Stochastic dynamic simulation of the Boltzmann equation for electron swarms in glow discharges

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A stochastic simulation method is proposed which allows efficient treatment of the Boltzmann equation. Interesting quantities (e.g., the time evolution of electron energy, the electron energy distribution function, and the electron velocity distribution function) are evaluated with the help of a stochastic simulation, which generates realizations of the underlying stochastic process, referred to as the dynamic Monte Carlo simulation (DMCS) method. The DMCS technique proposed here does not require knowledge of the cumulative free-flight distribution, in contrast to both the direct simulation Monte Carlo (DSMC) and the more efficient "null collision" Monte Carlo method. A helium discharge was used as an application for the DMCS technique. Transport properties as well as the electron energy distribution function and the electron velocity distribution function for homogeneous dc and rf cases are presented.

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I. INTRODUCTION

Knowledge of the electron energy distribution function (EEDF) in gas discharges is of crucial importance in predicting electron-transport properties and electron-impact reaction kinetics. The EEDF permits us to determine essential parameters, such as ionization rates, mean electron energy, etc., from a given set of collision cross sections. In the literature one may read that the nonequilibrium characteristics of electron transport can be treated by either Boltzmann equation solvers or Monte Carlo simulations. Both approaches are employed to give the characteristics of an electron swarm under certain conditions. However, Monte Carlo simulations are usually not conceived as Boltzmann equation solvers. This study will show that the Monte Carlo technique developed here emanates from the Boltzmann equation.

Electron statistics are predicted either statistically, employing Monte Carlo techniques to handle collisions (particles-in-cell–Monte Carlo collision simulations [1]), or numerically ("convective schemes" [2]), using techniques that are capable of resolving the EEDF as a function of space and time.

Finite difference methods (FDMs) and finite element methods (FEMs) have also been employed to solve the Boltzmann equation. The electron energy distribution function is usually expanded into spherical harmonics and it is approximated by a finite number of terms [3–6]. The most popular two-term expansion [4] of the EEDF is limited to (a) a relatively small electric field to neutral species density ratio E/N to ensure small perturbations to the isotropic part of the EEDF and (b) rf frequencies less than the momentum exchange frequencies. Time modulation of the quantities of interest can be provided by solving for the time-dependent EEDF until a steady state is reached [6]. For explicit FDM or FEM schemes the most severe restriction is the Courant-Friedrichs-Lewy (CFL) criterion for the time step. The CFL criterion dictates a time step small enough to ensure that no particle can cross more than one mesh per time step. Even when implicit schemes are invoked (relaxing the CFL constraint) the computational efficiency is lost when collisions are accounted for, rendering the matrices dense or banded with large bandwidths.

All electron-impact-associated processes within the electron Monte Carlo simulation (EMCS) are implanted either by using the direct simulation Monte Carlo (DSMC) method or the comparatively more efficient "null collision" Monte Carlo (NCMC) method proposed by Skullerud [7]. Both schemes require the inclusion of the free-flight-time cumulative distribution $\mathcal{P}(\tau^{FF})$ as an input. The major drawback of the DSMC method is the fact that only certain functional dependences of the cross sections can be treated efficiently, in the sense that $\mathcal{P}$ can easily be solved with respect to free flight time τ^{FF}. The NCMC method introduces the concept of the null collision cross section, which has no physical significance [8], but allows the straightforward calculation of τ^{FF}, due to the specially selected functional form of $\mathcal{P}$.

Sommerer and Kushner [9] have divided the electron energy range of interest into energy intervals, each one of which is assigned a null collision cross section so that the total collision frequency ν_{total} is constant over the corresponding energy interval. This collective handling of the electrons relieves the EMCS of computationally expensive floating point operations and it is evident that the efficiency of the scheme is dependent on the proportion of null collision events. Both the DSMC and the NCMC methods introduce a dilemma in the way to handle the energy crossing of inelastic thresholds either by an energy increase or decrease within the free-flight regime, since such occurrences modify $\mathcal{P}$ upon which the free-flight time τ^{FF} is based. Neutral Monte Carlo simulations do

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not impose such ambiguity, since between collisions there is no gain or loss in kinetic energy to affect the collision cross section.

