Comparison of the DSMC Method with an Exact Solution of the Boltzmann Equation

J. M. Montanero and A. Santos

Departamento de Física, Universidad de Extremadura, Spain

Abstract

Results obtained from the Direct Simulation Monte Carlo method are compared with an exact solution of the Boltzmann equation for Maxwell molecules in a far from equilibrium shear flow state. In the simulations, Bird's and Nanbu's schemes have been used with different values for the number of particles N. It is observed that for small values of N ($N < 500$) both schemes give incorrect results, the discrepancies being larger in the case of Nanbu's scheme. For $N = 5 \times 10^4$ both schemes agree reasonably well with the exact solution, but Bird's scheme consumes less computer time.

1 Introduction

The Direct Simulation Monte Carlo (DSMC) method [1] has proved in the last two decades to be an important tool to study a large variety of phenomena in rarefied gases. In order to be useful, the DSMC method must be efficient (from a computer point of view) and reliable (in the sense of capturing as many features of the Boltzmann equation as possible). This compromise has led to a number of different versions of the DSMC method, the most relevant of which are Bird's scheme [1] and Nanbu's scheme [2].

Nanbu has shown [3] that, if the parameters of the simulations are chosen properly, both schemes reproduce correctly an exact solution of the spatially homogeneous Boltzmann equation for Maxwell molecules. the so-called BKW-mode [4]. Nevertheless, the BKW-mode is a state relatively close to equilibrium that relaxes in a simple way, so that a more stringent test of the DSMC method is desirable.

The aim of this paper is to perform a comparison of the DSMC method with an *exact* solution of the Boltzmann equation which applies for states *arbitrarily* far from equilibrium. Such a solution is briefly described in §2. The main differences between Bird's and Nanbu's schemes of the DSMC method, as well as some technical details of our simulations, are given in §3. The results of the comparison are presented in §4. Finally, §5 summarizes the main conclusions.

2 Uniform shear flow

Let us consider a flow characterized by a constant density n, a spatially homogeneous temperature T, and a linear profile of the x-component of the flow velocity $\mathbf{u}$ along the y-axis:

$$\mathbf{u} = a\, y\, \hat{\mathbf{x}}\,, \tag{2.1}$$

a being the (constant) shear rate, which measures the departure from equilibrium. The above state is usually referred to as uniform shear flow, since it can be seen as spatially homogeneous in the Lagrangian frame of reference. Thus, the Boltzmann equation becomes

$$\frac{\partial}{\partial t} f - a V_y \frac{\partial}{\partial V_x} f = J[f,f]\,, \tag{2.2}$$

where $\mathbf{V} = \mathbf{v} - \mathbf{u}$ is the peculiar velocity. The hierarchy of moment equations associated to eqn. (2.2) can be recursively solved in the case of Maxwell molecules. The time evolution of the second and the third degree moments is explicitly given in Ref. [5]. For instance, the temperature evolves according to

$$\begin{aligned} T(t) = \; & T_0\, e^{\lambda t^*} \tfrac{1}{1+3\lambda} \Big\{ (1+\lambda)^2 + \lambda e^{-(1+\frac{3}{2}\lambda)t^*} \\ & \times \Big[(1-\lambda)\cos(\omega t^*) - \tfrac{\lambda(5+3\lambda)}{\omega} \sin(\omega t^*) \Big] \Big\}\,, \end{aligned} \tag{2.3}$$

if the initial condition is that of local equilibrium. Here, $t^* = t/\tau$, where τ is a convenient mean free time and

$$\lambda(a) = \frac{4}{3} \sinh^2 [\frac{1}{6} \cosh^{-1}(1 + 9a^2\tau^2)]\,, \tag{2.4}$$

$$\omega(a) = [\lambda(1 + \frac{3}{4}\lambda)]^{1/2}\,. \tag{2.5}$$

The fourth degree moments have also been evaluated recently [6,7]. For instance, if $a = 6.45\tau^{-1}$, one has [7]

$$\begin{aligned} \langle V^4 \rangle = \; & (2k_BT/m)^2 \{182.7 - 178.2e^{-0.0215t^*} + e^{-5.82t^*}[0.46\cos(2.83t^*) \\ & + 3.03\sin(2.83t^*)] - 0.014e^{-4.40t^*} - e^{-7.48t^*}[0.012\cos(1.75t^*) \\ & + 0.011\sin(1.75t^*)] + e^{-9.52t^*}[0.64\cos(4.65t^*) - 0.42\sin(4.65t^*)] \end{aligned} \tag{2.6}$$

if the initial condition is such that the second degree moments grow exponentially in time as $e^{\lambda t^*}$.

