The moment-guided Monte Carlo method

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SUMMARY

In this work we propose a new approach for the numerical simulation of kinetic equations through Monte Carlo schemes. We introduce a new technique that permits to reduce the variance of particle methods through a matching with a set of suitable macroscopic moment equations. In order to guarantee that the moment equations provide the correct solutions, they are coupled to the kinetic equation through a nonequilibrium term. The basic idea, on which the method relies, consists in guiding the particle positions and velocities through moment equations so that the concurrent solution of the moment and kinetic models furnishes the same macroscopic quantities. Copyright © 2010 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The Boltzmann equation provides a kinetic description of gases and more generally of particle systems. In many applications, the correct physical solution for a system far from thermodynamical equilibrium, such as, for instance, rarefied gases or plasmas requires the resolution of the Boltzmann equation [1]. The numerical simulation of the Boltzmann equation with deterministic techniques presents several drawbacks due to difficulties in treating the collision terms and to the large dimension of the problem. The distribution function depends on seven independent variables: three coordinates in physical space, three coordinates in velocity space and time. As a consequence, probabilistic techniques such as Direct Simulation Monte Carlo (DSMC) methods are extensively used in real situations due to their large flexibility and low computational cost compared with finite volume, finite difference or spectral methods for kinetic equations [2–5]. On the other hand, DSMC solutions are affected by large fluctuations. Moreover, in nonstationary situations it is impossible to use time averages to reduce fluctuations and this leads to either poorly accurate solutions or computationally expensive simulations.
More generally, Monte Carlo (MC) methods are frequently used in many real applications to simulate physical, chemical and mathematical systems [6]. We quote [3] for an overview on efficient and low variance MC methods. For applications of variance reduction techniques to kinetic equation, we mention the works of Homolle and Hadjiconstantinou [7, 8]. We mention also the research papers by Boyd and Burt [9] and Pullin [10], in which a low diffusion particle method was developed for simulating compressible inviscid flows. We finally quote the results obtained by two of the authors [11] on the construction of efficient and low variance methods for kinetic equations in transitional regimes.

The basic idea described in this paper consists in reducing the variance of MC methods by forcing particles to match prescribed sets of moments given by the solution of deterministic equations. In order to provide the correct solution, the moment equations are coupled to the DSMC simulation of the Boltzmann equation through a kinetic correction term, which takes into account departures from thermodynamical equilibrium.

We remark that the general methodology described here is independent from the choice of the collisional kernel (Boltzmann, Fokker–Planck, BGK, etc.). However, we point out that additional improvements can be obtained with hypotheses on the structure of the distribution function, on the type of considered kernel and on the type of resolution methods used for the kinetic and fluid equations.

In the present paper we will focus on the basic matching technique, which consists in matching the kinetic solution to that obtained by the deterministic solution of the first three moment equations. The idea is that the deterministic solution of the moment equation (through finite volume or finite difference techniques) leads to a more accurate solution, in terms of statistical fluctuations, than the DSMC method. Therefore, we constrain the DSMC method to match the moments obtained through the deterministic resolution of the moment equations in such a way that the higher accuracy of the moment resolution improves the accuracy of the DSMC method. We experimentally show that this is indeed the case.

We leave an in-depth discussion of possible higher order matching extensions to future works. For simplicity, in the numerical tests, we will make use of a BGK collision term. However, the formulation of the method is general and extensions to the full Boltzmann interaction term are possible without changing the structure of the algorithm as explained in details in the paper. Results in the case of the Boltzmann operator and improvements of the basic technique described here will be presented in [12].

The remainder of the paper is organized as follows. In the next section we recall some basic notions on the Boltzmann equations and its fluid limit. The details of the numerical method are described in Section 3. In Section 4 numerical examples, which demonstrate the capability of the method, are presented. Finally some future developments and remarks are detailed in the last section.

2. THE BOLTZMANN EQUATION AND ITS FLUID LIMIT

We consider equations of the following form:

\[ \partial_t f + v \cdot \nabla_x f = Q(f, f) \]  \hspace{1cm} (1)

with initial data

\[ f|_{t=0} = f_{\text{init}}. \]  \hspace{1cm} (2)

where \( f(x, v, t) \) is a nonnegative function describing the time evolution of the distribution of particles with velocity \( v \in \mathbb{R}^d \) and position \( x \in \Omega \subset \mathbb{R}^d \) at time \( t > 0 \). The operator \( Q(f, f) \) describes particles interactions and is assumed to satisfy the local conservation properties

\[ \langle m \, Q(f, f) \rangle = 0, \]  \hspace{1cm} (3)
where we define integrals over the velocity space as follows:

\[ \int_{\mathbb{R}^d} \psi \, dv =: \langle \psi \rangle \quad (4) \]

and \( m(v) = (1, v, |v|^2/2) \) are the collision invariants. Integrating (1) against its invariants in velocity space leads to the following set of conservation laws:

\[ \partial_t (mf) + \nabla_x (vmf) = 0. \quad (5) \]