Hunter [10], performing an EMCS in molecular hydrogen, divided the time between collisions into 1–100 intervals to account for the large differences in the mean collision time before and after a mean free path has been traversed. A comparative study by Reid [11] showed that, even though the NCMC method introduces a dummy collision event (null collision), no significant impact on the results obtained was observed when compared to the more physically reasonable DSMC scheme.

Once the free-flight time is established, at the end of the interval the type of the collision event that takes place must be determined. Usually it is assumed that the probability of a process occurring is proportional to its cross section normalized by the total cross section. Subsequently all relative cross sections are summed up to unity and a random number uniformly distributed in [0,1] decides the nature of the collision event [9–21].

The present paper proposes a Monte Carlo simulation that is dictated by the Boltzmann equation itself. The procedure that we introduce here is referred to as the dynamic Monte Carlo simulation (DMCS) technique. The advantage is that, contrary to other Monte Carlo schemes, the DMCS does not require knowledge of the cumulative free-flight distribution to decide the free-flight time after which the simulated particle inevitably suffers a collision (null or real). The DMCS technique requires only a set of collision cross sections that describe the underlying stochastic process. The free-flight-time interval is not input as a stochastic process, in contrast to the DSMC and the NCMC methods. In fact, the cumulative free-flight distribution is a result of the DMCS.

II. DESCRIPTION OF THE MODEL

The goal of this paper is to develop a technique that will allow efficient treatment of the electron–neutral-species (e-n) interactions, based on a stochastic process that is described by the Boltzmann equation. The main features of the plasmas considered are a low ionization degree ($n_e/N<10^{-5}$, where n_e is the electron density and N is the gas density), and an electron temperature, T_e, higher than the background gas temperature. The technique employed, for the stochastic interpretation of the Boltzmann equation, is referred to as the dynamic Monte Carlo simulation.

A. Derivation of the algorithm

The motion of the electrons in the swarm is assumed to be affected by externally applied electric and magnetic fields and by collisions of the electrons with the particles in the ambient gas. These external forces and collisions cause time-dependent changes in the electron velocity distribution function, which can be described by the Boltzmann equation [22–24]

$$\frac{\partial f}{\partial t}+\mathbf{u}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{u}}=\left[\frac{\partial f}{\partial t}\right]_{\text{col}}, \tag{1}$$

where f is the electron velocity distribution function, $\mathbf{r}$ is the spatial location, $\mathbf{u}$ is the electron velocity, $\mathbf{F}$ is the externally applied force field $\mathbf{F}=e(\mathbf{E}+\mathbf{u}\times\mathbf{B})$, where $\mathbf{E}$ is the external electric field, $\mathbf{B}$ is the magnetic field, e is the electric charge, and m is the electron mass. The right-hand side of Eq. (1) is referred to as the collision integral and is written as [25]

$$\left[\frac{\partial f(\mathbf{r},u,\vartheta,\varphi)}{\partial t}\right]_{\text{col}}=\sum_j\sum_i\int\int\int[f(\mathbf{r},u',\vartheta',\varphi')f_j(\mathbf{r},\mathbf{u}_j')|\mathbf{u}'-\mathbf{u}_j'|\sigma_{ij}(|\mathbf{u}'-\mathbf{u}_j'|,\chi)\delta(u-g(u',\varepsilon_{ij},\chi))d\mathbf{u}_j'$$
$$-f(\mathbf{r},u,\vartheta,\varphi)f_j(\mathbf{r},\mathbf{u}_j)|\mathbf{u}-\mathbf{u}_j|\sigma_{ij}(|\mathbf{u}-\mathbf{u}_j|,\chi)\delta(u'-g(u,\varepsilon_{ij},\chi))d\mathbf{u}_j]du'd\Omega', \tag{2}$$

