (12) is to replace high order terms of a suitable well-posed power series expansion by the local equilibrium. We will call this class of schemes *Time Relaxed* (TR) schemes. Here we will first derive the schemes as presented in [7] and then we will show how it is possible to generalize this approach.

3.1 Derivation

Let us consider a differential system of the type

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} [P(f, f) - \mu f] \tag{15}$$

with the same initial condition (2) and where $\mu \neq 0$ is a constant and P a bilinear operator.

Let us replace the time variable t and the function $f = f(v, t)$ using the equations

$$\tau = (1 - e^{-\mu t/\varepsilon}), \qquad F(v, \tau) = f(v, t) e^{\mu t/\varepsilon}. \tag{16}$$

Then F is easily shown to satisfy

$$\frac{\partial F}{\partial \tau} = \frac{1}{\mu} P(F, F) \tag{17}$$

with $F(v, \tau = 0) = f_0(v)$.

Now, the solution to the Cauchy problem for (17) can be sought in the form of a power series

$$F(v,\tau) = \sum_{k=0}^{\infty} \tau^k f_k(v), \qquad f_{k=0}(v) = f_0(v) \tag{18}$$

where the functions f_k are given by the recurrence formula

$$f_{k+1}(v) = \frac{1}{k+1} \sum_{h=0}^{k} \frac{1}{\mu} P(f_h, f_{k-h}), \quad k = 0, 1, \dots \tag{19}$$

Making use of the original variables we obtain the following formal representation of the solution to the Cauchy problem (12)

$$f(v,t) = e^{-\mu t/\varepsilon} \sum_{k=0}^{\infty} \left(1 - e^{-\mu t/\varepsilon}\right)^k f_k(v). \tag{20}$$

Remark 3.1 The method was originally developed by Wild [19] to solve the Boltzmann equation for Maxwellian molecules. Here we describe the method under more general hypothesis on P, as derived in [7]. We emphasize that the representation (20) is not unique and other well-posed power series expansions can be obtained in a similar way [7].

Finally, note that expansion (20) continues to hold also if μ is a function of v. Unfortunately this choice leads to nonconservative schemes.

From this representation, a class of numerical schemes can be naturally derived.

In [7] the following class of numerical schemes, based on a suitable truncation for $m \geq 1$ of (20), has been constructed

$$f^{n+1}(v) = e^{-\mu \Delta t/\varepsilon} \sum_{k=0}^{m} \left(1 - e^{-\mu \Delta t/\varepsilon}\right)^k f_k^n(v) + \left(1 - e^{-\mu \Delta t/\varepsilon}\right)^{m+1} M(v), \tag{21}$$

where $f^n = f(n\Delta t)$ and Δt is a small time interval. The quantity M (referred as the local Maxwellian associated to f) is the asymptotic stationary solution of the equation.

It can be shown that the schemes obtained in this way are of order m in time. Furthermore, we have [7] the following

Proposition 3.1 *The schemes defined by (21) satisfy*

i) conservation:

If $P(f,g)$ is a non negative bilinear operator such that there exist some functions $\phi(v)$ with the following property

$$\int_{R^3} P(f,f)\phi(v)\, dv = \mu \int_{R^3} f\phi(v)\, dv, \tag{22}$$

and the initial condition f^0 is a non negative function, then f^{n+1} is nonnegative for any $\mu\Delta t/\varepsilon$, and satisfies

$$\int_{R^3} f^{n+1}\phi(v)\, dv = \int_{R^3} f^n \phi(v)\, dv. \tag{23}$$

ii) asymptotic preserving (AP):

For any $m \geq 1$, we have

$$\lim_{\mu\Delta t/\varepsilon \to \infty} f^{n+1} = M(v). \tag{24}$$

3.2 Application to the Boltzmann equation

Now we apply the previous general approach to the Boltzmann equation and related kinetic models. To this aim, we will need a bound on the loss term, which is essential in most numerical methods.

Let us consider the space homogeneous problem

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} Q(f, f). \tag{25}$$

Problem (25) can be written in the form (15) taking

$$P(f, f) = Q^+(f, f) + f(v) \left(\mu - \int_{I\!R^3} \int_{S^2} \sigma(|v - v_*|, \omega) f(v_*)\, d\omega\, dv_* \right), \tag{26}$$

where

$$Q^+(f, f,) = \int_{I\!R^3} \int_{S^2} \sigma(|v - v_*|, \omega) f(v') f(v'_*)\, d\omega\, dv_*, \tag{27}$$

and the constant μ must satisfy

$$\mu \geq \int_{I\!R^3} \int_{S^2} \sigma(|v - v_*|, \omega) f(v_*)\, d\omega\, dv_*. \tag{28}$$

In general, the previous condition cannot be satisfied for all $v \in I\!R^3$. The usual way to overcome this difficulty is to replace the kernel σ with the bounded kernel σ_b

$$\sigma_b(|v - v_*|, \omega) = \min \left\{ \sigma(|v - v_*|, \omega), \bar{\sigma} \right\}, \quad \bar{\sigma} > 0.$$

In this case it is enough to choose $\mu = 4\pi\rho\bar{\sigma}$ in order to satisfy (28).

Note that, in a particle method, there is a natural bound $\bar{\sigma}$ on the cross section due to the finite number of velocities and therefore it is always possible to satisfy Eq.(28).

It is a simple exercise to verify that Proposition 3.1 holds with $\phi(v) = 1, v, v^2$.

Let us consider the first order scheme, in which $f_k, k \geq 2$ is substituted by the local Maxwellian (8). With the notations of the previous sections, the scheme reads

$$f^{n+1}(v) = (1 - \tau) f^n(v) + \tau(1 - \tau) f_1^n(v) + \tau^2 M(v), \tag{29}$$

where $\tau = 1 - e^{-\mu\Delta t/\varepsilon}$. The results from the last two subsections show that the approximation defined by (29) is well-defined independently of the Knudsen number, and by proposition 3.1, has the correct moments, and converges towards the correct fluid-dynamic limit.

Remark 3.2 In the case of Maxwell molecules the method considerably simplifies. In fact, since the collision kernel does not depend on the relative velocity $\sigma_{\bar{\sigma}} = \sigma_b(\omega)$ we simply have $P(f, f) = Q^+_{\bar{\sigma}}(f, f)$ and $\mu = 4\pi\rho\bar{\sigma}$ where

$$\bar{\sigma} = \frac{1}{4\pi} \int_{S^2} \sigma_{\bar{\sigma}}(\omega) d\omega. \tag{30}$$

3.3 Generalized TR schemes

The approach we have seen in the previous sections can be generalized using different weight functions to combine the influence of the high order coefficients appearing in the Wild sum (20). In general such schemes can be written as

$$f^{n+1} = \sum_{k=0}^{m} A_k f_k + A_{m+1} M, \tag{31}$$

where the coefficients f_k are given by Eq. (19).