Equilibrium functions for the operator \( Q(f, f) \) (i.e. solutions of \( Q(f, f) = 0 \)) are local Maxwellian of the form

\[ M_f(\rho, u, T) = \frac{\rho}{(2\pi T)^{d/2}} \exp\left(-\frac{|u-v|^2}{2T}\right). \quad (6) \]

where \( \rho, u, T \) are the density, mean velocity and temperature of the gas at position \( x \) and at time \( t \)

\[ \rho = \int_{\mathbb{R}^d} f \, dv, \quad u = \frac{1}{\rho} \int_{\mathbb{R}^d} vf \, dv, \quad T = \frac{1}{d\rho} \int_{\mathbb{R}^d} |v-u|^2 f \, dv. \quad (7) \]

In the sequel we will denote by

\[ U = (\rho, u, T), \quad E[U] = M_f. \quad (8) \]

Clearly we have

\[ U = \langle mE[U] \rangle. \quad (9) \]

Now, when the mean free path between the particles is very small compared with the typical length scale of the experiment, the operator \( Q(f, f) \) is large and we can rescale the space and time variables in (1) as

\[ x' = \varepsilon x, \quad t' = \varepsilon t, \quad (10) \]

to obtain

\[ \partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f), \quad (11) \]

where \( \varepsilon \) is a small parameter proportional to the mean free path and the primes have been omitted to keep notations simple.

Passing to the limit for \( \varepsilon \to 0 \) leads to \( f \to E[U] \) and thus we have a closed hyperbolic system of equations for the macroscopic variables \( U \)

\[ \partial_t U + \nabla_x F(U) = 0, \quad (12) \]

with \( F(U) = \langle vmE[U] \rangle \).

3. THE MOMENT GUIDED MONTE CARLO METHODS

For the sake of simplicity, in this work, we consider the problem in one dimension both in physical and velocity spaces. Extensions to multidimensional problems are straightforward and will be considered in [12]. The starting point of the method is the following micro–macro decomposition

\[ f = E[U] + g. \quad (13) \]

The function \( g \) represents the nonequilibrium part of the distribution function. From the definition above, it follows that \( g \) is in general nonpositive. Moreover, since \( f \) and \( E[U] \) have the same moments we have

\[ \langle mg \rangle = 0. \quad (14) \]
Now $U$ and $g$ satisfy the coupled system of equations

$$\partial_t U + \partial_x F(U) + \partial_x (v \langle mg \rangle) = 0, \tag{15}$$

$$\partial_t f + v \partial_x f = Q(f, f). \tag{16}$$

We skip the elementary proof of the above statement and refer to [13] for details on the decomposition of the distribution function and the coupled systems which it is possible to derive.

Our goal is to solve the kinetic equation with a MC method, and concurrently the fluid equation with any type of finite difference or finite volume scheme, where the correction term $\partial_x (v \langle mg \rangle)$ is evaluated using particle moments. The two Equations (15)–(16), except for numerical errors, give the same results in terms of macroscopic quantities. It is natural to assume that the set of moments obtained from the fluid system represents a better statistical estimate of the true moments of the solution, since the resolution of the moment equations does not involve any stochastic process.

Thus, we can summarize the method in the following way. At each time step $t^n$

1. Solve the kinetic equation (16) with an MC scheme and obtain a first set of moments $U^n = \langle mf^n \rangle$.
2. Solve the fluid equation (15) with a finite volume/difference scheme using particles to evaluate $\partial_x (v \langle mg \rangle)$ and obtain a second set of moments $U^{n+1}$.
3. Match the moments of the kinetic solution with the fluid solution through a transformation of the samples values $f^{n+1} = T(f^n)$ so that $\langle mf^{n+1} \rangle = U^{n+1}$.
4. Restart the computation to the next time step.

For Step 1, one can use any MC method (or more generally any low accurate but fast solver). Steps 2 and 3 of the above procedure require great care since they involve the evaluation of $\partial_x (v \langle mg \rangle)$ and the moment matching procedure.

Finally let us note that, in principle, it is possible to improve the method, adding to system (15) additional equations for the time evolution of higher order moments and we get

$$\partial_t \langle m_n f \rangle + \partial_x \langle vm_n f \rangle = \langle m_n Q(f, f) \rangle \tag{17}$$

with $m_n = v^n$ and $n \geq 3$. The solution of (17) with a finite volume/difference scheme, which in the general case is not straightforward, will provide a better estimate of the moments which are used in the moment matching [14–16].

We will call this general class of methods as MG MC schemes. In the sequel, we briefly focus on steps 2 and 3 of the above procedure.