where the velocities of the electron distribution function f are expressed in spherical coordinates for simplicity, Ω' is the solid angle ($d\Omega'=\sin\vartheta' d\vartheta' d\varphi'$), $u=(u_x^2+u_y^2+u_z^2)^{1/2}$ is the electron speed, σ_{ij} is the collision cross section for a collision of type i between an electron and a particle of type j, and δ is a Dirac delta function, included in the definition of the transition rate to ensure the conservation of both energy and momentum. Electron-electron collisions are not considered to be significant at low ionization levels ($n_e/N<10^{-5}$). Hence f_j does not represent the EEDF. The angles ϑ and φ represent the polar and azimuthal angles in the spherical coordinate system, respectively. The collision cross section depends on both the magnitude of the relative velocities of the interacting particles and the scattering angle χ,

$$\chi:=\cos^{-1}\left[\frac{(\mathbf{u}-\mathbf{u}_j)}{|\mathbf{u}-\mathbf{u}_j|}\cdot\frac{(\mathbf{u}'-\mathbf{u}_j')}{|\mathbf{u}'-\mathbf{u}_j'|}\right]. \tag{3}$$

Equation (3) actually has nine independent variables, depending on the integral in which it appears. The function χ depends on $\mathbf{u}$, $\mathbf{u}'$, and $\mathbf{u}_j'$ in the first integral and on $\mathbf{u}$, $\mathbf{u}'$, and $\mathbf{u}_j$ in the second. The fourth vector appearing in Eq. (3) is given in terms of the other three vectors such that momentum is conserved ($m\mathbf{u}'+m_j\mathbf{u}_j'=m\mathbf{u}+m_j\mathbf{u}_j$, where m and m_j are the mass of the electron and the collision partner, respectively).

The first term of the collision integral Eq. (2) describes the repopulation of the six-dimensional phase-space volume $d\mathbf{r}\,du\,d\vartheta\,d\varphi$, whereas the second term describes the depopulation of the volume $d\mathbf{r}\,du\,d\vartheta\,d\varphi$. Transitions between phase locations can occur, provided that the Dirac δ functions are satisfied.

We have used shorthand notation for the electron velocity distribution function, which we interpret as a conditional probability density normalized to the electron number defined as

$$f(\mathbf{r},u,\vartheta,\varphi)d\mathbf{r}\,du\,d\vartheta\,d\varphi$$
$$\equiv f(\mathbf{r},u,\vartheta,\varphi;t|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0;t_0)d\mathbf{r}\,du\,d\vartheta\,d\varphi$$
$$:=\text{Prob}\{\text{that a given electron has a position between } \mathbf{r} \text{ and } \mathbf{r}+d\mathbf{r}\ ,$$
speed between u and $u+du$, polar angle of velocity between ϑ and $\vartheta+d\vartheta$,
and azimuthal angle of velocity between φ and $\varphi+d\varphi$ at time t ,
given that it had position $\mathbf{r}_0$, speed u_0, polar angle ϑ_0 ,and azimuthal angle φ_0 at time $t_0\}\times N_e$. (4)

The symbol := means "is defined as" and N_e is the total number of electrons. The interpretation of f as a conditional probability is consistent with the fact that the Boltzmann equation describes a Markovian process, as can be verified by its satisfaction of the Chapman-Kolmogorov equation. The local electron density $n_e(\mathbf{r})$ is given by

$$n_e(\mathbf{r})=\int\int\int f(\mathbf{r},u,\vartheta,\varphi)du\,d\vartheta\,d\varphi\ . \tag{5}$$

Analogous relations hold for $f_j(\mathbf{r},\mathbf{u}_j)$ (integrated over $d\mathbf{u}_j$).

