A remark on the finite number of particles effect in Monte Carlo methods for kinetic equations

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Monte Carlo methods are the most popular methods for solving problems in kinetic theory [2, 5]. In this short remark we emphasize some of the side effects due to the use of conservative methods over a finite number of statistical samples (particles) in the simulation. The most relevant aspect is that the steady states of the system are compactly supported and thus they cannot be Maxwellian (or any other non compactly supported statistics) unless the number of particles goes to infinity. These aspects are studied numerically with the help of a simple one-dimensional space homogeneous kinetic model.

1 Introduction

The numerical solution of kinetic equations is usually performed through statistical simulation methods such as Monte Carlo [3]. The reason for this is twofold, on the one hand probabilistic techniques provide an efficient toolbox for the simulation due to the reduced computational cost when compared with deterministic schemes, on the other hand the evolution of the statistical samples follows the microscopic binary interaction dynamics thus providing all the relevant physical properties of the system. Traditionally the methods are considered extremely efficient when dealing with stationary problems. In such case, in fact, fluctuations can be eliminated by taking subsequent averages of the solution after then a certain ”stationary time” has been reached. Here we show, with the help of a simple one-dimensional system, that this averaging procedure does not guarantee convergence towards the correct steady state due to finite number of particles correlations introduced by the microscopic conservation laws. Similar analysis for rarefied gas dynamics have been done in [9, 6].

1.1 The model equation

We will consider a simple one–dimensional kinetic model, where the binary interaction between particles obey to the law

$$v' = v\cos\theta - w\sin\theta, \qquad w' = v\sin\theta + w\cos\theta, \tag{1}$$

where $\theta \in [-\pi, \pi]$ is a collision parameter. The microscopic energy after the binary interaction rule is conserved

$$(v')^2 + (w')^2 = v^2 + w^2, \tag{2}$$

whereas momentum is not.

Let $f(v,t)$ denote the distribution of particles with velocity $v \in \mathbb{R}$ at time $t \geq 0$. The kinetic model can be easily derived by standard methods of kinetic theory, considering that the change in time of $f(v,t)$ depends on a balance between the gain and loss of particles with velocity v due to binary collisions. This leads to the following integro-differential equation of Boltzmann type [4],

$$\frac{\partial f}{\partial t} = \int_{\mathbb{R}} \int_{-\pi}^{\pi} \frac{1}{2\pi} \left(f(v')f(w') - f(v)f(w) \right) d\theta \, dw. \tag{3}$$

As a consequence of the binary interaction the second momentum of the solution is conserved in time, whereas the first momentum is preserved only if initially it is equal to zero. For this model one can show that the stationary solution $f_\infty(v)$ is the Maxwell density

$$f_\infty(v) = \frac{1}{\sqrt{2\pi}} e^{-v^2/2}. \tag{4}$$

A standard Monte Carlo method for this equation can be easily derived using either Bird’s or Nanbu’s algorithm for Maxwell molecules [2, 5]. The two algorithms differ mainly in the way the time discretization is treated, but not in the way collisions (sampling from the collision integral operator) are performed. Our results do not differ for the two methods.

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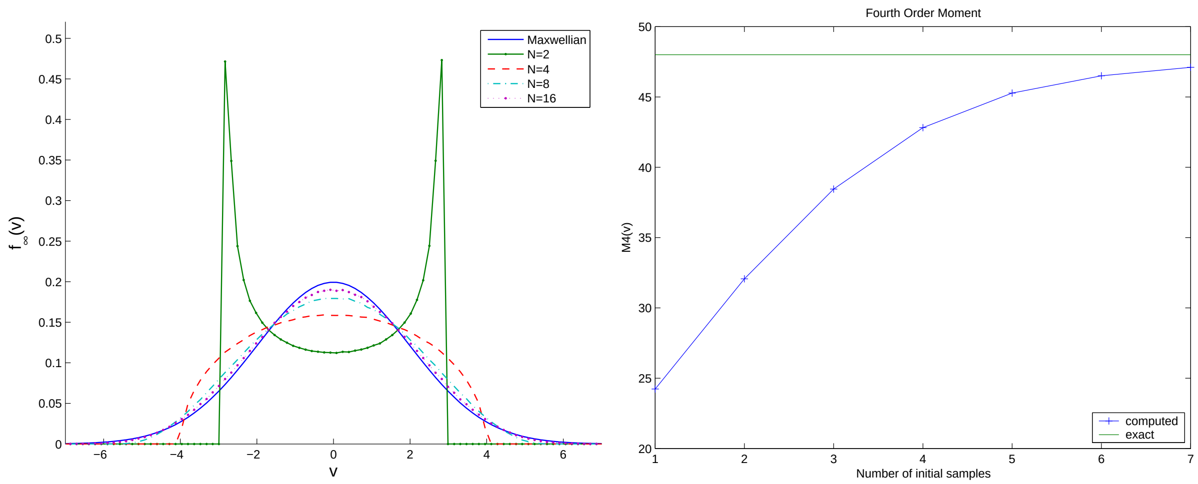

Fig. 1 Equilibrium states for different finite sets of particles vs Maxwellian (left) and equilibrium value of the fourth order moment for the different finite sets of particles.

2 Numerical results

The problem we consider here is related to the effect of the finite number of particles in Monte Carlo simulations. Note that given a set of particles $v_1, v_2, \ldots, v_N$ with energy $E = \frac{1}{2}\sum_{i=1}^{N} v_i^2$, we have the inequality

$$|v_i| \leq R_N = \sqrt{2EN}. \tag{5}$$

As a consequence of this, any particle dynamic, namely any transformation of the type

$$v_i' = \phi_i(v_1, \ldots, v_N), \quad i = 1, \ldots, N, \tag{6}$$

that preserves exactly energy is such that the particle solution remains compactly supported in $[-R_N, R_N]$ at any time. This implies that the distribution of such particles cannot be Maxwellian (or any other non compactly supported statistics) unless the particles number goes to infinity. This is exactly what happens if we use the so-called Nanbu-Babovsky [1] strategy of performing collisions by pairs so that the Monte Carlo methods are exactly conservative and not conservative in the mean. We report in Figure 1 (left) the numerical distribution of the finite sets of particles in the case of the one-dimensional Maxwell model (3). The results have been obtained taking initially Maxwellian samples with zero mean and energy 4 and then averaging in time over the Monte Carlo solutions to the equation. For very small numbers of particles it is remarkable that the computed distribution differ considerably from the expected Maxwellian. The different fourth order moments of the corresponding steady solutions are then plotted in Figure 1 (right) against the exact fourth order moment of the Maxwellian. We point out that such small particle numbers can be present is some cells when one consider fully non homogeneous rarefied gas flow simulations and thus, even if the transport part can affect the nature of these correlations, a particular care has to be taken when averaging over such small numbers. Similar conclusion are valid also for different kinetic models where the steady state statistics is not compactly supported like in granular gases, plasma physics, quantum kinetic theory, traffic flows and economic models.

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