3.1. Solution of the moment equations

In this section we discuss the discretization of the moment equations. We will, at the end of the section, suggest some approaches that can possibly be used to improve the method in the nearby future. Our scope, in the construction of the numerical scheme, is to take advantage from the knowledge of the Euler part of the moment equations

$$\partial_t U + \partial_x F(U) + \partial_x (v \langle mg \rangle) = 0. \tag{18}$$

Euler equations

Thus, the method is based on solving first the set of compressible Euler equations, for which many efficient numerical methods have been developed in the literature, and then considering the discretization of the kinetic flux $\partial_x (v \langle mg \rangle)$. To that aim, for the space discretization of the compressible Euler equations we use a second-order MUSCL central scheme, whereas a backward discretization is used for the time derivative in all cases

$$\frac{U_i^m - U_i^n}{\Delta t} + \frac{\psi_{i+1/2}(U^n) - \psi_{i-1/2}(U^n)}{\Delta x} = 0. \tag{19}$$
The discrete flux reads
\[
\psi_{i+1/2}(U^n) = \frac{1}{2} (F(U^n_i) + F(U^n_{i+1})) - \frac{1}{2} \sigma_i (U^n_{i+1} - U^n_i) + \frac{1}{2} (\sigma^n_{i+1} - \sigma^n_i),
\]
where
\[
\sigma^n_{i+1} = (F(U^n_{i+1}) \pm \alpha U^n_{i+1} - F(U^n_i) \mp \alpha U^n_i) \phi_{\epsilon}(\lambda^n_{i \pm})
\]
with \(\phi_{\epsilon}\) being a modified slope limiter. Classical slope limiters, based on the total variation arguments, determine which regions of the domain can be solved by a second-order method and which regions need a first-order method to avoid the onset of numerical oscillations. Following the same principle, we define a modified limiter which takes into account also the departure from the thermo-dynamical equilibrium of the gas. Thus, to switch from the second to the first-order discretization, we have:
\[
\phi_{\epsilon}(\chi) = \phi_L(\chi) \beta,
\]
where \(\phi_L(\chi)\) is the van Leer limiter
\[
\phi_L(\chi) = \frac{|\chi| + \chi}{1 + \chi},
\]
and
\[
\beta = \begin{cases} 
1 & \text{if } \sum_i |\lambda^n_i| < \beta_{th} \sum_i |F_3(U_i^n)| \\
0 & \text{if } \sum_i |\lambda^n_i| > \beta_{th} \sum_i |F_3(U_i^n)| 
\end{cases}
\]
with \(\beta_{th}\) being a given threshold value, while
\[
\lambda_i = \int_{\mathbb{R}^3} |v|^2 \beta^n_i \, dv
\]
and \(F_3(U)\) is the energy flux. Note that in the one-dimensional case the nonequilibrium mass and momentum fluxes are identically zero. The MUSCL second-order scheme is then used when \(\lambda\) is small and when \(\phi_L = 1\), whereas the first-order scheme is used otherwise. In the above equations \(\alpha\) is equal to the larger eigenvalue of the Euler system in the fluid limit, whereas it is equal to \(\Delta x/\Delta t\) in the large Knudsen regimes (\(\beta = 0\)). The variable \(\lambda^n_{i \pm}\) is defined as follows:
\[
\lambda^n_{i \pm} = \frac{F(U^n_i) \pm \alpha U^n_i - F(U^n_{i-1}) \mp \alpha U^n_{i-1}}{F(U^n_{i+1}) \pm \alpha U^n_{i+1} - F(U^n_i) \mp \alpha U^n_i}
\]
where the above ratio of vectors is defined componentwise. This method, as shown in the tests, does not increase fluctuations and, at the same time, guarantees a lower level of numerical dissipation in the results.

We now discuss how to discretize the nonequilibrium term \(\dot{\varepsilon}_m < v_m g >\). To this aim, the same space first-order discrete derivative is used as for the hydrodynamic flux \(F(U)\). The nonequilibrium term \(<v_m (f - E[U])>\) is computed by taking the difference between the moments of the particle solution and those of the Maxwellian equilibrium. Thus the final scheme, for the moment equations, reads
\[
\frac{U^n_{i+1} - U^n_i}{\Delta t} + \frac{\psi_{i+1/2}(U^n) - \psi_{i-1/2}(U^n)}{\Delta x} + \frac{\Psi_{i+1/2}(<v_m g^n>) - \Psi_{i-1/2}(<v_m g^n>)}{\Delta x} = 0,
\]
where \(\psi_{i+1/2}(U^n)\) can be either first or second order, whereas \(\Psi_{i+1/2}(<v_m g^n>)\) is always first order. In our method, in addition to the mass momentum and energy equations, we consider the third-order moment evolution equation. In this case, like in (17), we have the additional problem of evaluating the source term that now appears at the right-hand side. At the particle level this can
be done by simply measuring the variations of higher order moments in each cell during particle collisions. Thus, the discretized third-order moment equation is performed in two steps, where the second one reads

\[
\frac{\langle m_3 f^n_{i+1/2} \rangle - \langle m_3 f^n_{i} \rangle}{\Delta t} + \frac{\Psi_{i+1/2}(\langle m_3 f^n \rangle) - \Psi_{i-1/2}(\langle m_3 f^n \rangle)}{\Delta x} = 0,
\]