Alternatively, the collision integral Eq. (2) can be written in the form reminiscent of a master equation as

$$\left[\frac{\partial f(\mathbf{r},u,\vartheta,\varphi}{\partial t}\right]_{\text{col}} = \sum_j\sum_i\int\int\int[f(\mathbf{r},u',\vartheta',\varphi')W_{ij}(\mathbf{u}|\mathbf{u}') - f(\mathbf{r},u,\vartheta,\varphi)W_{ij}(\mathbf{u}'|\mathbf{u})] \times du'd\vartheta'd\varphi' , \tag{6}$$

where the transition rate W_{ij} is defined as

$$W_{ij}(\mathbf{u}|\mathbf{u}')=\int f_j(\mathbf{r},\mathbf{u}_j')|\mathbf{u}-\mathbf{u}_j'|\sigma_{ij}(|\mathbf{u}-\mathbf{u}_j'|,\chi) \times\delta(u-g(u',\varepsilon_{ij},\chi))\sin\chi\,d\mathbf{u}_j' . \tag{7}$$

The transition rate W_{ij} has a straightforward stochastic interpretation. Roughly speaking, Eq. (7) represents the probability with which an electron that suffers a collision with particle j abruptly changes its velocity from $\mathbf{u}'$ to $\mathbf{u}$. The master equation (6) is used to develop an algorithm for the stochastic trajectory of an electron that generates realizations of the underlying stochastic process.

Now we assume that the velocity of the collision partner is small compared to the velocity of the electron. This allows us to make the scattering cross section a function of $\mathbf{u}$ and $\mathbf{u}'$ only and not of the velocities of particle j. In fact, the scattering angle χ is just the angle between the pre- and post-collision electron velocity vectors and ε_{ij} corresponds to the electron energy loss when it suffers an elastic collision i (e.g., excitation and ionization) associated with particle j.

When Eq. (2) is inserted into the Boltzmann equation [Eq. (1)], and Eq. (1) is integrated over $\mathbf{u}_j'$ and $\mathbf{u}_j$ we obtain

$$\frac{\partial f(\mathbf{r},u,\vartheta,\varphi)}{\partial t}+\mathbf{u}\cdot\frac{\partial}{\partial\mathbf{r}}f(\mathbf{r},u,\vartheta,\varphi)+\frac{\mathbf{F}}{m}\cdot\frac{\partial}{\partial\mathbf{u}}f(\mathbf{r},u,\vartheta,\varphi) = \sum_j\sum_i\int\int[n_j\sigma_{ij}(u',\chi)u'\delta(u-g(u',\varepsilon_{ij},\chi))f(\mathbf{r},u',\vartheta',\varphi')-n_j\sigma_{ij}(u,\chi)u\,\delta(u'-g'(u,\varepsilon_{ij},\chi))f(\mathbf{r},u,\vartheta,\varphi)]du'd\Omega' , \tag{8}$$

where n_j represents the particle density of the collision partner.

In order to integrate the first term on the right-hand side of Eq. (8) over du' we must specify the form of the Dirac δ function, which as already mentioned is the result of conservation of both momentum and energy and can be written as [23]

$$g(u',\varepsilon_{ij},\chi):=\left\{u'^2\left[1-\frac{2m}{m_j}(1-\cos\chi)\right]-\frac{2\varepsilon_{ij}}{m}\right\}^{1/2} , \tag{9}$$

where m_j is the mass of the collision partner ($m\ll m_j$). The quantity g is the speed of the electron after the collision. The second term on the right-hand side of Eq. (8) is independent of the dummy variable u', hence the integration is straightforward.

For a straightforward integration of Eq. (8) over du', we performed a transformation of variables on the Dirac δ function, which results in

$$\delta(u-g(u',\varepsilon_{ij},\chi))=\left[\frac{\partial g}{\partial u'}\right]^{-1}\delta(g'(u,\varepsilon_{ij},\chi)-u') , \tag{10}$$

where $g'(u,\varepsilon_{ij},\chi)$ represents the electron speed before the collision and has a form similar to that of Eq. (10) [22] (replace m with $-m$). For simplicity, in the remainder of the derivation g and g' will not be presented as functions of all their arguments but only of u' and u, respectively. By inserting Eq. (10) into Eq. (8) and then performing the integration over du' we obtain

$$\left[\frac{\partial f(\mathbf{r},u,0,0)}{\partial t}\right]_{\text{col}} = \sum_j \sum_i \left[n_j \int_0^{2\pi}\int_0^{\pi} \sigma_{ij}(g'(u),\chi) g'(u) \left[\frac{\partial g(u')}{\partial u'}\right]^{-1}_{u'=g'(u)} f(\mathbf{r},g'(u),\chi,\varphi')\,d\chi\,d\varphi' - n_j f(\mathbf{r},u,0,0) u 2\pi \int_0^{\pi} \sigma_{ij}(u,\chi)\sin\chi\,d\chi \right], \tag{11}$$

where the integration over the angles is to be performed in the spherical coordinate system, where the z axis of the velocity points in the direction of $\mathbf{u}$ (thus $\vartheta=\varphi=0$, $\vartheta'=\chi$, and φ' represents the azimuthal angle in the new coordinate system).