The weights $A_k = A_k(\tau)$ are nonnegative function that satisfy the following properties

Proposition 3.2 *Let the weights $A_k = A_k(\tau)$ be nonnegative functions such that*

i) consistency:

$$\lim_{\tau\to 0} A_1(\tau)/\tau \;=\; 1, \quad \lim_{\tau\to 0} A_k(\tau)/\tau = 0, \quad k = 2, \dots, m+1 \tag{32}$$

ii) conservation:

$$\sum_{k=0}^{m+1} A_k = 1 \quad \tau \in [0,1], \tag{33}$$

iii) asymptotic preserving (AP):

$$\lim_{\tau\to 1} A_k(\tau) = 0, \quad k = 0, \dots, m \tag{34}$$

then (31) is a consistent discretization of problem (15) that satisfies proposition 3.1.

The proof is a simple exercise and we leave it to the reader.

A choice of functions which satisfies the previous requirements is given by

$$A_k = (1-\tau)\tau^k, \; k = 0, \dots, m, \quad A_{m+1} = \tau^{m+1}, \tag{35}$$

which correspond to the scheme (21). A better choice of parameters is [13]

$$A_k = (1-\tau)\tau^k, \; k = 0, \dots, m-1, \quad A_m = 1 - \sum_{k=0}^{m} A_k - A_{m+1}, \quad A_{m+1} = \tau^{m+2}, \tag{36}$$

which corresponds to take $f_{m+1} = f_m$, $f_k = M$, $k \geq m+2$ in (20).

However, other choices are possible and it is an open problem the determination of the *optimal* set of functions A_k that satisfies the previous requirements and guarantees the most accurate approximation.

3.4 Stability analysis of the TR schemes

In this paragraph we report some reults related to the stability of the TR schemes. In particular, we show that the first and second order TR schemes are L-stable [13].

Let us apply the TR scheme to the test equation

$$y' = \lambda y, \tag{37}$$

with $y(0) = 1$ and $\lambda \in C^-$.

The equation can be written in the form

$$y' = P(y, y) - \mu y,$$

with $P(f, g) = \frac{1}{2}(\mu + \lambda)(f + g)$, and μ is a positive constant such that $|\lambda| < \mu$. The numerical solution after one time step is given by

$$y^1 = \sum_{k=0}^{m} A_k y_k. \tag{38}$$

The $m+1$ term vanishes because the equilibrium solution is zero. The term y_k can be explicitly computed by applying the formula (19). A simple calculation yields

$$y_k = \frac{1}{k!} \prod_{j=1}^{k} (j + a) = \frac{\Gamma(k + 1 + a)}{\Gamma(k + 1)\, \Gamma(1 + a)}, \quad k = 0, \ldots, m \tag{39}$$

where $a = \lambda/\mu$ and Γ denotes the usual Γ-function. The numerical solution after one time step, called the *function of absolute stability*, is therefore a function of a real parameter τ and a complex parameter a

$$R_m(\tau, a) = \sum_{k=0}^{m} A_k(\tau) y_k(a),$$

where $\tau = 1 - \exp(-\mu \Delta t)$ is the relaxed time, and a is a complex number $a \in C^-, |a| \leq 1$. Here we give definitions of A- and L-stability which are the natural generalization of the standard definition [8] to the case where the function of absolute stability depends on an additional real parameter.

Definition 3.1 *:*
i) *We say that the scheme is A-stable if*

$$|R(\tau, a)| \leq 1 \quad \forall \tau \in [0, 1],\ a \in C^-, |a| \leq 1.$$

ii) *We say that the scheme is L-stable if it is A-stable and*

$$\lim_{\tau \to 1} R(\tau, a) = 0, \quad \forall a \in C^-, |a| \leq 1.$$

It is clear that, because of the asymptotic preserving properties, if a TR scheme is A-stable it is also L-stable.

Here we recall the main result about the stability of first and second order TR schemes with weights given by (35).

The functions of absolute stability for these schemes are

$$\begin{aligned} R_1(\tau, a) &= (1-\tau)[1+\tau(1+a)], \quad (40) \\ R_2(\tau, a) &= (1-\tau)[1+\tau(1+a)+\frac{1}{2}\tau^2(1+a)(2+a)]. \quad (41) \end{aligned}$$

We have the following [13]

Theorem 3.1 *The schemes defined by (35) for $m=1$ and $m=2$ are A-stable, i.e.*

$$|R_1(\tau, a)| \leq 1, \forall \tau \in [0,1],\ a \in C^-, |a| \leq 1,$$

$$|R_2(\tau, a)| \leq 1, \forall \tau \in [0,1], a \in \Omega_a \equiv \{z \in C : \Re z \leq 0, |z| \leq 1\}.$$

4 Time Relaxed Monte Carlo (TRMC) methods

In this section we describe the *Time Relaxed Monte Carlo* (TRMC) method for the evolution of the density function f. We shall include the description of classical DSMC no-time counter algorithm, so that it will be easier to make a comparison between the new formulation and the previous one.

We develop the algorithms first in the simple case of constant cross sections (Maxwellian molecules) and then for the Boltzmann equation for Variable Hard Sphere gas.

4.1 DSMC methods

Here we will describe the classical DSMC method in the general framework we have introduced in the previous sections. More specifically, we consider the Nanbu-Babovsky algorithm [11], [1].

The kinetic equations we are considering can be written in the form

$$\frac{\partial f}{\partial t} = \frac{1}{\epsilon}[P(f,f) - \mu f]. \quad (42)$$

In particular, for the Boltzmann equation for Maxwellian molecules we have $P(f,f) = Q^+(f,f)$ (see Remark 3.2), whereas for general kernels with cut-off $P(f,f)$ is given by (26).

We assume that f is a probability density, i.e.

$$\rho = \int_{I\!R^3} f(v,t)\, dv = 1.$$

Let us discretize time, and denote by $f^n(v)$ an approximation of $f(v, n\Delta t)$. The forward Euler scheme applied to Eq. Eq. (42) writes

$$f^{n+1} = (1 - \frac{\mu \Delta t}{\epsilon}) f^n + \frac{\mu \Delta t}{\epsilon} \frac{P(f^n, f^n)}{\mu}. \quad (43)$$

This equation has the following probabilistic interpretation: a particle with velocity v_i will not collide with probability $(1-\mu\Delta t/\epsilon)$, and it will collide with probability $\mu\Delta t/\epsilon$, according to the collision law described by $P(f^n, f^n)(v)$.

We remark here that the probabilistic interpretation of Eq. Eq. (43) breaks down if $\Delta t/\epsilon$ is too large, because the coefficient of f^n on the right hand side may become negative. This implies that the time step becomes extremely small when approaching the fluid dynamic limit. Therefore the classical DSMC method becomes almost unusable near the fluid regime.

For clarity of exposition, let us consider first kinetic equations for which $P(f,f) = Q^+(f,f)$, i.e. the collision kernel does not depend on the relative velocity of the particles.

An algorithm based on this probabilistic interpretation was proposed by Nanbu [11].

