Numerical study of a direct simulation Monte Carlo method for the Uehling-Uhlenbeck-Boltzmann equation

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Abstract. In this paper we describe a DSMC algorithm for the Uehling-Uhlenbeck-Boltzmann equation in terms of Markov processes. This provides a unifying framework for both the classical Boltzmann case as well as the Fermi-Dirac and Bose-Einstein cases. By numerical experiments we study the sensitivity of the algorithm to the number of simulation particles and to the discretization of the velocity space, when approximating the steady state distribution.

INTRODUCTION

The recent landmark experiments of Bose-Einstein condensation have generated significant interest in quantum ideal gases (see [8] and references therein). Kinetic theory is useful in the study of a quantum gas, especially when the particle dynamics can be decomposed into two-body collisions and a mean field potential. For this regime, Uehling and Uhlenbeck [16] extended the Boltzmann equation to quantum systems by including the Pauli factor. In the spatially homogeneous case, this equation takes the form

$$\begin{aligned}\frac{\partial}{\partial t} f(t,v) \quad = \quad & \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, B(v,w,e) \Big[(1+\theta f(t,v))\,(1+\theta f(t,w))\, f(t,v^*)\, f(t,w^*) - \\ & (1+\theta f(t,v^*))\,(1+\theta f(t,w^*))\, f(t,v)\, f(t,w) \Big], \end{aligned} \tag{1}$$

with initial condition $f(0,v) = f_0(v)$.

The postcollision velocities corresponding to $v, w \in \mathcal{R}^3$ are

$$v^*(v,w,e) = v + e\,(e, w-v)\,, \quad w^*(v,w,e) = w - e\,(e, w-v)\,, \qquad e \in \mathcal{S}^2\,, \tag{2}$$

where $\mathcal{S}^2 \subset \mathcal{R}^3$ is the unit sphere, and $(.,.)$ denotes the scalar product in the Euclidean space $\mathcal{R}^3$. The function B is the collision kernel, which, in case of hard sphere molecules, takes the form $B(v,w,e) = \text{const}\,|(e, w-v)|$. Note that $n = \int_{\mathcal{R}^3} f_0(v)\, dv$ is the average number of physical particles per unit volume in position space. Equation (1) includes (namely for $\theta = 0$) the **Boltzmann** equation of classical statistics as a special case. It differs from the latter in the case of **Bose-Einstein** statistics ($\theta = +1$) and in the case of **Fermi-Dirac** statistics ($\theta = -1$). The case $\theta = +1$ has been studied recently in [14].

Direct simulation Monte Carlo (DSMC) has been the most widely used numerical algorithm for the classical Boltzmann equation [4]. Stochastic particle algorithms for the Uehling-Uhlenbeck-Boltzmann (UUB) equation were first developed to simulate the Fermi-Dirac dynamics of nucleons during heavy ion collisions [3], [2], [5]. These numerical methods were later reformulated into a DSMC-based framework by Lang, et al. [12]. Similar Monte Carlo algorithms have been used to study the dynamics of cooling [17] and trapping [6] in Bose-Einstein condensation. Dense gas corrections to the UUB equation have been modelled using the Consistent Boltzmann Algorithm [1], a dense gas variant of DSMC. This algorithm has been used to include

virial corrections to UUB simulations [11], [15]. Its asymptotic properties in the Boltzmann case have been studied in [9].

In this paper we describe a DSMC algorithm for the Uehling-Uhlenbeck-Boltzmann equation in terms of Markov processes. This provides a unifying framework for both the classical Boltzmann case as well as the Fermi-Dirac and Bose-Einstein cases. Using numerical experiments we study the sensitivity of the algorithm to the number of simulation particles and to the discretization of the velocity space, when approximating the steady state distribution.

The paper is organized as follows. In Section 2 we give a detailed description of the DSMC algorithm starting from a corresponding Markov jump process. Section 3 contains results of numerical experiments for both the Fermi-Dirac and Bose-Einstein cases. We calculate approximations to the equilibrium solution using the particle algorithm. We study the error depending on the numerical parameters like particle number or number of cells in the velocity space.