We may develop a stochastic algorithm from Eq. (11) by integrating it over t from t_0 to $t_0+\Delta t$, to obtain a discretized stochastic trajectory of a single electron. The left-hand side of Eq. (8) is a straightforward Liouville equation and describes the flight of the electron between collisions. Thus, during the time step Δt, the electron moves deterministically under the influence of the electric field

$$\mathbf{u}(t_0+\Delta t)=\mathbf{u}(t_0)+\frac{1}{m}\int_{t_0}^{t_0+\Delta t}\mathbf{F}(t)dt \approx \mathbf{u}(t_0)+\frac{\mathbf{F}(t_0)}{m}\Delta t\ ,$$

$$\mathbf{r}(t_0+\Delta t)=\mathbf{r}(t_0)+\int_{t_0}^{t_0+\Delta t}\mathbf{u}(t)dt \approx \mathbf{r}(t_0)+\mathbf{u}(t_0)\Delta t\ . \tag{12}$$

However, during the small time interval, there is a probability that the electron collides with a gas particle, which causes an abrupt change in the velocity of the electron. For the moment we ignore the deterministic part of the Boltzmann equation and integrate both sides of Eq. (11) over t from t_0 to $t_0+\Delta t$. We also expand the electron probability density function in a Taylor series in the variable t about t_0 and perform the integration over t, keeping terms only to order Δt:

$$\begin{aligned} &f(\mathbf{r},u,0,0;t_0+\Delta t|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0;t_0) \\ &=f(\mathbf{r},u,0,0;t_0|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0;t_0)\left\{1-\Delta t\sum_{i,j} n_j u_0 2\pi\int_0^{\pi}\sigma_{ij}(u_0,\chi)\sin\chi\,d\chi\right\} \\ &+\Delta t\sum_{i,j} n_j g'(u)\int_0^{2\pi}\int_0^{\pi}\sigma_{ij}(g'(u),\chi)\left[\frac{\partial g(u')}{\partial u'}\right]^{-1}_{u'=g'(u)} f(\mathbf{r},g'(u),\chi,\varphi'|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0)\,d\chi\,d\varphi'\ . \end{aligned} \tag{13}$$

However, by definition of the conditional probability, we may write

$$f(\mathbf{r},u,\vartheta,\varphi;t_0|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0;t_0)=\delta(\mathbf{r}-\mathbf{r}_0)\delta(u-u_0)\delta(\vartheta-\vartheta_0)\delta(\varphi-\varphi_0)N_e\ . \tag{14}$$

When Eq. (14) is inserted into Eq. (13), we obtain

$$\begin{aligned} &N_e^{-1}f(\mathbf{r},u,0,0;t_0+\Delta t|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0;t_0) \\ &=\delta(\mathbf{r}-\mathbf{r}_0)\delta(u-u_0)\delta(\vartheta_0)\delta(\varphi_0)\left[1-\Delta t\sum_{i,j} n_j u_0 2\pi\int_0^{\pi}\sigma_{ij}(u_0,\chi)\sin\chi\,d\chi\right] \\ &+\delta(\mathbf{r}-\mathbf{r}_0)\Delta t\sum_{i,j} n_j\sigma_{ij}(g'(u),\vartheta_0)g'(u)\left[\frac{\partial g(u)}{\partial u'}\right]^{-1}_{u'=g'(u)}\delta(g'(u)-u_0)\ . \end{aligned} \tag{15}$$