In its first version, Nanbu's algorithm was not conservative, i.e. energy and momentum were conserved only in the mean, but not at each collision. A conservative version of the algorithm was introduced by Babovsky [1]. Instead of selecting single particles, independent particle pairs are selected, and conservation is maintained at each collision. The expected number of particles that collide in a small time step Δt is $N\mu\Delta t/\epsilon$, and the expected number of collision pairs is $N\mu\Delta t/2\epsilon$. The algorithm is the following

Algorithm 4.1 (DSMC for Maxwell molecules)

- compute the initial velocity of the particles, $\{v_i^0, i = 1, \ldots, N\}$, by sampling them from the initial density $f_0(v)$
- for $n = 1$ to n_{TOT}
  given $\{v_i^n, i = 1, \ldots, N\}$,
    - compute $\{v_i^{n+1}\}$ as follows:
    - set $N_c = \mathrm{Iround}(\mu N\Delta t/(2\epsilon))$
    - select N_c pairs (i,j) uniformly among all possible pairs, and for those
      - perform the collision between i and j, and compute v_i' and v_j' according to the collisional law
    - set $v_i^{n+1} = v_i'$, $v_j^{n+1} = v_j'$
    - set $v_i^{n+1} = v_i^n$ for all the particles that have not been selected

  end for

During each step, all the other $N - 2N_c$ particle velocities remain unchanged. Here by $\mathrm{Iround}(x)$ we denote a suitable integer rounding of a positive real number x. In our algorithm we choose

$$\mathrm{Iround}(x) = \begin{cases} [x] & \text{with probability} \quad [x] + 1 - x \\ [x] + 1 & \text{with probability} \quad x - [x] \end{cases}$$

where $[x]$ denotes the integer part of x.

The post-collisional velocities are computed through relations

$$v_i' = \frac{v_i + v_j}{2} + \frac{|v_i - v_j|}{2}\omega, \quad v_j' = \frac{v_i + v_j}{2} - \frac{|v_i - v_j|}{2}\omega, \tag{44}$$

where ω is chosen uniformly in the unit sphere, according to

$$\omega = \begin{pmatrix} \cos\phi \sin\theta \\ \sin\phi \sin\theta \\ \cos\theta \end{pmatrix}, \quad \theta = \arccos(2\xi_1 - 1), \quad \phi = 2\pi\xi_2, \tag{45}$$

and ξ_1, ξ_2 are uniformly distributed random variables in $[0, 1]$.

Note that this approach is equivalent to sample the post collisional velocity according to $P(f, f)/\mu$, where $\mu = 4\pi\sigma$ and σ is the constant cross section.

The above algorithm has to be modified when the scattering cross section is not constant. In this case, a simple algorithm is obtained by using an upper bound $\bar{\sigma}$ of the scattering cross section and acceptance-rejection technique

Algorithm 4.2 (DSMC for VHS molecules)

- compute the initial velocity of the particles, $\{v_i^0, i = 1, \ldots, N\}$,
  by sampling them from the initial density $f_0(v)$
- for $n = 1$ to n_{TOT}
  given $\{v_i^n, i = 1, \ldots, N\}$,
  - ∘ compute an upper bound $\bar{\sigma}$ for the cross section
  - ∘ set $\mu = 4\pi\bar{\sigma}$
  - ∘ set $N_c = \text{Iround}(\mu N \Delta t/(2\epsilon))$
  - ∘ select N_c dummy collision pairs (i, j) uniformly
    among all possible pairs, and for those
    - ∘ compute the relative cross section $\sigma_{ij} = \sigma(|v_i - v_j|)$
    - ∘ if $\bar{\sigma}$ Rand $< \sigma_{ij}$
      - ∘ perform the collision between i and j, and
        compute v_i' and v_j' according to the collisional law
      - ∘ set $v_i^{n+1} = v_i'$, $v_j^{n+1} = v_j'$
  - ∘ set $v_i^{n+1} = v_i^n$ for all the particles that have not collided

  end for

The new velocities v_i' and v_j' are computed using Eqs. (44) and (45).

The upper bound $\bar{\sigma}$ should be chosen as small as possible, to avoid inefficient rejection, and it should be computed fast.

An upper bound can be derived taking $\bar{\sigma}$ as

$$\sigma_{\max} = \max_{v_i, v_j} \sigma(|v_i - v_j|). \tag{46}$$

Classically, since this computation would require $O(N^2)$ operations, instead of (46) it is preferable to use an upper bound of $\sigma_{\max}$ given by

$$\sigma_{\max} \leq \bar{\sigma} = \sigma(2\Delta v), \quad \Delta v = \max_i |v_i - \bar{v}|, \quad \bar{v} = \sum_i v_i/N. \tag{47}$$

For general collisional kernel, the algorithm is slightly modified by introducing the angular dependence. In this case the collision is always performed, and the new velocities are extracted according to the differential cross section. Then a rejection is used to decide whether the collision is accepted.

Remark 4.1 Note that if the time step is small enough, only a small fraction of particles, let us say N_c, will collide. The computational cost of the collisions is therefore $O(N_c)$. On the other hand the cost of the computation of the upper bound $\bar{\sigma}$ is $O(N)$, which may be much larger than $O(N_c)$. A possible way to overcome this difficulty is to update at each time step the value of the upper bound $\bar{\sigma}$ only if it increases. This may be done as follows. During the computation of the collision between particles i and j, let $\tilde{v}_i$ and $\tilde{v}_j$ denote the new particle velocities. Then the quantity Δv is updated according to

$$\Delta v = \max(\Delta v, |\tilde{v}_i - \bar{v}|, |\tilde{v}_j - \bar{v}|). \tag{48}$$

At the end of the collision loop, the upper bound on the cross section is computed as

$$\bar{\sigma} = \sigma(2\Delta v).$$

In a space non homogeneous calculations, assuming that there are several collisional time steps during a convection time step, the bound can be computed according to Eq. (47) the first time, and then updated as described above.

4.2 TRMC methods

The first order TRMC algorithm is based on the TR schemes

$$f^{n+1} = A_0 f^n + A_1 f_1 + A_2 M \tag{49}$$

The probabilistic interpretation of the above equation is the following: a particle extracted from f^n will not collide with probability A_0, it will collide with another particle extracted from f^n with probability A_1, or it will be replaced by a particle sampled from a Maxwellian with probability A_2.

In this formulation the probabilistic interpretation holds uniformly in $\mu\Delta t/\epsilon$, at variance with standard DSMC, which requires $\mu\Delta t/\epsilon < 1$. Furthermore, as $\mu\Delta t/\epsilon \to \infty$, the distribution at time $n+1$ is sampled from a Maxwellian. In this limit, the density f^{n+1} relaxes immediately to its equilibrium distribution. In a space non homogeneous case, this would be equivalent to the particle method for Euler equations proposed by Pullin [15].

The Monte Carlo scheme described above are conservative in the mean. It is possible to make it exactly conservative by selecting collision pairs uniformly, rather than individual particles, and by using a suitable algorithm for sampling a set of particles with prescribed momentum and energy from a Maxwellian [16].