DESCRIPTION OF THE ALGORITHM

We introduce a Markov process

$$Z(t) = \Big(V_1(t), \dots, V_N(t)\Big), \qquad t \geq 0\,,$$

defined by the infinitesimal generator

$$\mathcal{A}(\Phi)(z) = \frac{n}{2N} \sum_{1 \leq i \neq j \leq N} \int_{\mathcal{S}^2} Q(z,i,j,e) \Big[\Phi(J(z,i,j,e)) - \Phi(z)\Big] de\,, \tag{3}$$

where

$$z = (v_1, \dots, v_N) \in \big(\mathcal{R}^3\big)^N = \mathcal{Z} \tag{4}$$

and N is the number of simulation particles. The jump transformation is (cf. (2))

$$[J(z,i,j,e)]_k = \begin{cases} v_k & \text{, if} \quad k \neq i,j\,, \\ v^*(v_i,v_j,e) & \text{, if} \quad k = i\,, \\ w^*(v_i,v_j,e) & \text{, if} \quad k = j\,. \end{cases} \tag{5}$$

The intensity function has the form

$$Q(z,i,j,e) = Y\left(\frac{n}{N}\sum_{k=1}^{N} g(v^*(v_i,v_j,e),v_k), \frac{n}{N}\sum_{k=1}^{N} g(w^*(v_i,v_j,e),v_k)\right) B(v_i,v_j,e)\,, \tag{6}$$

where g is some mollifying kernel,

$$g(v,w) = g(w,v) \geq 0\,, \qquad \int_{\mathcal{R}^3} g(v,w)\, dw = 1\,, \tag{7}$$

intended for approximating Dirac's delta-function. The concrete form of g as well as of the non-negative function Y will be specified later (cf. (14), (16) below).

For numerical purposes, we rewrite the generator (3) in the form

$$\mathcal{A}(\Phi)(z) = \int_{\mathcal{Z}} \Big[\Phi(\bar{z}) - \Phi(z)\Big]\, \hat{\mathcal{Q}}(z, d\bar{z})\,,$$

where

$$\hat{\mathcal{Q}}(z, d\bar{z}) = \tag{8}$$
$$\frac{n}{2N} \sum_{1 \leq i \neq j \leq N} \int_{\mathcal{S}^2} \Big\{\delta_{J(z,i,j,e)}(d\bar{z})\, Q(z,i,j,e) + \delta_z(d\bar{z}) \Big[\hat{Y}(z)\, \hat{B}(z) - Q(z,i,j,e)\Big]\Big\}\, de$$

and δ denotes the Dirac measure. The functions $\hat{B}$ and $\hat{Y}$ are such that (cf. (6))

$$Y\left(\frac{n}{N}\sum_{k=1}^{N} g(v^*(v_i,v_j,e),v_k), \frac{n}{N}\sum_{k=1}^{N} g(w^*(v_i,v_j,e),v_k)\right) \le \hat{Y}(z), \qquad \forall\, z\in\mathcal{Z}, \tag{9}$$

and

$$B(v_i,v_j,e) \le \hat{B}(z), \qquad \forall\, 1\le i\ne j\le N, \quad e\in\mathcal{S}^2, \quad z\in\mathcal{Z}. \tag{10}$$

Thus, the pathwise behaviour of the process is as follows. Coming to a state (4), the process stays there for a **random waiting time**, which has an exponential distribution with the parameter (cf. (8))

$$\hat{\pi}(z) = \hat{\mathcal{Q}}(z,\mathcal{Z}) = 2\pi\, n\, \hat{Y}(z)\, \hat{B}(z)\,(N-1). \tag{11}$$

Then the process jumps into a state $\bar{z}$, which is distributed according to the jump distribution

$$\hat{\pi}(z)^{-1}\,\hat{\mathcal{Q}}(z,d\bar{z}) = \\ \frac{1}{N\,(N-1)}\sum_{1\le i\ne j\le N}\frac{1}{4\pi}\int_{\mathcal{S}^2}\left\{\delta_{J(z,i,j,e)}(d\bar{z})\,\frac{Q(z,i,j,e)}{\hat{Y}(z)\,\hat{B}(z)} + \delta_z(d\bar{z})\left[1-\frac{Q(z,i,j,e)}{\hat{Y}(z)\,\hat{B}(z)}\right]\right\}.$$

Consequently, first the parameters i,j and e, are generated **uniformly**. Given i,j and e, the jump is **fictitious**, i.e. the new state is $\bar{z}=z$, with probability

$$1-\frac{Q(z,i,j,e)}{\hat{Y}(z)\,\hat{B}(z)}. \tag{12}$$

Otherwise, the new state is $\bar{z}=J(z,i,j,e)$.