(28)

and where \( f^* \) is the solution of the first step, the collision step, which depends on the type of collisional operator. We will describe this step in the numerical test section below in the case of a BGK-type kernel. The main advantage of considering additional moment equations is that this reduces the fluctuations in the evaluations of the macroscopic quantities \( U \). Indeed, in the extended moment system, particles play a role only in the evaluation of higher order terms \( \langle v^p f \rangle, p > 3 \) and not directly on the evolution of the hydrodynamics quantities.

As a conclusion for this section, we discuss some possible improvements that will be developed in future works [12]. To this aim, we observe that the decomposition of the flux term into an equilibrium and a nonequilibrium part can be further exploited. Indeed, as an effect of the guided MC technique, the only remaining source of fluctuations in the moment equations is due to the nonequilibrium term \( \hat{c}_x \langle vmg \rangle \). Thus, instead of using the same numerical scheme as for the flux \( \hat{c}_x \langle F_U \rangle \), we can develop a specific discretization method which further reduces the variance of these fluctuations. We can consider cell averages of the form

\[
\frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \hat{c}_x \langle vmg \rangle \, dx = \frac{\langle vmg \rangle|_{x=x_{i+1/2}} - \langle vmg \rangle|_{x=x_{i-1/2}}}{\Delta x}, \quad m = (1, v, |v|^2),
\]

with \( \langle vmg \rangle = \langle vmf \rangle - F(U) \). The integral over the velocity space can be evaluated by summing over the particles

\[
\langle vmf \rangle|_{x=x_{i+1/2}} \approx \frac{1}{N} \sum_{j \in I_{i+1/2}} B(p_j - x_{i+1/2})m_j,
\]

(30)

where \( p_j \) and \( v_j \) represent the position and velocity of the \( j \)th particle, \( m_j = (1, v_j, |v_j|^2) \), \( I_{i+1/2} \) a given space interval of size \( h \) (typically \( h \geq \Delta x \)) containing \( x_{i+1/2} \) and \( B \geq 0 \) is a suitable weight function s.t.

\[
\int_{\mathbb{R}} B(x) \, dx = 1.
\]

For example, \( B(x) = 1/h \) if \( |x| \leq h/2 \) and \( B(x) = 0 \) elsewhere gives rise to a simple sum of the particles moments in the interval \( I_{i+1/2} \) known as the ‘Nearest Grid Point’ procedure in plasma physics [17]. Smoother reconstructions can be recovered by convolving the samples with a bell-shaped weight like a B-spline [18]. Note that the value \( h \) has a strong influence on the fluctuations in the reconstructed function, and in general should be selected as a good compromise between fluctuations and resolution.

3.2. The moment matching

In the present work we restrict ourselves to the following linear transformation: let a set of velocities \( v_1, \ldots, v_J \) with first two moments \( \mu_1 \) and \( \mu_2 \) be given. Suppose better estimates \( \sigma_1 \) and \( \sigma_2 \) of the same moments are available (using the moment equation). We can apply the transformation described in [3]

\[
v_i^* = (v_j - \mu_1)/c + \sigma_1 \quad c = \sqrt{\frac{\mu_2 - \mu_1^2}{\sigma_2 - \sigma_1^2}}, \quad i = 1, \ldots, J
\]

(31)

to get

\[
\frac{1}{J} \sum_{j=1}^{J} v_j^* = \sigma_1, \quad \frac{1}{J} \sum_{j=1}^{J} (v_j^*)^2 = \sigma_2.
\]
Of course this renormalization is not possible for the moment of order zero (the mass density). Let us denote by $\mu_0$ an estimate of the zero-order moment and by $\sigma_0$ its better evaluation by the moment equations.

Among the possible techniques that can be used to restore a prescribed density we choose to replicate or discard particles inside the cells. Other possibilities are to deal with weighted particles, move particles among cells according to some interpolation procedure or reconstruct the probability distribution starting from samples and resample particles. We leave a deeper analysis of possible alternate choices to future works.