The conservative version of the methods can be formalized in the following algorithm

Algorithm 4.3 (First order TRMC for VHS molecules)

- compute the initial velocity of the particles, $\{v_i^0, i = 1, \ldots, N\}$, by sampling them from the initial density $f_0(v)$
- for $n = 1$ to n_{TOT}
  given $\{v_i^n, i = 1, \ldots, N\}$,
  - ∘ compute an upper bound $\bar{\sigma}$ of the cross section
  - ∘ set $\tau = 1 - \exp(-\rho\bar{\sigma}\Delta t/\epsilon)$
  - ∘ compute $A_1(\tau)$, $A_2(\tau)$
  - ∘ set $N_c = \mathrm{Iround}(NA_1/2)$
  - ∘ perform N_c dummy collisions, as in Algorithm 4.2
  - ∘ set $N_M = \mathrm{Iround}(NA_2)$
  - ∘ select N_M particles among those that have not collided, and compute their mean momentum and energy
  - ∘ sample N_M particles from the Maxwellian with the above momentum and energy, and replace the N_M selected particles with the sampled ones
  - ∘ set $v_i^{n+1} = v_i^n$ for all the $N - 2N_c - N_M$ particles that have not been selected

  end for

A second order Monte Carlo scheme is obtained by the TR scheme

$$f^{n+1} = A_0 f^n + A_1 f_1 + A_2 f_2 + A_3 M, \tag{50}$$

with

$$f_1 = \frac{P(f^n, f^n)}{\mu}, \quad f_2 = \frac{P(f^n, f_1)}{\mu}.$$

Given N particles distributed according to f^n, the probabilistic interpretation of scheme (50) is the following: NA_0 particles will not collide, NA_1 will be sampled from f_1 (as in the first order scheme), NA_2 will be sampled from f_2, i.e. $NA_2/2$ particles sampled from f^n will undergo dummy collisions with $NA_2/2$ particles sampled from f_1, and NA_3 particles will be sampled from a Maxwellian.

Once again, the methods can be made conservative using the same techniques adopted in the first order scheme. The various steps of the method can be summarized in the following algorithm.

Algorithm 4.4 (Second order TRMC for VHS molecules)

- compute the initial velocity of the particles, $\{v_i^0, i = 1, \ldots, N\}$, by sampling them from the initial density $f_0(v)$
- for $n = 1$ to n_{TOT}
  given $\{v_i^n, i = 1, \ldots, N\}$,

- ∘ compute an upper bound $\bar{\sigma}$ of the cross section
- ∘ set $\tau = 1 - \exp(-\rho\bar{\sigma}\Delta t/\epsilon)$
- ∘ compute $A_1(\tau)$, $A_2(\tau)$,$A_3(\tau)$
- ∘ set $N_1 = \text{Iround}(NA_1/2)$, $N_2 = \text{Iround}(NA_2/4)$
- ∘ select $N_1 + N_2$ dummy collision pairs (i, j) uniformly among all possible pairs, and for those
  - ∘ compute the relative cross section $\sigma_{ij} = \sigma(|v_i - v_j|)$
  - ∘ if $\bar{\sigma}$ Rand $< \sigma_{ij}$
    - ∘ perform the collision between i and j, and compute v_i' and v_j' according to the collisional law
    - ∘ set $v_i^{n+1} = v_i'$, $v_j^{n+1} = v_j'$ for $2N_1$ particles
- ∘ select $2N_2$ particles from f^n
- ∘ perform the collision of these selected particles with the remaining $2N_2$ particles that have collided once
- ∘ update the velocity of the $4N_2$ particles with the outcome of the $2N_2$ collisions (of particles that have never collided before with particles that collided once)
- ∘ set $N_M = \text{Iround}(NA_3)$
- ∘ replace N_M particles with samples from Maxwellian, as in Algorithm 4.3
- ∘ set $v_i^{n+1} = v_i^n$ for all the $N - 2N_1 - 4N_2 - N_M$ particles that have not been selected

end for

Simlarly higher order TRMC methods can be constructed. For example a third order scheme is obtained from

$$f^{n+1} = A_0 f^n + A_1 f_1 + A_2 f_2 + A_3 f_3 + A_4 M, \tag{51}$$

with

$$f_1 = \frac{P(f^n, f^n)}{\mu}, \quad f_2 = \frac{P(f^n, f_1)}{\mu}, \quad f_3 = \frac{1}{2\mu}[P(f^n, f_2) + P(f_1, f_1)].$$

We omit for brevity the details of the resulting Monte Carlo algorithm.

We remark here that the TR scheme is a direct consequence of the time discretization of the Boltzmann equation. In this respect it is not crucial to select a particular Monte Carlo scheme in order to perform the comparison. Here we considered a commonly used Monte Carlo scheme. If a different technique is used to model the collision, then the same technique could be used in conjunction with TR discretization.

5 Numerical Results

In this section we present some numerical results for the new time relaxed Monte Carlo (TRMC) method and compare them with standard DSMC method.

5.1 Space homogeneous results

First we consider homogeneous test problems for the Kac equation [9], and for the Boltzmann equation for Maxwell molecules. Exact solutions are known in these special situations and so we can compare the accuracy of the different schemes. In our tests we have performed a single run, with a number of particles sufficiently large to control the effects of the fluctuations. We express the results as a function of the scaled time variable t/ϵ which we denote again by t in order to simplify the notations.

5.1.1 Test I: Kac equation

In the first test we compare the different Monte Carlo methods using an exact solution of the Kac equation [9]. This test is used to check the accuracy of the methods using different time steps.

The Kac equation is a simplified one-dimensional model of the Boltzmann equation for Maxwell molecules characterized by

$$Q(f,f)(v) = \frac{1}{2\pi}\int_0^{2\pi}\int_{I\!R}[f(v')f(v'_*) - f(v)f(v_*)]\,dv_*\,d\theta, \tag{52}$$

where

$$v' = v\cos\theta - v_*\sin\theta, \qquad v'_* = v\sin\theta + v_*\cos\theta. \tag{53}$$

An exact solution for this equation is [10]

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

with $C(t) = 3 - 2\exp(-\sqrt{\pi}t/16)$.

The previous TR schemes can be applied directly to (52) taking

$$P(f,f) = \frac{1}{2\pi}\int_0^{2\pi}\int_{I\!R^3} f(v')f(v'_*)\,dv_*\,d\theta, \tag{54}$$

and $\mu = \rho$.

The density function f has been reconstructed on a regular grid, by convolving the particle distribution by a suitable mollifier [6]

$$f(V_I) = \frac{1}{N}\sum_{j=1}^{N} W_H(V_I - v_j), \tag{55}$$

where

$$\{V_I = V_{\min} + I\Delta V, I = 1,\ldots,N_g\}.$$

The smoothing function $W_{\rm H}$ is given by

$$W_{\rm H}(x) = \frac{1}{H}W\left(\frac{x}{H}\right), \quad W(x) = \begin{cases} 3/4 - x^2 & \text{if } |x| \le 0.5, \\ (x-3/2)^2/2 & \text{if } 0.5 < |x| \le 1.5, \\ 0 & \text{otherwise.} \end{cases}$$

The value $H = 0.2$ has been selected as a good compromise between fluctuations and resolution. The simulations are performed for $t \in [0, 8]$ by starting with $N = 5 \times 10^4$ particles.

In Fig. 1 we present the numerical results obtained at time $t = 2$ for the different schemes with the same time step $\Delta t = 1.0$ which represents the upper bound for stability of DSMC.

It is evident that all TRMC schemes gives a better representation of the solution especially near the local extrema (top).