For calculating the quantity (12), one needs to evaluate the **empirical density** (cf. (6))

$$\hat{f}(z,v) \;=\; \frac{n}{N}\sum_{k=1}^{N} g(v,v_k), \tag{13}$$

for $v=v^*(v_i,v_j,e)$ and $v=w^*(v_i,v_j,e)$. Note that (7) implies

$$\int_{\mathcal{R}^3}\hat{f}(z,v)\,dv = n, \qquad \forall z\in\mathcal{Z}.$$

For numerical purposes, it is convenient to introduce some partition $\mathcal{V}_l, l=1,...,M$, of the velocity space and to use the function

$$g(v,w) = \sum_{l=1}^{M}\frac{1}{|\mathcal{V}_l|}\,\chi_{\mathcal{V}_l}(v)\,\chi_{\mathcal{V}_l}(w), \tag{14}$$

where χ denotes the indicator function. Let $N_l, l=1,...,M$, be the number of particles with velocities in cell $\mathcal{V}_l$. Then the empirical density (13) takes the form

$$\hat{f}(z,v) = \frac{n\,N_{l(v)}}{N\,|\mathcal{V}_{l(v)}|}, \qquad v\in\mathcal{R}^3, \tag{15}$$

where $l(v)$ denotes the number of the cell to which v belongs. Note that the function (15) is constant in each cell.

The following algorithm is obtained.

0. Generate the initial state z so that (13) approximates f_0 for large N.

1. Given z calculate the time step

$$\frac{1}{2\pi\, n \hat{Y}(z)\, \hat{B}(z)\, (N-1)}$$

according to (11).

2. Generate $i\,, j\,, e$ uniformly and calculate

$$v_i^* = v^*(v_i, v_j, e)\,, \qquad v_j^* = w^*(v_i, v_j, e)$$

according to (5).

3. With probability (12), i.e. if

$$\frac{Y(\hat{f}(z, v_i^*), \hat{f}(z, v_j^*))}{\hat{Y}(z)}\, \frac{B(v_i, v_j, e)}{\hat{B}(z)} \;\leq\; \mathrm{RAND}\,,$$

go to **1.**

4. Replace $v_i\,, v_j$ by $v_i^*\,, v_j^*$.

5. Update $\hat{B}\,, \hat{f}\,, \hat{Y}$ and go to **1.**

Some remarks: First, in the Boltzmann case $Y \equiv 1$, the procedure differs slightly from standard DSMC. This is due to the fact that in general Y depends on e so that this parameter also must be generated **before** the rejection. Second, note that the function $\hat{Y}$ in (9) can be adapted during the process of computation, similar to the adaption of the function $\hat{B}$ in (10) depending on the maximum relative velocity. Third, even if $M = \infty$, the sum (14) remains finite. Alternatively, one considers the set outside some (big) ball in the velocity space as the last cell. The empirical density is there approximated by zero. Finally, the limiting equation (as $N \to \infty$) for this Markov process is the UUB equation (1), for the choice

$$Y(x, y) = (1 + \theta\, x)\, (1 + \theta\, y)\,, \qquad x, y \in \mathcal{R}\,. \tag{16}$$

The derivation will be presented elsewhere.

NUMERICAL EXPERIMENTS

The equilibrium density for the UUB equation takes the form [7,Ch. 17.5]

$$p(v) = \frac{1}{A \exp(\alpha\, \|v\|^2) - \theta}\,, \tag{17}$$

where $A > \max(\theta, 0)$ and $\alpha > 0$. Note that, in case $\theta > 0$ and $A \to \theta$, some delta-like distribution is obtained (Bose-Einstein condensation), while in case $\theta < 0$ and $A \to 0$, an approximate uniform distribution is obtained (Fermi level). For $A \to \infty$ distributions in both cases are close to a Maxwellian (with mean $\sim A^{-1}$). Finally, in case $\theta = 0$, a pure Maxwellian is obtained.