In order to recover the moment $\sigma_0$, in the case $\mu_0 > \sigma_0$, we can use a discarding procedure. Note that we would like to eliminate exactly the following number of particles:

$$N_p = \frac{\mu_0 - \sigma_0}{m_p},$$

where $m_p$ is the mass of a single particle. In general, the precise match is impossible, since the particles mass is kept fixed in time, and $N_p$ cannot be an integer. A fixed mass $m_p$ implies that

$$\mu_0 = N_1 m_p, \quad \sigma_0 = N_2 m_p$$

with $N_1$ and $N_2$ being integers such that $N_1 > N_2$. $N_1$ and $N_2$ are the number of particles in the cell before and after the matching. Moreover, since the estimate $\sigma_0$ is not in general an integer multiple of $m_p$, a mismatch $e$ such that $e < \pm m_p$ is unavoidable. Thus, we can simply eliminate from the cell a suitable stochastic integer approximation of $\tilde{N}_p$:

$$N_p = \text{Iround} \left( \frac{\mu_0 - \sigma_0}{m_p} \right),$$

where Iround($x$) is a stochastic rounding defined as

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

with $[x]$ being the integer part of $x$.

In the opposite case, in which the mass of the particles inside a cell is lower than the mass prescribed by the fluid equations $\mu_0 < \sigma_0$, the situation is less simple. In this situation, since the distribution function is not known analytically, it is not possible to sample new particles without introducing correlations between samples. In this case we need to replicate

$$N_p = \text{Iround} \left( \frac{\sigma_0 - \mu_0}{m_p} \right)$$

particles. Note that this is done by allowing repetitions. After the generation step, samples are relocated uniformly inside each spatial cell.

Now we briefly discuss the possibility of forcing samples to follow higher order prescribed moments. To this aim, observe that, the moment matching procedure has infinite possible solutions, since the number of particles inside a cell is larger than the number of the constraints. However, we aim at finding a transformation which possibly preserves the Gaussian distribution. The only operations, which obey this constraint, are linear transformations such as (31), i.e. shifts and homotheties of the particle velocities.

However, if we slightly relax the constraint of preservation of the Gaussian distribution, we can reformulate the problem in the following terms: find a suitable transformation that leads to the required moments with the minimal changes in the distribution function. In the general case, this request has a nontrivial answer which can be recovered by solving an appropriate nonlinear system of equations with several constraints at each time step for every cell. For this reason, an efficient implementation of this procedure is still an open question.
4. NUMERICAL RESULTS

In the present section we report some numerical results of the moment-guided (MG) method on different test cases obtained using a simplified BGK model for the kinetic equation. First, we perform an accuracy test using a smooth periodic solution and then we consider three classical shock problems. In all the tests, we compared the MG solution with the standard MC solution and with the direct deterministic solution to the BGK equations based on a discrete velocity model (DVM) [19].

4.1. The moment-guided DSMC method applied to the BGK model

In this paragraph we detail a possible algorithm, which merges the techniques described in the previous sections, in the case of the simplified BGK collision operator.

As usual the starting point of MC methods is given by a time splitting [18] between free transport and collision, which in the case of the BGK operator is substituted by a relaxation towards the equilibrium

\[ \hat{\partial}_t f + v \cdot \nabla_x f = 0, \]  

and collision, which in the case of the BGK operator is substituted by a relaxation towards the equilibrium

\[ \hat{\partial}_t f = \frac{1}{\epsilon} (f - E[U]). \]  

In MC simulations the distribution function \( f \) is discretized by a finite set of particles

\[ f = \sum_{i=1}^{N} m_p \delta(x - x_i(t)) \delta(v - v_i(t)), \]  

where \( x_i(t) \) represents the particle position and \( v_i(t) \) represents the particle velocity. During the transport step then, the particles move to their next positions according to

\[ x_i(t + \Delta t) = x_i(t) + v_i(t) \Delta t, \]  

where \( \Delta t \) is such that an appropriate CFL condition holds.

The collision step changes the velocity distribution and, in this simplified case, the space homogeneous problem admits the exact solution at time \( t + \Delta t \)

\[ f(t + \Delta t) = e^{-\Delta t/\epsilon} f(t) + (1 - e^{-\Delta t/\epsilon}) E[U](t). \]  

The relaxation step of a MC method for the BGK equation consists in replacing randomly selected particles with Maxwellian particles with probability \( (1 - e^{-\Delta t/\epsilon}) \). Thus

\[ v_i(t + \Delta t) = \begin{cases} 
  v_i(t) & \text{with probability } e^{-\Delta t/\epsilon}, \\
  E[U](v) & \text{with probability } 1 - e^{-\Delta t/\epsilon},
\end{cases} \]  

where \( E[U](v) \) represents a particle sampled from the Maxwellian distribution with moments \( U \).

Thus, finally, at each time step the MG MC method reads as follows:

(i) transport and collide particles (40)–(42);
(ii) solve the first three moment equations (27) and the additional equation for the third-order moment (28);
(iii) match the computed mass, momentum and energy of the particle solution (Section 3.2) to those computed with the moment equations.