Fig. 2 shows the results of the L^2-norm of the error for the same test. At the bottom of the same figure we show how it is possible to use larger time steps in TRMC schemes with respect to DSMC without any deterioration of the accuracy.

5.1.2 Test II: Maxwell molecules

Next we perform the same kind of accuracy test in the case of the Boltzmann equation for Maxwell molecules in the two-dimensional case. An exact solution to this equation [10] is given by

$$f(v,t) = \frac{1}{2\pi C}\left[1 - \frac{1}{C}(1-C)\left(1 - \frac{v^2}{2C}\right)\right]\exp\left(-\frac{v^2}{2C}\right), \tag{56}$$

where $C(t) = 1 - (1/2)\exp(-t/8)$.

The comparison with the exact solution is obtained by reconstructing the function on a regular grid of spacing $\Delta v = 0.25$ by the "weighted area rule".

All the simulations have been performed for $t \in [0, 16]$ by starting with $N = 10^5$ particles.

In Fig. 3 we show the L^2 norm of the error in time for both DSMC and TRMC schemes. In the first picture we report the results obtained with the same time step $\Delta t = 1.0$. The results confirm the gain of accuracy of the TRMC methods on the transient time scale. Next the results obtained with different time steps, chosen in such a way that the different methods are almost equivalent, are also reported.

5.2 Shock wave profiles

The last test problem deals with the numerical solution of the space non homogeneous Boltzmann equation for hard sphere molecules (VHS, for $\alpha = 1$) with $C_\alpha = 1$. We present some numerical results for one-dimensional stationary shock profiles. In particular we have computed the structure of the shock for different Knudsen numbers, from the rarefied regime up to the fluid limit. In all our numerical tests the gas is initially at the upstream equilibrium state in the left half-space and in the downstream equilibrium state in the right-half space. The upstream state is determined from the downstream state using the Rankine-Hugoniot relations [18].

In the present calculations, the downstram state is characterized by

$$\rho = 1.0, \quad T = 1.0, \quad M = 3.0,$$

where M is the Mach number of the shock. The downstream mean velocity is then given by

$$u_x = -M\sqrt{(\gamma T)}, \quad u_y = 0,$$

with $\gamma = 2$ since we have considered a 2D gas in velocity space.

The infinite physical space is truncated to the finite region $[-7.5, 7.5]$. A suitable stabilizing tecnique [2] has been used to keep the number of particles constant during the time evolution. We report the result obtained with the different schemes using 50 space cells and 500 particles in each downstream cell. Since we are computing a stationary solution after a fixed initial time, we can strongly improve the accuracy of the Monte Carlo solution by averaging in time the solution itself. To this aim we started the statistics accumulation at time $t = 5$ and we average up to $t = 20$ which correspond approximatively to 1500 results. The reference solution in the rarefied and intemediate regime is obtained using the DSMC method with 200 space cells and 500 particles in each downstream cell and averaging over approximatively 8000 results. All the results are reported on the space interval $[-4.5, 4.5]$.

In Fig. 4 we plot the result obtained in the rarefied regime ($\epsilon = 1$) using the different Monte Carlo methods. The computational cost of the methods is comparable since here we are far from the fluid limit. As expected, the results show that essentially the TRMC methods and the DSMC method are equivalent and provid a good description of the rarefied shock.

Next we consider the intermediate regime ($\epsilon = 0.1$). In this simulation the time step of the DSMC method is 10 times smaller then the time step used in TRMC methods. The result show that, despite the larger time step, the accuracy of the solution obtained with TRMC schemes is essentially the same of DSMC (see Fig. 5).

Finally we give the result of the computations close to the Euler limit ($\epsilon = 10^{-6}$). The profiles obtained with the TRMC methods are reported in Fig. 6. Due to the small Knudsen number the DSMC method is unusable in practice in this test. Note that the TRMC methods are all equivalent to Pullin method. Thus we have plotted only one approximate solution.

Conclusion and future works

In this paper a new family of schemes is proposed for the numerical solution of the Boltzmann equation.

The schemes have been tested on several problems for the Boltzmann equation, and they provide good results compared with standard Monte Carlo methods.

There is still a lot to do to improve the accuracy and robustness of the schemes. In particular, the optimal choice of the coefficients $A_k, k = 1, \ldots, \bar{m}$ is still an open problem. Several possibilities are presently under consideration. The first one corresponds to choose the coefficients in such a way that some moments of the distribution function for Maxwelliam molecules are computed exactly. It is well known, in fact, exact closure for the moment equations is possible in the case of Maxwellian molecules [20]. The same coeffients could then be used for VHS molecules.

A second alternative is to compute several terms of the Wild sum expansion. If the weights of the expansion decay fast enaough, the computation can be done very efficiently by a recursive algorithm, even for large values of k. The recursive tree can eventually be truncated, and the corresponding value of f_k substituted by sampling from a Maxwellian. Such approach is very promising, and is considered in [14].

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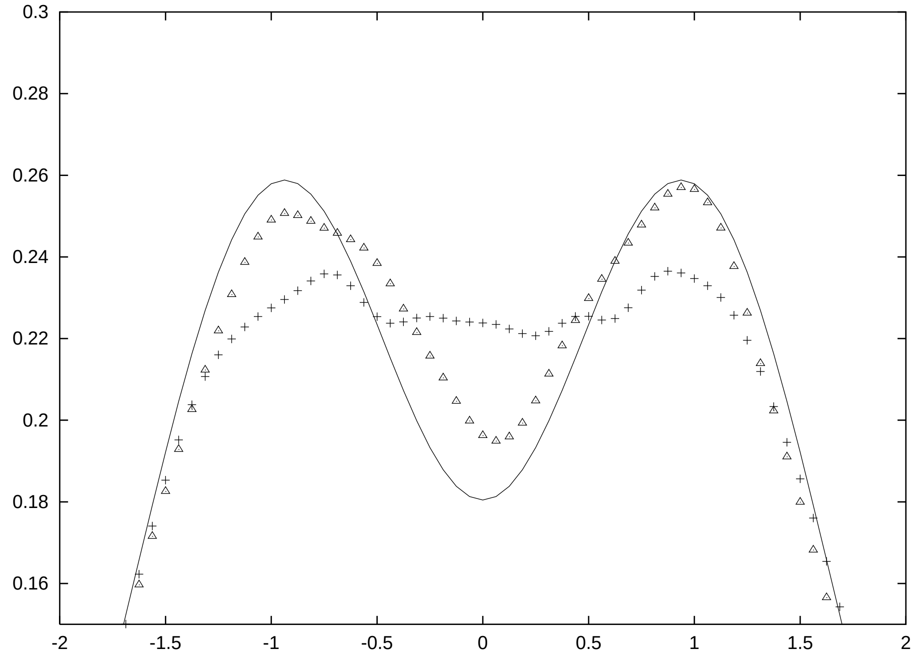