Since the equilibrium density is isotropic, it will be useful to consider the speed distribution, defined as

$$\tilde{p}(u) = \frac{4\pi u^2}{A \exp(\alpha\, u^2) - \theta}\,, \tag{18}$$

where $u = \|v\|$. Note that the speed distribution is merely $p(v)$ given in (17) integrated over angle.

Fermi-Dirac case

Figure 1 (left) shows the steady state speed distribution (18) measured in the simulation of a gas of Fermi-Dirac particles ($\theta = -1$). The parameters in this case are $A = 0.01$ and $\alpha = 1$, which corresponds to a temperature of $0.21\, T_F$ where T_F is the Fermi temperature [10]. The simulation used $N = 10^4$ particles and

$M = 10^4$ velocity cells[1] , which were cubic with a width of $\Delta v = 0.45$. Note that for this choice of parameters we find good agreement with the expected equilibrium distribution.

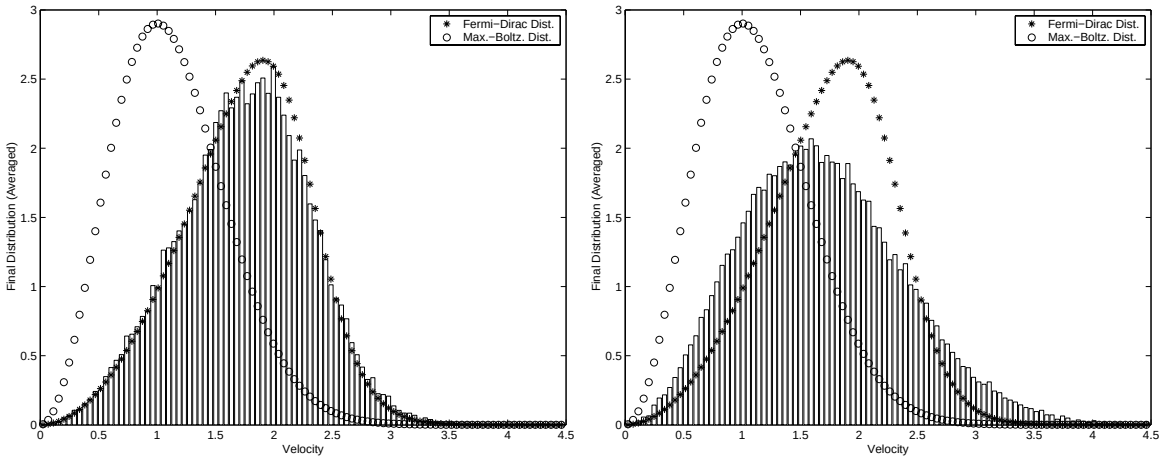

FIGURE 1. *Steady-state speed distribution in a Fermi-Dirac gas. Data from a simulation with $N = 10^4$ particles and $M = 10^4$ (left) or $M = 10^6$ (right) velocity cells is shown as histogram bars; expected distribution shown by asterisks. The Maxwell-Boltzmann distribution for a gas with the same kinetic energy is shown, by open circles, for comparison.*

To quantify this agreement, the square integrated difference between the measured and expected speed distribution was evaluated as,

$$E(N,M) = \int_0^\infty [\tilde{p}(u) - \tilde{p}_s(u;N,M)]^2 \, du$$

where $\tilde{p}_s$ is the estimated steady state distribution from the simulation. For the results shown in Fig. 1 this error was 0.031. For comparison, one finds an integrated square difference of about 10^{-5} in a comparable simulation of a Maxwell-Boltzmann gas (i.e., standard DSMC).[2] As the value of E also varies with the parameters A and α, we use the normalized error defined as $\bar{E}(N,M) = E(N,M)/E(10^4,10^4)$.

Interestingly, increasing the number of velocity cells can *reduce* the accuracy of the distribution, as seen in **Figure 1 (right)**, which is similar to the left figure but with the number of velocity cells increased to $M = 10^6$ (and the cell size reduced to $\Delta v = 0.09$). When the number of cells is significantly larger than the number of particles, Fermi exclusion is not accurately modelled.