3 DSMC method

The DSMC method simulates the stochastic process associated to the Boltzmann equation, interpreted as a master equation for the velocity

distribution function f [2]. Since the probability per unit of time for a transition $(\mathbf{r},\mathbf{v}) \to (\mathbf{r}',\mathbf{v}')$ depends on f itself, one must estimate it by considering a system of N particles. Furthermore, the results are averaged over an ensemble of M members. In the method, the free motion and the collisions are uncoupled over the time step Δt. In the collision stage, a representative set of collisions is chosen, so that pre-collision velocities are replaced by random post-collision velocities. For further details we refer the reader to Refs. [1,2]. The main difference between Bird's and Nanbu's DSMC schemes appears in the collision stage. This is specially apparent in the case of Maxwell molecules, for which the collision rate per particle ρ is constant. In Bird's scheme, the steps in the collision stage can be summarized as follows:

1. Choose at random $N' = \frac{1}{2} N \rho \Delta t$ collisional pairs.
2. Assign post-collision velocities to both particles of each pair.

On the other hand, the steps in Nanbu's scheme are:

1. Choose at random k colliding particles, where the number k is sampled from the binomial distribution $P(k) = \binom{N}{k} p^k (1-p)^{N-k}$, with $p = \rho \Delta t (N-1)/N$.
2. Choose at random a collision partner for each colliding particle.
3. Assign post-collision velocities to the colliding particles (but not to their partners)

We have used both schemes to simulate eqn. (2.2). Since eqn. (2.2) is spatially homogeneous (in the Lagragian frame), it is not necessary to store the coordinates of the particles. Instead, the free motion stage consisted of applying a nonconservative (inertial) force $\mathbf{F} = -maV_y\hat{\mathbf{x}}$ on each particle of velocity $\mathbf{V}$. The simulations have been performed with a cut-off value $\beta_0 = 3$ for the dimensionless impact parameter. The number of particles has been $N = 15, 25, 50, 500, 5 \times 10^4$. Finally, the time step and the number of members in the ensemble have been $\Delta t = 0.000294\tau$ and $M = 1.25 \times 10^6 N^{-1}$ (in the simulations for the second degree moments) or $\Delta t = 0.00294\tau$ and $M = 3.75 \times 10^6 N^{-1}$ (in the simulations for the fourth degree moments).

4 Results

Figure 1 shows the time dependence of the relative deviation between the simulation temperature T_s and the exact temperature T_e, eqn. (2.3), for a shear rate $a = 6\tau^{-1}$. We observe that the magnitude of the deviations tends to increase with time and is significant if N is not sufficiently large. Bird's scheme tends to overestimate the temperature, while the opposite happens with Nanbu's scheme. On the other hand, the deviations are smaller in the case of Bird's scheme. For instance, at $t = 5\tau$ and $N = 50$, the error in the temperature is about 0.8% in Bird's scheme and about 8% in Nanbu's