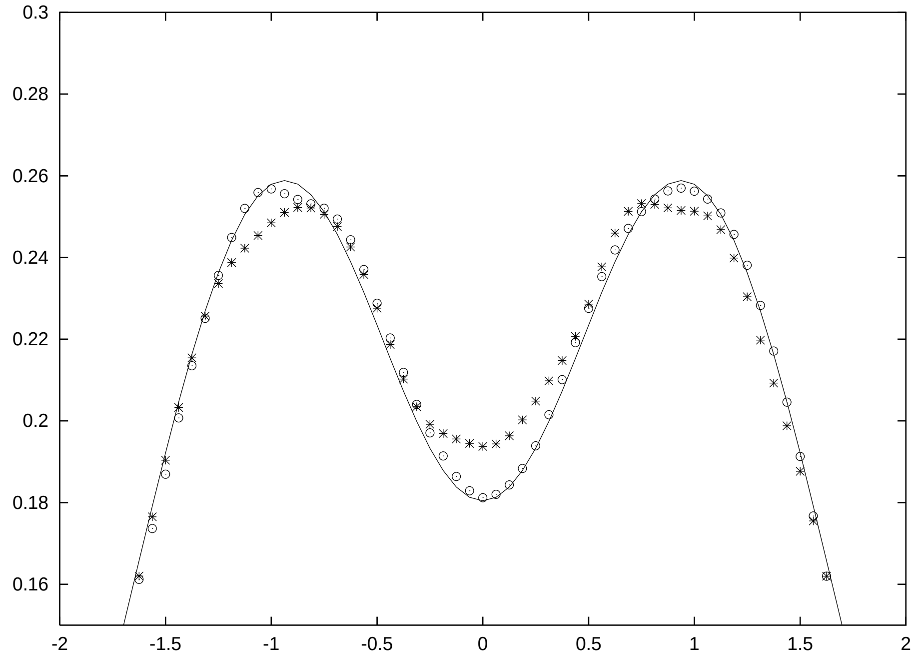

Figure 1: Test I (Kac equation). Details of the distribution function at time $t = 2.0$ for $\Delta t = 1.0$. Exact (line), DSMC ($+$), first order TRMC ($\triangle$), second order TRMC ($*$), third order TRMC ($\circ$).

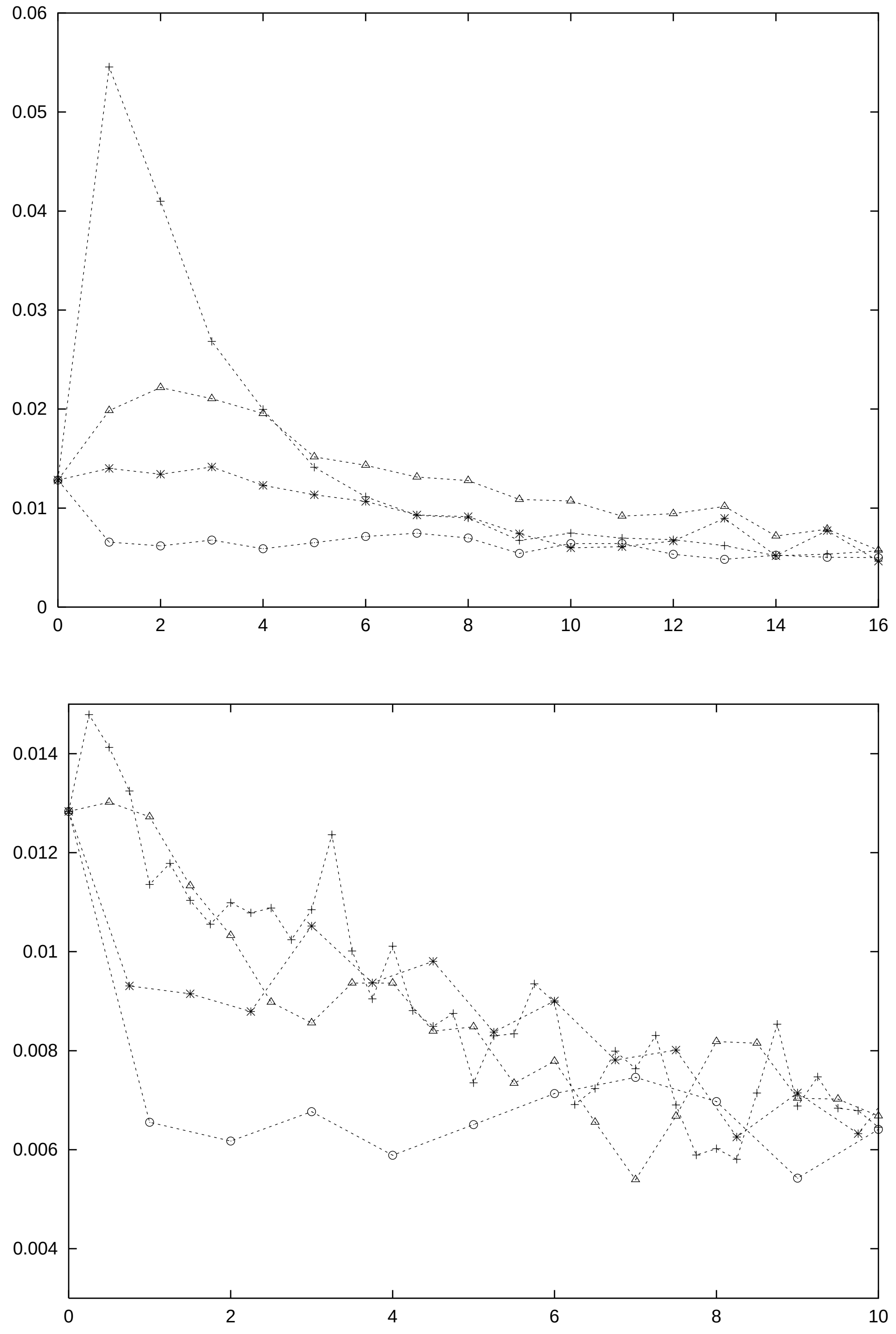

Figure 2: Test I (Kac equation). L^2 norm of the error vs time. Exact (line), DSMC (+), first order TRMC ($\triangle$), second order TRMC ($*$), third order TRMC ($\circ$). Top: time step $\Delta t = 1.0$. Bottom: DSMC with $\Delta t = 0.25$, first order TRMC with $\Delta t = 0.5$, second order TRMC with $\Delta t = 0.75$, third order TRMC3 with $\Delta t = 1.0$.