This effect is confirmed in **Figure 2 (left)**, which shows the normalized error as a function of the number of cells for various values of N. On the other hand, for a given number of cells the error plateaus when $N \geq M$, as shown in **Figure 2 (right)**. Roughly speaking, the error is minimum when $N \approx M$ and when we take the number of particles equal to the number of cells we find that the $\bar{E} \approx N^{-1}$, as shown in **Figure 3**. One also finds that even when $N = M \approx 300$ the distribution retains a strong quantum signature, when compared with the corresponding Maxwell-Boltzmann distribution (dashed line in **Figure 3**). Note that all of these results are for simulations using the parameters $A = 0.01$ and $\alpha = 1$; for different values of the parameters we expect quantitatively different errors (e.g., $\bar{E}$ decreases as A increases) but qualitatively similar dependence on N and M.

Bose-Einstein case

Figure 4 (left) shows the steady state speed distribution (18) measured in the simulation of a gas of

[1] Actually the value of M is rounded to the nearest cubic integer, e.g., for $M = 10^5$ the number of velocity cells is actually $97336 = 46^3$.

[2] The error goes to zero, independent of N ($N > 1$) as the number of samples goes to infinity, that is, standard DSMC exactly reproduces the Maxwell-Boltzmann distribution.

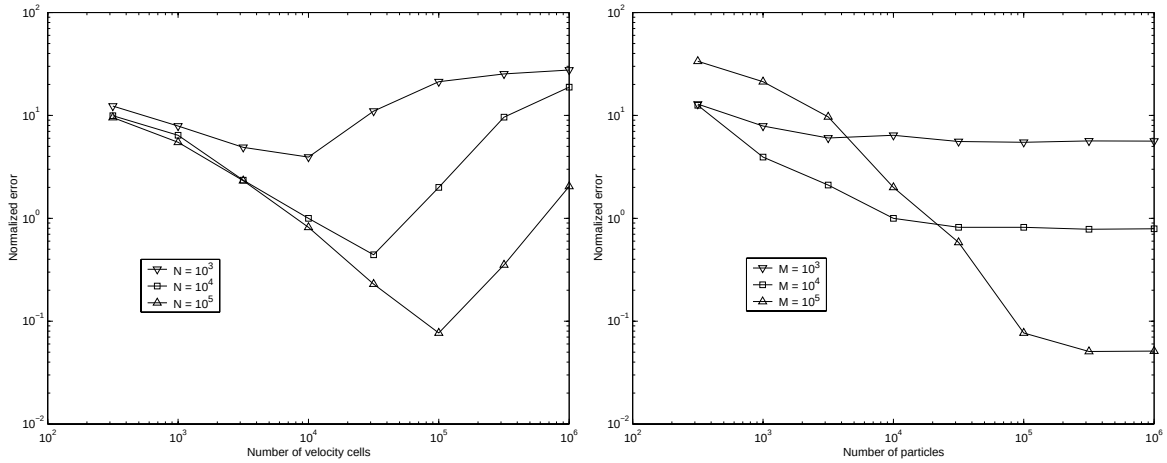

FIGURE 2. *Normalized error, $\bar{E}(N,M)$, in the steady-state Fermi-Dirac speed distribution as a function of the number of velocity cells (left) and as a function of the number of particles (right).*