Moments are reconstructed by simple summation formulas in each cell; fluxes are then obtained by interpolation on the grid points and then discretized with Lax–Friedrichs type central schemes of second order as described in the previous sections.
Figure 1. Statistical error test: solution at $t = 0.05$ for density (top), velocity (middle) and temperature (bottom). MC method (left), Hydro Guided MC method (right). Knudsen number vary from $\varepsilon = 10^{-1}$ to $\varepsilon = 10^{-4}$. Squares indicate errors for $\varepsilon = 10^{-1}$, diamonds for $\varepsilon = 10^{-2}$, circles for $\varepsilon = 10^{-3}$, whereas crosses indicate errors for $\varepsilon = 10^{-4}$.

Remark 1
After the relaxation step (41), the perturbation term can be rewritten as

$$g(t + \Delta t) = f(t + \Delta t) - E[U(t + \Delta t)] = e^{-\Delta t/\varepsilon} f(t) + (1 - e^{-\Delta t/\varepsilon}) E[U(t)]$$

$$- E[U(t + \Delta t)] = e^{-\Delta t/\varepsilon} (f(t) - E[U(t)]) = e^{-\Delta t/\varepsilon} g(t),$$

(43)
Figure 2. Steady shock: solution at $t = 0.3$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 5 \times 10^{-2}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line.

As $\Delta t/\varepsilon$ grows, which means that the system approaches the equilibrium, the contribution of the kinetic term vanishes even though it is evaluated through particles. This does not happen if we...
only compute the kinetic term $\hat{c}_s(v_{mg})$ from the particles without considering the structure of the distribution function $f$. This dramatically decreases fluctuations when the Knudsen number is small.

Since this property is related to the BGK structure and we aim at a method that can be applied to the full Boltzmann equation, we do not take advantage of it in the numerical results. We leave the possibility to extend this idea to the Boltzmann equation using time relaxed Monte Carlo (TRMC) methods [20] to future investigations.

Figure 3. Steady shock: solution at $t = 0.3$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 10^{-4}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line.
4.2. Accuracy test

First we report on the results of a stochastic error analysis with respect to the number of particles. As reference solution we considered the average of $M$ independent realizations

$$\overline{U}_{MC} = \frac{1}{M} \sum_{i=1}^{M} U_{i,MC}$$  \hfill (45)
Figure 5. Unsteady shock: solution at $t = 0.065$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 10^{-3}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Two hundred particles for cell.

and

$$U_{MG} = \frac{1}{M} \sum_{i=1}^{M} U_{i,\text{MG}},$$

(46)

where the two subscripts MC and MG indicate, respectively, the reference solution for the MC method and for the MG method. Only for this test first-order discretizations are used to evaluate the fluxes in the moment equations. In addition, we use two different reference solutions since the
two schemes present different discretization errors and thus they converge, when the number of particles goes to infinity, to different discretized solutions. The difference between the two large particle limit solutions (MC and MG MC) is mainly due to the different numerical dissipations introduced by the two methods. Some figures, which compare the two methods for increasing number of particles, will be shown in the case of the unsteady shock and the Sod test which follow in the next paragraphs. The two reference solutions are obtained by fixing the time step and mesh size and letting the number of particles go to infinity. The number of samples used to compute the

Figure 6. Unsteady shock: solution at $t=0.065$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 10^{-2}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Two hundred particles for cell.
Figure 7. Unsteady shock: solution at $t = 0.065$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 10^{-1}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Two hundred particles for cell.

'exact' solution is on average 20 000 per cell, whereas the number of cells is 100. The time step is $10^{-3}$ when the Knudsen number lies between $10^{-3}$ and $10^{-1}$ and $10^{-4}$ when the Knudsen is equal to $10^{-4}$. In this way, both reference solutions contain negligible stochastic error. At the same time, both solutions involve space and time discretization errors. However, the amount of such errors does not change when the number of particles varies. Therefore, by comparing solutions obtained with a given $\Delta t$, $\Delta x$, but with a finite number of particles to reference solutions obtained
Figure 8. Unsteady shock: solution at $t=0.065$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 10^{-2}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Four hundred particles for cell.

with the same $\Delta t$, $\Delta x$, but with a very large number of particles, we obtain a true measure of the error originating from the stochastic nature of the method. Then, we measure the quantity

$$\Sigma^2(N) = \frac{1}{M} \sum_{i=1}^{M} \sum_{j=1}^{j_{\text{max}}} (U_{i,j} - \bar{U}_j)^2,$$

(47)
Figure 9. Unsteady shock: solution at $t = 0.065$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided method MG (right). Knudsen number $\varepsilon = 10^{-1}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Four hundred particles for cell.