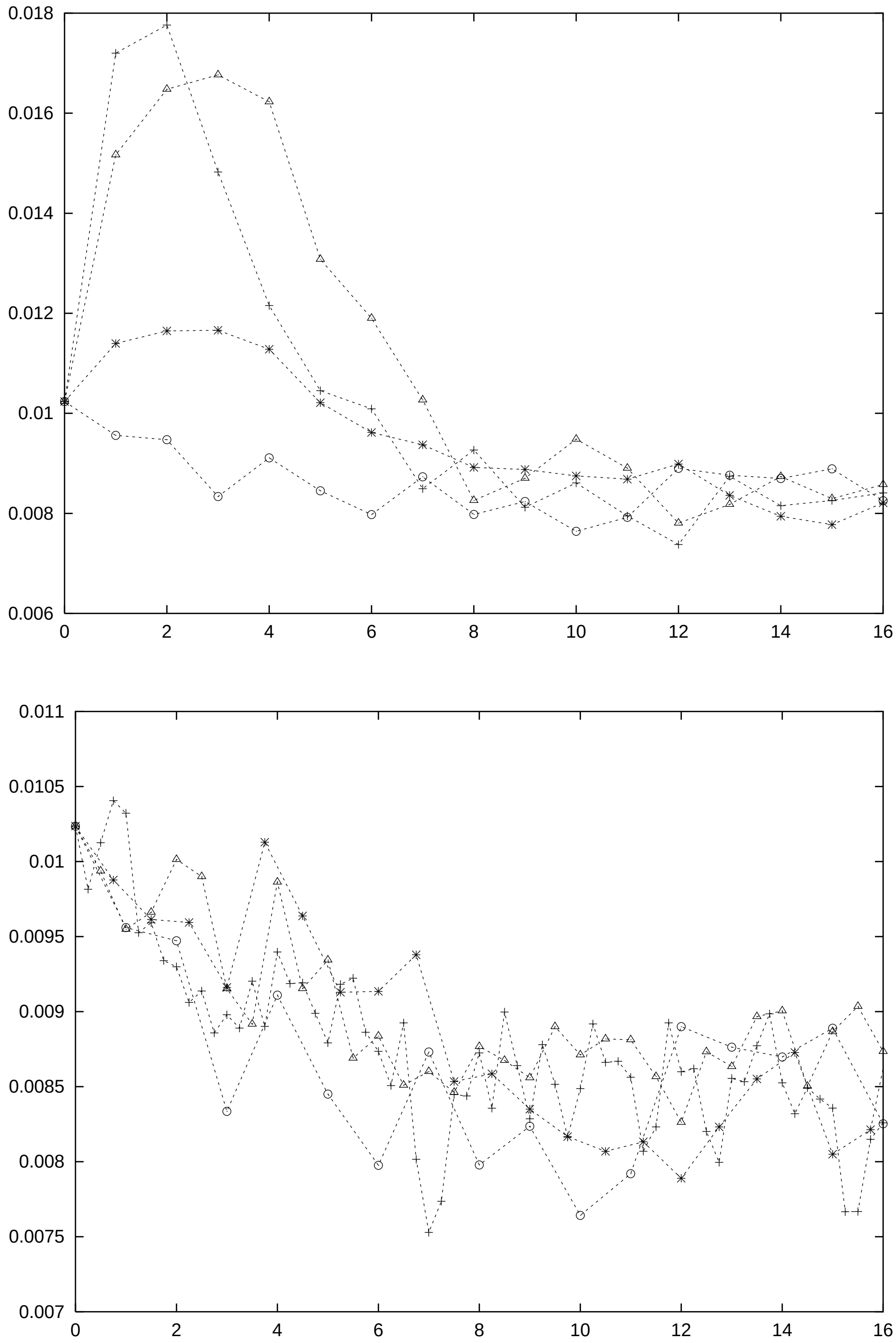

Figure 3: Test II (Maxwell molecules). L^2 norm of the error vs time. Exact (line), DSMC (+), first order TRMC ($\triangle$), second order TRMC ($*$), third order TRMC ($\circ$). Top: time step $\Delta t = 1.0$. Bottom: DSMC with $\Delta t = 0.25$, first order TRMC with $\Delta t = 0.5$, second order TRMC with $\Delta t = 0.75$, third order TRMC3 with $\Delta t = 1.0$.

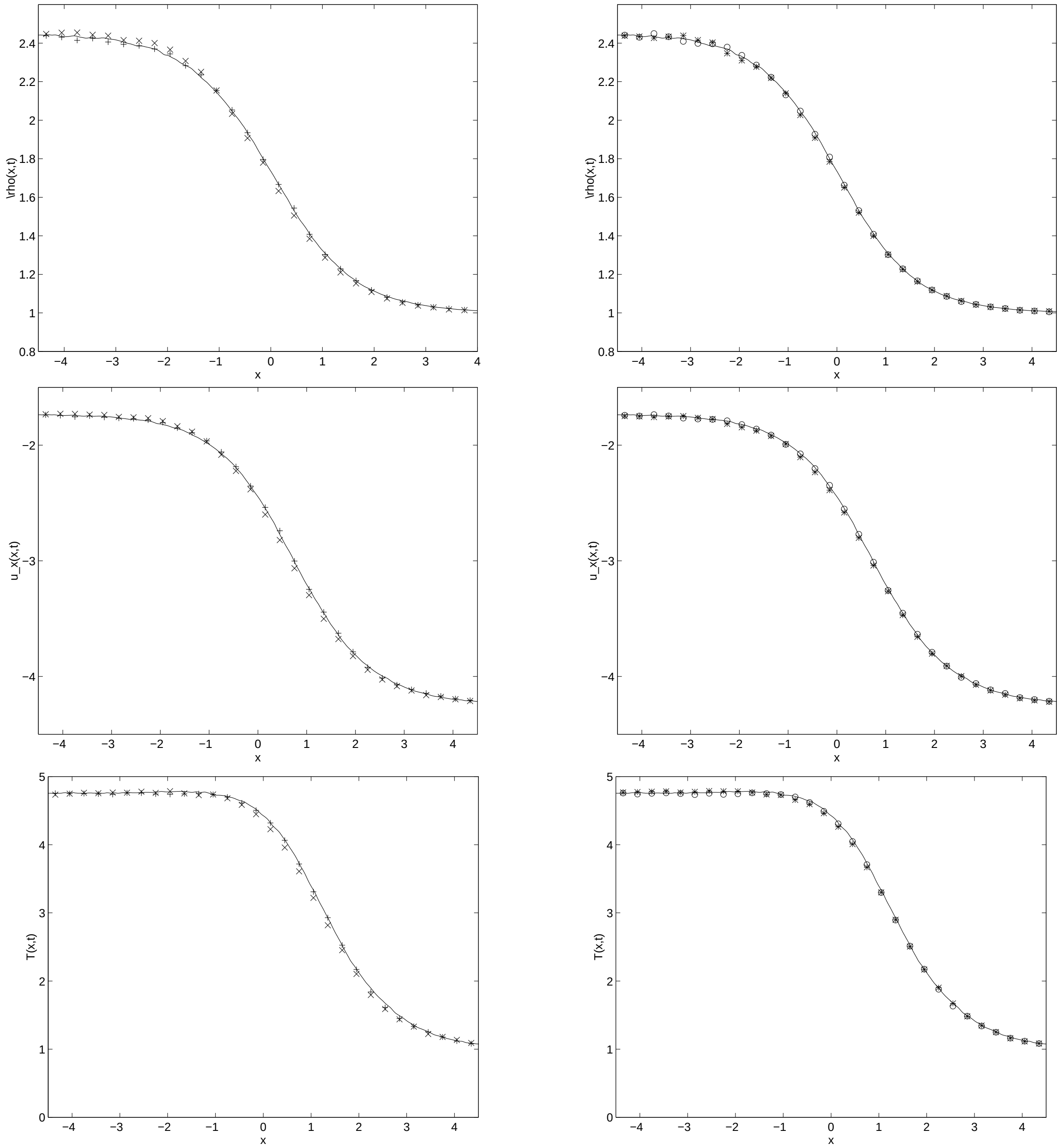

Figure 4: Shock wave profiles (rarefied regime): DSMC(+) and first order TRMC ($\times$) (left column), second order ($*$) and third order ($\circ$) TRMC (right column) for $\epsilon = 1.0$ and $\Delta t = 0.025$. From top to bottom: ρ, u,T.