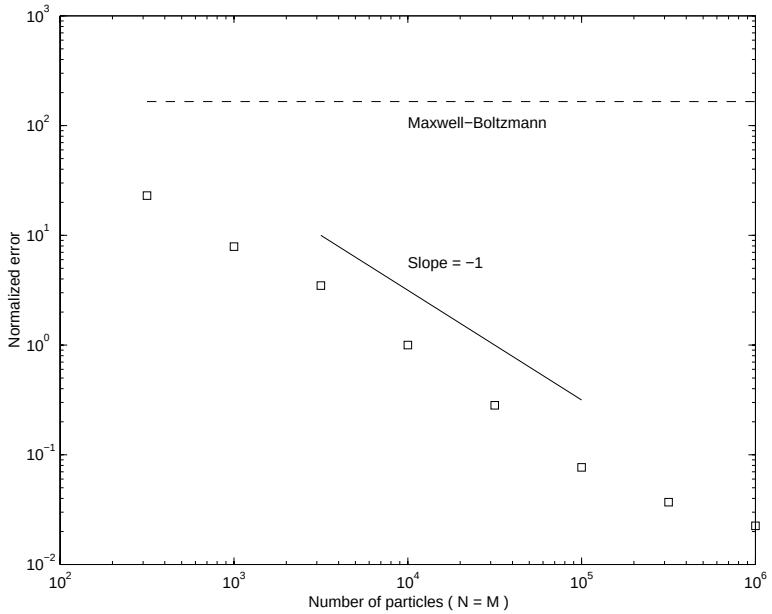

FIGURE 3. *Normalized error, $\bar{E}(N,M)$, in the steady-state Fermi-Dirac speed distribution as a function of $N = M$. For comparison, the error for a Maxwell-Boltzmann distribution (i.e., open circles in Fig. 1) is shown as a dashed line.*

Bose-Einstein particles ($\theta = 1$). The parameters in this case are $A = 1.01$ and $\alpha = 1$, which corresponds to a temperature of $1.08T_c$ where T_c is the critical temperature [10]. The simulation parameters are $N = 10^4$, $M = 10^4$ and $\Delta v = 0.38$. Although the agreement with the expected distribution is poor, **Figure 4 (right)** shows that the agreement is very good when N and M are increased to 10^6 (and Δv reduced to 0.08).

Figure 5 (left) shows that in these simulations of a Bose-Einstein gas, the normalized error drops with increasing number of velocity cells until $M \approx 100N$. On the other hand, for a given number of cells $\bar{E}(N,M)$ is approximately constant in N, as shown in **Figure 5 (right)**, when $N > M/10$. Finally, graphing $\bar{E}(N,M)$ versus $N = M$ (**Figure 6**) shows that the error decreases with N except for in the smallest simulations ($N \leq 10^3$). For those simulations the error plateaus at approximately that of a DSMC simulation for a

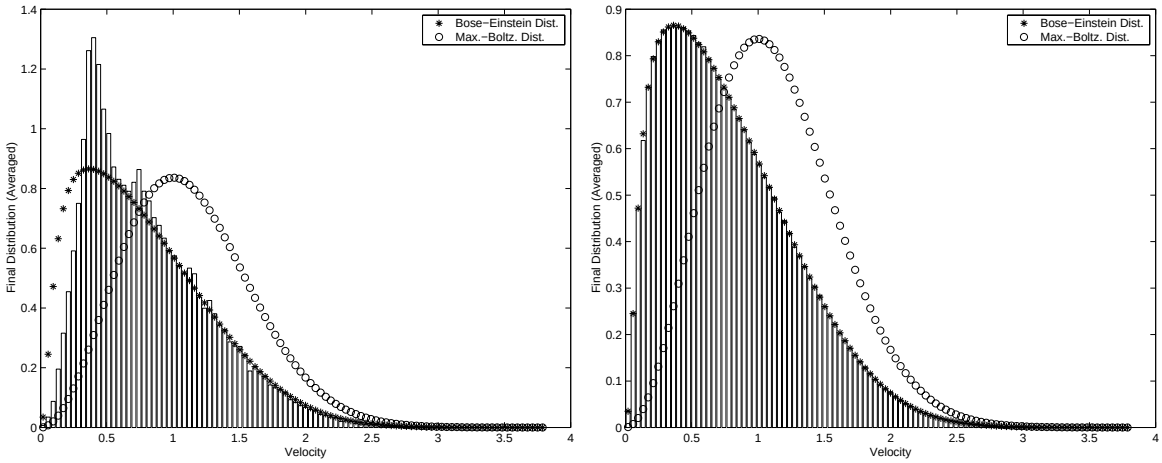

FIGURE 4. *Steady-state speed distribution in a Bose-Einstein simulation with $N = 10^4$ particles and $M = 10^4$ velocity cells (left) and with $N = 10^6$ particles and $M = 10^6$ cells.*

Maxwell-Boltzmann gas (i.e., $\theta = 0$), though the distribution is *not* Maxwellian. Again, all of the Bose-Einstein simulations used the parameters $A = 1.01$ and $\alpha = 1$; for different values of the parameters we expect quantitatively different errors (e.g., $\bar{E}$ decreases as A increases) but qualitatively similar dependence on N and M.