where $\overline{U}_j$ represents the reference solution and $j_{\text{max}}$ represents the number of mesh point. The test consists of the following initial data:

$$
\rho(x, 0) = 1 + a_\rho \sin \frac{2\pi x}{L},
$$

$$
u(x, 0) = 1.5 + a_\nu \sin \frac{2\pi x}{L},$$

$$\frac{1}{2} \int f |v|^2 \, dv = W(x, 0) = 2.5 + a_W \sin \frac{2\pi x}{L},$$

(48)

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Figure 10. Sod shock tube test: solution at $t = 0.05$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided MG method (right). Knudsen number $\varepsilon = 10^{-4}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Two hundred particles for cell.

with

$$a_0 = 0.3, \quad a_u = 0.1, \quad a_W = 1.$$  

This test problem gives rise to a periodic smooth solution in the interval $t \in [0, 5 \times 10^{-2}]$. The results of this test in log–log scale are shown in Figure 1. On the left, we reported the stochastic error for the pure MC and on the right for the MG method. From top to bottom, the errors for the three macroscopic quantities are depicted for different values of the Knudsen number. For the MC case, the stochastic error does not substantially change with respect to the Knudsen number.
and shows a convergence rate approximatively equal to $\frac{1}{2}$. At variance, for the MG method, errors decrease as the Knudsen number diminishes and the convergence rate of the method seems to increase achieving larger values (between 0.5 and 1). This behavior is due to the fact that, for large Knudsen numbers, the kinetic part of the solution, $g$, is not negligible and evaluated through the DSMC method. On the contrary, close to thermodynamical equilibrium, $g \rightarrow 0$, which means that the MC component of the solution carries only fluctuations but no information. It is remarkable that, in all analyzed regimes, the stochastic error of the MG method is smaller than that of the pure particle solver.
Figure 12. Sod shock tube test: solution at \( t = 0.05 \) for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided MG method (right). Knudsen number \( \varepsilon = 10^{-2} \). Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Two hundred particles for cell.

4.3. Steady shock test

As a second test case we consider the classical stationary shock wave problem. The gas is initially divided into two uniform left and right Maxwellian states separated by a discontinuity at \( x = 0.5 \). The two states are related by the Rankine–Hugoniot relations. For the upstream flow, the density value is \( \rho = \frac{9}{5} \), the mean velocity \( u = -\frac{5}{3} \sqrt{3} \), and the pressure \( p = 13 \). For the downstream flow the density is equal to \( \rho = 1 \), the mean velocity to \( u = -3 \sqrt{3} \) and the pressure to \( p = 1 \). The number of cells is equal to 200 while the time step is given by the minimum between the Knudsen number,
the ratio of $\Delta x$ over the maximum velocity owned by the particles and the ratio of $\Delta x$ over the larger eigenvalues of the compressible Euler system. The final time is 0.3, the number of particles for cell is on average 200 (i.e. the total number of particles inside the domain is $200^2$ allocated proportionally to the mass in each cell). Figures 2 and 3 consider the same initial data with different initial Knudsen number values, respectively, $\varepsilon = 5 \times 10^{-2}$ and $\varepsilon = 10^{-4}$.

In the figures we report the density, the mean velocity and the temperature from top to bottom, with the pure MC solver (on the left) and MG method (on the right). In addition, we represent solutions of the compressible Euler equations and as the reference solution we used a DVM for
Figure 14. Sod shock tube test: solution at $t = 0.05$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided MG method (right). Knudsen number $\varepsilon = 10^{-2}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Eight hundred particles for cell.

The two figures show a large reduction in fluctuations especially for the small Knudsen number case. We observe also both for the MG method and the MC method a small shift to the right for the density and the velocity profile in the large Knudsen case (Figure 2) compared with the reference solution, whereas the temperature profile is slightly steeper around 0.8 for the MG method. To this aim, we remark that a shift phenomenon has already been observed and discussed by Ohwada [21] in 1993. To prevent the onset of this phenomenon in numerical simulation, a stabilization technique is normally used. In the present paper we did not make use of such techniques which have to be probably designed for this particular class of hybrid methods.
Figure 15. Sod shock tube test: solution at $t = 0.05$ for the density (top), velocity (middle) and temperature (bottom). MC method (left), moment-guided MG method (right). Knudsen number $\varepsilon = 10^{-1}$. Reference solution: dash dotted line. Euler solution: continuous line. Monte Carlo or moment guided: circles plus continuous line. Eight hundred particles for cell.

in a different way respect to classical finite volume methods. We defer a detailed analysis on this problem to a future work.