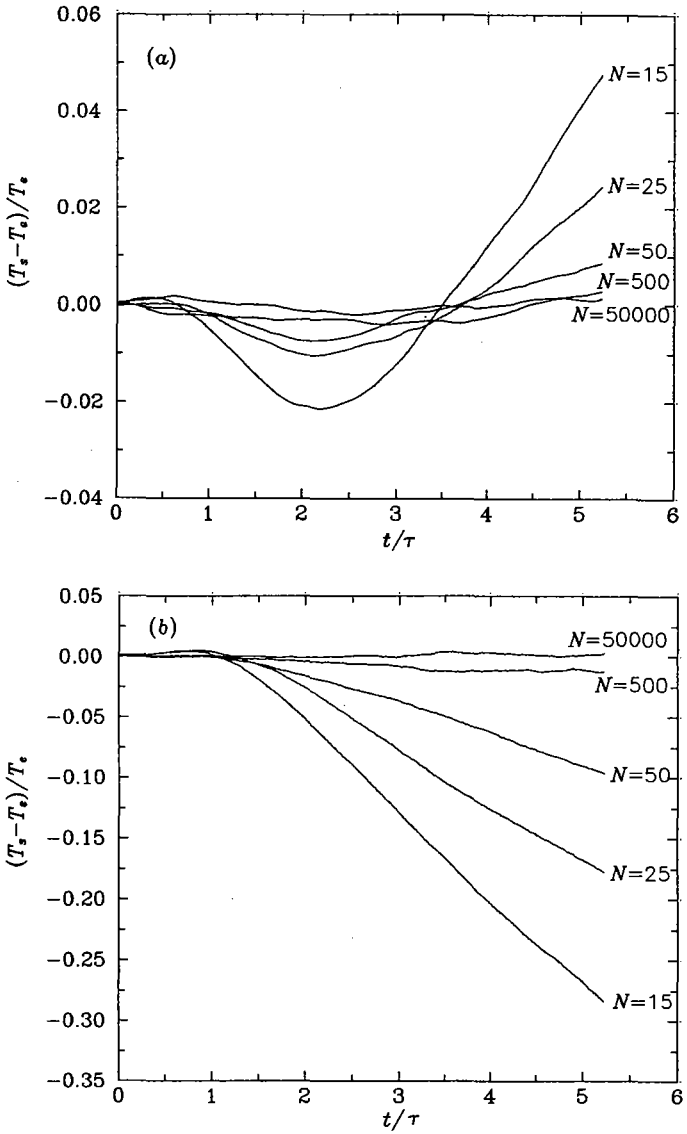

Figure 1. Time evolution of the relative difference between the temperature measured in the simulations, T_s, and the exact temperature, T_e, for several values of N by using (a) Bird's scheme and (b) Nanbu's scheme. The shear rate is $a = 6\tau^{-1}$.

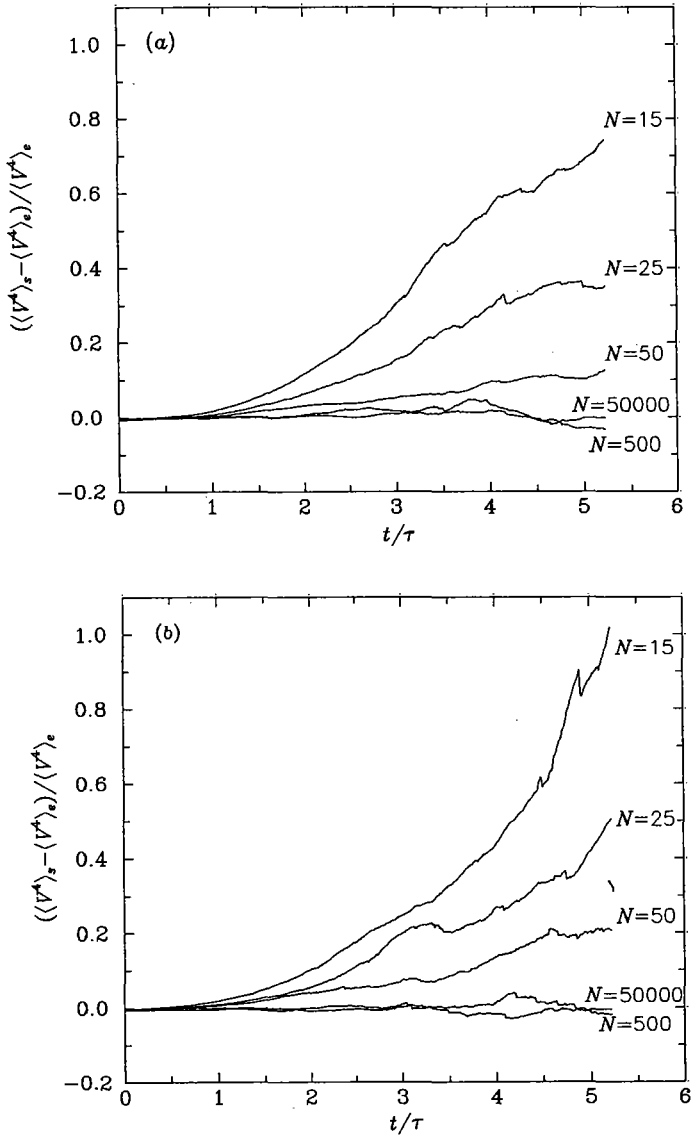

Figure 2. Same as in Fig. 1 but for the fourth moment $\langle V^4\rangle$. The shear rate is $a = 6.45\tau^{-1}$.

scheme.

Figure 2 shows a similar comparison, but for the fourth moment $\langle V^4 \rangle$. The shear rate is now $a = 6.45\tau^{-1}$, so that the exact moment, $\langle V^4 \rangle_e$, is given by eqn. (2.6). Again, the deviations increase with time if N is not sufficiently large and are more important in the case of Nanbu's scheme. For instance, at $t = 5\tau$ and $N = 50$, the error in $\langle V^4 \rangle$ is about 12% in Bird's scheme and about 20% in Nanbu's scheme. In contrast to what happens with the temperature, however, the sign of the deviations is the same in both schemes.