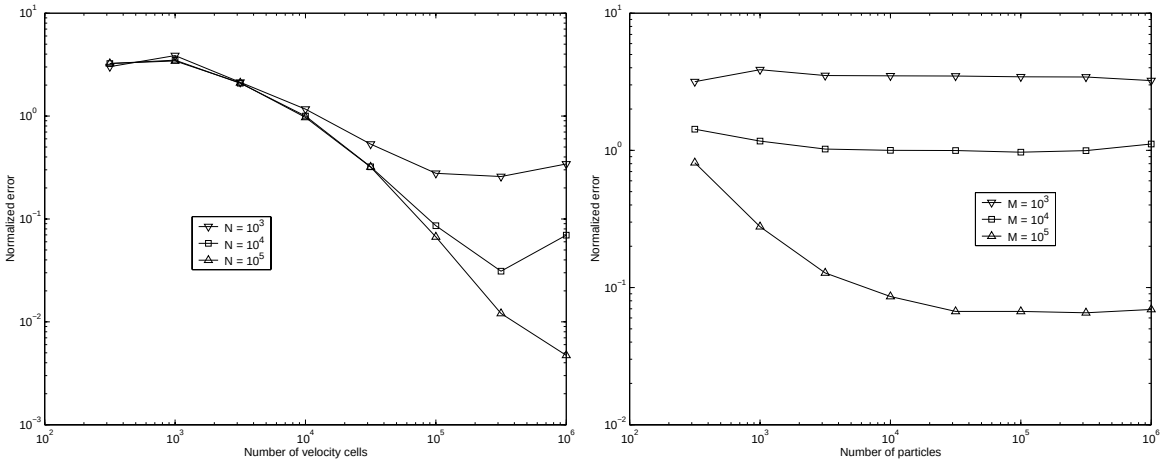

FIGURE 5. *Normalized error, $\bar{E}(N, M)$, in the steady-state Bose-Einstein speed distribution as a function of the number of velocity cells (left) and as a function of the number of particles (right).*

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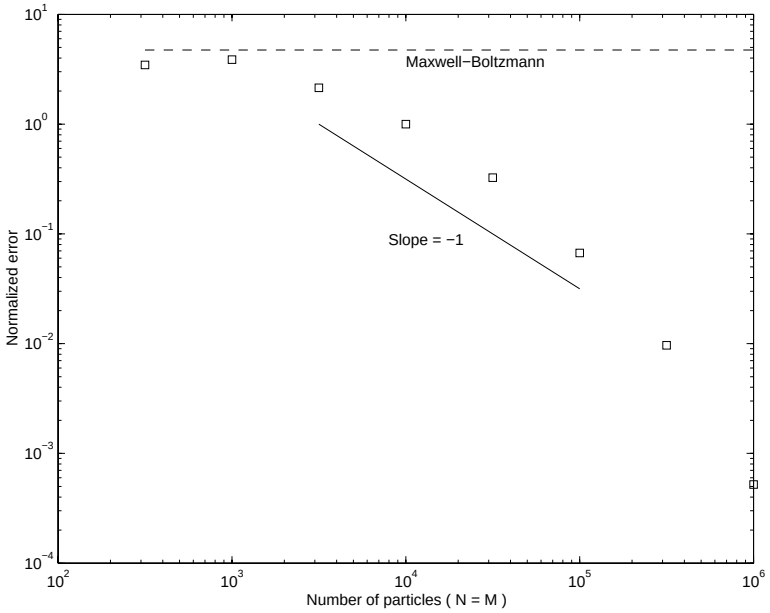

FIGURE 6. *Normalized error, $\bar{E}(N,M)$, in the steady-state Bose-Einstein speed distribution as a function of $N = M$. For comparison, the error for a Maxwell-Boltzmann distribution (i.e., open circles in Fig. 4) is shown as a dashed line and $\bar{E} = N^{-1}$ as a solid line.*

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