4.4. Unsteady shock test

Next we consider an unsteady shock test case. This choice reflects the fact that the method is specifically aimed at situations in which the classical variance reduction technique using time averaging cannot be used or turns out to be useless, since time averaging or using more particles leads to the same computational effort.
Figures 4–7 consider the same initial data for the density \( \rho = 1 \), the mean velocity \( u = -1 \) and the temperature \( T = 1 \) with different initial Knudsen number values, ranging from \( \varepsilon = 10^{-4} \) to \( \varepsilon = 10^{-1} \). At the beginning of the simulation 200 particles per cell are used, the number of cells is 200 while the time step is given by the minimum between the Knudsen number, the ratio of \( \Delta x \) over the maximum velocity owned by the particles and the ratio of \( \Delta x \) over the larger eigenvalues of the compressible Euler system. Each figure depicts the density, the mean velocity and the temperature from top to bottom, with the pure MC solver (on the left) and the MG method (on the right).

In addition, we represent solutions of the compressible Euler equations and as reference solution we used a DVM for the BGK equation [19]. These figures show a large reduction in fluctuations especially for small Knudsen numbers for the MG method in comparison with the standard MC method. In Figures 8 and 9 we report the same simulations of Figures 6 and 7 (i.e. the Knudsen number equal to \( 10^{-1} \) and \( 10^{-2} \)) where the number of initial particles is doubled, which means 400 particles on an average for a cell. These figures show that the MG method approaches the solution furnished by the DVM also in the case of large Knudsen values. Moreover, thanks to the high-order discretization of the moment equations the physical accuracy is almost the same of the MC method in the fluid limit, which means that the shock is well represented.

4.5. Sod shock tube

Finally we look at the classical Sod shock tube test. Again this choice relies on the fact that the method is specifically aimed at unsteady problems in which the classical time averaging technique turns out to be useless. Figures 10–13 consider the same initial data for the density \( \rho = 1 \) upstream and \( \rho = 0.125 \) downstream of the initial shock, the mean velocity \( u = 0 \) in all the domain and the temperature: \( T = 5 \) upstream and \( T = 4 \) downstream of the shock. Different initial Knudsen number values are considered in the test, which range from \( \varepsilon = 10^{-4} \) to \( \varepsilon = 10^{-1} \) while the number of cell is 200. Two hundred particles per cell are used on an average, more precisely 200\(^2\) particles are present at the beginning of the simulation and then distributed accordingly to the density in each cell. Finally the time step is given by the minimum between the Knudsen number, the ratio of \( \Delta x \) over the maximum velocity of the particles and the ratio of \( \Delta x \) over the larger eigenvalues of the compressible Euler equations. As for the unsteady shock test each figure depicts the density, the mean velocity and the temperature from top to bottom, with the pure MC solver (left) and the MG method (right). A reference solution obtained through a discrete velocity scheme [19] is represented in each figure as well as the solution of the compressible Euler equations. The figures show good results for all ranges of Knudsen numbers in terms of reduction in fluctuations. The high-order solver permits to improve the accuracy of the solution in the fluid limit without introducing additional fluctuations for large Knudsen. Finally, Figures 14 and 15 represent the same solution both for the MC and the MG method for Knudsen equal to \( \varepsilon = 10^{-1} \) and \( \varepsilon = 10^{-2} \) with 800 particles for cell on an average at the beginning of the simulation. These figures permit to show the convergence of the MG method towards the reference solution also in the case of larger Knudsen. Observe that, in all tests and different figures reported in the paper, the fluctuations which are present in the MG solution are less in comparison with the original MC method.

5. CONCLUSIONS

We have developed a new class of hybrid methods which aim at reducing the variance in MC schemes. The key idea consists in driving particle positions and velocities in such a way that moments given by the solution of the kinetic equation exactly match moments given by the solution of an appropriate set of moment equations. It is important to point out that the schemes that can be derived through this technique can be easily implemented in the existing MC codes through few modifications; adding a fluid solver and a routine for the moment matching.

Preliminary numerical results show reductions in fluctuations in all regimes compared with DSMC. The reduction becomes stronger as we approach equilibrium. Numerical convergence tests show better performances of the proposed method, in terms of stochastic error, compared with pure
MC schemes. For these problems the MG method seems very promising, leading to solutions that contain less fluctuations at a computational cost which is comparable to the cost of a traditional MC solver, and the addition of the cost of a macroscopic solver for the compressible Euler equations, which is usually computationally less expensive than the MC method.

Currently, we are working on extensions of the present method to the full Boltzmann equation in the multidimensional case. To this aim we plan to use both classical MC methods such as Bird or Nanbu methods [5] and TRMC techniques [20]. Moreover, we plan to explore other possible algorithms that can possibly further reduce fluctuations, such as matching higher order moments and/or using higher order closure of the hierarchy in order to solve a larger set of hydrodynamics equations, or using hybrid representations of the distribution function [4]. We hope to be able to present other results supporting this methodology in the near future [12].

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