5 Conclusions

In this paper we have compared the results for the second and fourth degree velocity moments obtained from the DSMC method in the uniform shear flow with an exact solution of the Boltzmann equation for Maxwell molecules [5,6,7]. By choosing the value of the shear rate, this state can be made arbitrarily far from equilibrium. Two schemes of the DSMC method have been used: Bird's [1] and Nanbu's [2]. The results show that when the simulation parameters (such as the time step and the cut-off in the impact parameter) are properly chosen, the DSMC method reproduces correctly the details of the solution of the Boltzmann equation, provided that the number of particles N is sufficiently large. For instance, an excellent agreement is found if $N = 5 \times 10^4$ [8].

In contrast to what one could expect [2], the errors associated to small values of N are more important in Nanbu's scheme than in Bird's. The two main differences between both schemes in the case of Maxwell molecules are: (i) in Bird's scheme the number of particles that change their velocities upon collision is fixed, while in Nanbu's scheme that number fluctuates; (ii) in Bird's scheme both particles involved in a collision change their velocities, while in Nanbu's scheme only one of the two particles modifies its velocity. We have checked that it is the latter point which actually has a remarkable influence. Results obtained from a hybrid scheme made of Bird's point (i) and Nanbu's point (ii) are hardly distinguishable from those obtained from Nanbu's scheme, and vice versa. Futhermore, from a practical point of view, Bird's scheme is preferable, since it consumes less computer time (about one half in our simulations) than Nanbu's scheme.

This work was supported by the DGICYT (Spain) through Grant No. PB91-0316. The research of J. M. M. has been supported by a predoctoral fellowship from the MEC (Spain).

Bibliography

1. Bird, G. A. (1976): *Molecular Gas Dynamics.* Clarendon Press, Oxford; Bird, G. A. (1994): *Molecular Gas Dynamics and the Direct Simulation of Gas Flows.* Clarendon Press, Oxford.
2. Nanbu, K. (1986): Theoretical Basis of the Direct Simulation Monte Carlo Method. *Proceedings of the 15th International Symposium on Rarefied Gas Dynamics*, edited by V. Boffi and C. Cercignani. B. G. Teubner, Stuttgart, 369–383.
3. Nanbu, K. (1980): Direct Simulation Scheme Derived from the Boltzmann Equation. I. Monocomponent Gases. *J. Phys. Soc. Jpn.* **49**, 2042–2049; Nanbu, K. (1983): Derivation from Kac's Master Equation of the Stochatic Laws for Simulating Molecular Collisions. *J. Phys. Soc. Jpn.* **52**, 4160–4165.
4. See, for instance, Ernst, M. H. (1981): Nonlinear Model-Boltzmann Equations and Exact Solutions. *Phys. Rep.* **78**, 1–171.
5. Truesdell, C. and Muncaster, R. G. (1980): *Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas.* Academic Press, New York, Ch. XIV.
6. Santos, A., Garzó, V., Brey, J. J. and Dufty, J. W. (1993): Singular Behavior of Shear Flow Far from Equilibrium. *Phys. Rev. Lett.* **71**, 3971–3974; **72**, 1392 (Erratum).
7. Santos, A. and Garzó, V. (1994): Exact Moment Solution of the Boltzmann Equation for Uniform Shear Flow. *Physica A*, submitted.
8. See Figs. 1 and 2 in Montanero, J. M. and Santos, A. (1994): Comparison of the DSMC Method with an Exact Solution of the Boltzmann Equation. *Book of Abstracts of the 19th International Symposium on Rarefied Gas Dynamics.*