The Dirac δ function $\delta(g'(u)-u_0)$ represents the condition that both momentum and energy should be conserved when a collision event occurs. This δ function is the term that allows us to predict the speed of an electron after it has suffered a collision. For the purpose of writing Eq. (15) in terms of probability functions we make use of the relation Eq. (10). Hence Eq. (15) can then be written as

$$\begin{aligned} N_e^{-1}f(\mathbf{r},u,0,0;t_0+\Delta t|\mathbf{r}_0,u_0,\vartheta_0,\varphi_0;t_0) &= \delta(\mathbf{r}-\mathbf{r}_0)\delta(u-u_0)\delta(\vartheta_0)\delta(\varphi_0)\left[1-\sum_{i,j}\mathcal{P}_{ij}^{C}(u_0)\right] \\ &+\delta(\mathbf{r}-\mathbf{r}_0)\sum_{i,j}\mathcal{P}_{ij}^{C}(u_0)\mathcal{P}_{ij}^{u}(u|u_0)\mathcal{P}_{ij}^{\chi}(\vartheta_0|u_0)\mathcal{P}^{\varphi}(\varphi_0)\ , \end{aligned} \tag{16}$$

where $\mathcal{P}_{ij}^{C}$, $\mathcal{P}_{ij}^{u}$, $\mathcal{P}_{ij}^{\chi}$, and $\mathcal{P}^{\varphi}$ correspond to the collision probability, the conditional probability for the electron speed, the scattering angle probability, and the azimuthal angle probability, respectively. Each probability is defined respectively by the formulas

$$\mathcal{P}_{ij}^{C}(u_0):=\Delta t n_j u_0 2\pi\int_0^{\pi}\sigma_{ij}(u_0,\chi')\sin\chi' d\chi'\ , \tag{17}$$

$$\mathcal{P}_{ij}^{u}(u|u_0):=\delta(u-g(u_0,\varepsilon_{ij,\chi}))\ , \tag{18}$$

$$\mathcal{P}_{ij}^{\chi}(\chi|u_0):=\sigma_{ij}(u_0,\chi)\sin\chi \Big/ \int_0^{\pi}\sigma_{ij}(u_0,\chi')\sin\chi' d\chi' , \tag{19}$$

$$\mathcal{P}^{\varphi}(\varphi):=\frac{1}{2\pi} . \tag{20}$$

For simplicity, the scattering and azimuthal angles ϑ_0 and φ_0 will be represented as χ and φ, respectively, in the remainder of the paper.

Equation (16) suggests a numerical stochastic algorithm for forward integration in time of the Boltzmann equation, since its stochastic interpretation is straightforward. Consider an electron that has position $\mathbf{r}_0$ and velocity $\mathbf{u}_0$ at time t_0. Equations (16) and (12) say that the position of the electron changes during a small time step Δt by $\mathbf{u}_0\Delta t$. The velocity changes by two mechanisms. First, $\mathbf{u}_0$ changes deterministically according to Eq. (12). Second, it may or may not undergo a collision during the time step. The probability that the electron does not undergo a collision is

$$\mathcal{P}^{NC}=1-\sum_{i,j}\mathcal{P}_{ij}^{C} , \tag{21}$$

in which case the velocity changes just according to Eq. (12) (free flight). However, the probability that the electron undergoes a collision of type i with a particle of type j is given by Eq. (17), in which case the scattering angle χ is picked from $\mathcal{P}_{ij}^{\chi}(\chi|u_0)$, the azimuthal angle φ picked from the distribution $\mathcal{P}^{\varphi}(\varphi)$, and the speed undergoes a change from u_0 to $u_0(1-(1-\cos\chi)m/m_j)$, if process i is elastic, and to $(u_0^2-2\varepsilon_{ij}/m)^{1/2}$ (where the effect of momentum transfer has been neglected as negligible when compared to ε_{ij}), if i corresponds to an inelastic process according to $\mathcal{P}_{ij}^{u}(u|u_0)$. Since we choose the z axis to point towards (as yet unknown) $\mathbf{u}$, by finding χ and φ we find the angle between $\mathbf{u}$ and $\mathbf{u}_0$. Since $\mathbf{u}_0$ is known, we then know the orientation of $\mathbf{u}$.