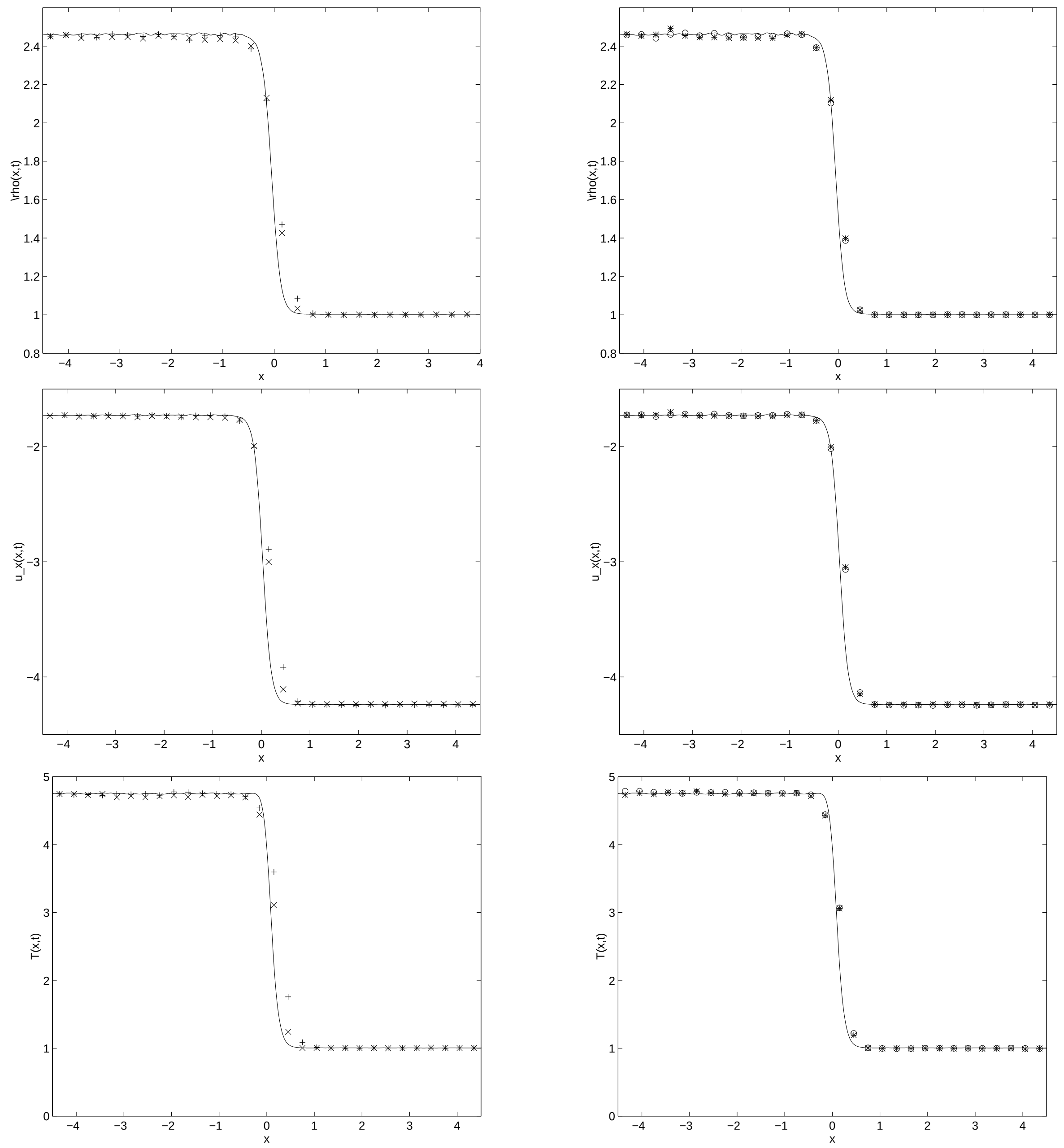

Figure 5: Shock wave profiles (intermediate regime): DSMC(+) and first order TRMC ($\times$) (left column), second order ($*$) and third order ($\circ$) TRMC (right column) for $\epsilon = 1.0$ and $\Delta t = 0.0025$ for DSMC, $\Delta t = 0.025$ for TRMC. From top to bottom: ρ, u,T.

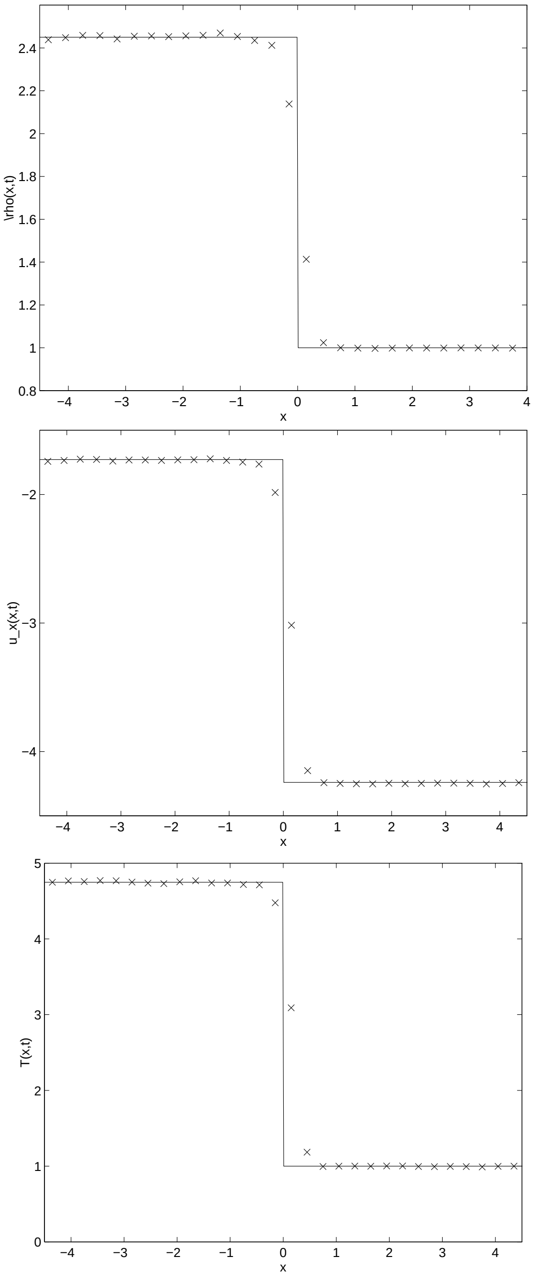

Figure 6: Shock wave profiles (fluid regime): first order TRMC ($\times$) for $\epsilon = 10^{-8}$ and $\Delta t = 0.025$. From top to bottom: ρ, u,T.