COMPARISION OF THE DSMC METHOD WITH AN EXACT SOLUTION OF THE BOLTZMANN EQUATION

J. M. Montanero and A. Santos
Departamento de Física, Universidad de Extremadura, E-06071, Badajoz, Spain

The Direct Simulation Monte Carlo (DSMC) method has proved to be an efficient tool to study a large variety of phenomena in rarefied gases. There are essentially two DSMC schemes: Bird's scheme [1] and Nanbu's scheme [2]. The main differences between both schemes are most apparent in the case of Maxwell molecules. In Bird's scheme, the steps in the collision stage are: (i) choose at random $N' = \frac{1}{2}N\rho\Delta t$ collisional pairs, where N is the number of particles in the system, Δt is the time-step, and ρ is the collision rate per particle; (ii) assign post-collision velocities to both particles of each pair. In Nanbu's scheme the steps are: (i) choose at random k colliding particles, where the number k is sampled from the binomial distribution $P(k) = \binom{N}{k}p^k(1-p)^{N-k}$, $p = \rho\Delta t(N-1)/N$; (ii) choose at random a collision partner for each colliding particle; (iii) assign post-collision velocities to the colliding particles (but not to their partners). It is generally believed that both DSMC methods reproduce correctly the solution of de Boltzmann equation (BE). In fact, both of them give results in agreement with the BKW-mode [2], an exact solution of the spatially homogeneous BE for Maxwell molecules. However, the scarcity of exact solutions of the BE for states arbitrarily far from equilibrium has prevented a more stringent test of the DSMC method.

In this contribution, we compare Bird's and Nanbu's schemes with an exact solution of the BE for Maxwell molecules in a non-homogeneous situation, the so-called uniform shear flow (USF); USF is characterized by a linear profile of the flow velocity, namely $u_x = ay$, $u_y = u_z = 0$, and uniform density n and temperature T [3]. The shear rate a measures the distance from equilibrium. In the simulations we have taken $N = 5\times 10^4$ particles, a cut-off value $\beta_0 = 3$ for the dimensionless impact parameter, and a time-step $\Delta t = 0.000294\ \tau$, τ being and effective mean free time; as a consequence, $\rho\Delta t = 0.004$. Figure 1 shows the time evolution of the reduced temperature $T^* = e^{-\lambda t}T(t)/T_0$ where T_0 is the initial temperature and $\lambda = \frac{4}{3}\tau^{-1}\mathrm{sh}^2[\frac{1}{6}\mathrm{ch}^{-1}(1+9(a\tau)^2)]$, for the case $a = 6\tau^{-1}$. The dashed line is the exact result [3], the solid line corresponds to results obtained from Nanbu's scheme, and the dotted line corresponds to Bird's scheme, in both cases by averaging over an ensemble of 15 members. We observe that both DSMC schemes describe very well the evolution of T^*, especially the transient regime.

The exact fourth-order moments for USF have been recently obtained [4]. This allows us to perform a stronger comparision with simulation. Figure 2 shows the time evolution of $M_4 = <(\mathbf{v}-\mathbf{u})^4>/(2k_BT/m)^2$ for $a = 6.45\tau^{-1}$. The meaning of the lines is as in Fig. 1, except that the number of members of the ensemble in the simulation is 75. The agreement of the theory and simulation is excellent. The degree of distortion of the state from equilibrium is measured by the fact that $M_4 = \frac{15}{4}$ at equilibrium and $\frac{63}{20} \le M_4 \le \frac{15}{4}$ in the BKW-mode.

We conclude that, when the simulation parameters are properly chosen, the DSMC method reproduces correctly the details of the solution of the BE. The scheme to be used is mainly a question of taste, although Bird's scheme usually consumes less computer time than Nanbu's scheme.

[1] G. A. Bird, *Molecular Gas Dynamics* (Clarendon, Oxford, 1976).
[2] K. Nanbu, in *Proceedings of the 15th International Symposium on Rarefied Gas Dynamics*, edited by V. Boffi and C. Cercignani (B. G. Teubner, Stuttgart, 1986), pp 369-383, and references therein.
[3] C. Truesdell and R. G. Muncaster, *Fundamentals of Maxwell's kinetic theory of a simple monatomic gas* (Academic Press, NY, 1980)
[4] A. Santos and V. Garzó, unpublished.

Figure 1

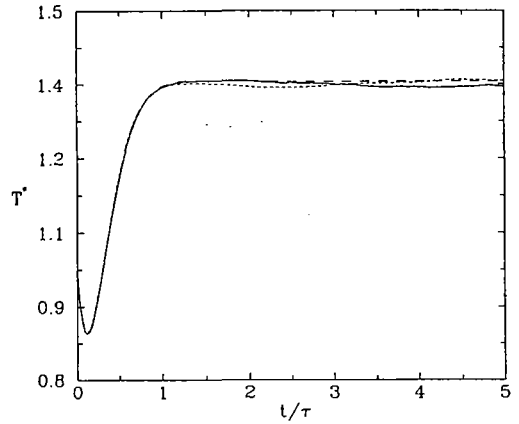

Figure 2