The proposed algorithm is to simulate an ensemble of electrons whose stochastic trajectory is generated by the above probabilities and a pseudorandom number generator. Desired averages, such as electron density, energy distribution, or velocity distribution of electrons, can be calculated from the ensemble. In most cases the initial distribution of the electrons is a Maxwellian distribution with an average energy of 1 eV.

Each time step requires at least one random number, and possibly three, for each electron in the ensemble. The first random number determines which type of collision occurs (or if none at all occurs). If no collision occurs during that time step, no other random numbers are drawn. If a collision does occur, the second random number determines the new velocity direction χ from the scattering cross section and the third number picks out the new velocity direction φ uniformly between 0 and 2π. The magnitude of the new velocity is determined deterministically, Eq. (18), from the type of collision. The method described is referred to as the dynamic Monte Carlo simulation.

B. The DMCS algorithm code interpretation

The first step in applying the above algorithm is to find the time step as it is dictated by the derivation of the DMCS technique. From the derivation of the technique the time step should be such that the second-order terms in Δt, in the Taylor expansion in Eq. (13), are not significant. A first approach though in deciding the time step is to make sure that $\mathcal{P}^{NC}$ is always positive over the energy range of interest. Note that a small Δt increases $\mathcal{P}^{NC}$ and a large Δt decreases $\mathcal{P}^{NC}$ (which means that the electron is more likely to suffer a collision at the end of a time step). Once the time step has been determined we compute the probability for each collision according to the prescription below. The electron velocity is then updated depending on the type of collision selected. Thereafter, the particles subject to the stochastic simulation are advanced in time by integrating Newton's equations of motion Eq. (12).

For all e-n interactions the collision probabilities depend on the local collision partner density and the speed of the actual electron. Note that all probabilities are automatically normalized so that

$$\mathcal{P}^{NC}+\sum_{i,j}\mathcal{P}_{ij}^{C}=1 , \tag{22}$$

where the sum is over all possible particles j and all possible collisions i. A random number $\mathcal{Y}$, chosen from a uniform distribution [0,1], determines whether the electron continues its trajectory unhindered

$$\mathcal{Y}\le\mathcal{P}^{NC} \tag{23}$$

or that the electron suffers a collision k, of a specific type i with particle j

$$\mathcal{P}^{NC}+\sum_{m=1}^{k-1}\mathcal{P}_m^{C}\le\mathcal{Y}\le\mathcal{P}^{NC}+\sum_{m=1}^{k}\mathcal{P}_m^{C} , \tag{24}$$

where the probabilities are now sorted in a vector form rather than a matrix form (each value for m corresponds to a unique pair i,j). Once the collision type has been determined, the velocity of the electrons is then updated based on the new speed dictated by Eq. (18), the scattering angle given by Eq. (19), and the azimuthal angle given by Eq. (20).

To account for production and loss mechanisms of electrons (e.g., ionization and attachment) that are not accounted for in the Boltzmann equation, simulated electrons are removed or added to the DMCS. However, for convenience we wish to maintain the number of simulated particles within a specified range (100–300). When the number of electrons increases beyond the maximum number of electrons that the DMCS is specified to handle, a number of electrons are rejected from the ensemble. The electrons removed are chosen at random so that the ensemble features are not perturbed. When the number of electrons decreases beyond the minimum required number for good statistics a number of new electrons are introduced into the ensemble with velocities dictated by the ensemble electron velocity distribution function (EVDF), which is continuously updated. However, the latter situation is rather rare since we are normally in-

terested in electron-swarm parameters under discharge conditions that a glow-discharge can be sustained. Thus the simulated electrons usually increase beyond the maximum number of electrons set to be handled by the DMCS. In this sense, the computationally expensive task of computing the EVDF usually can be avoided.

As the electron properties are evolved forward in time, the velocity components are recorded at prespecified phases of the simulation and statistics are accumulated. In order to obtain interesting quantities (e.g., average energy, rate coefficients, and drift velocity) we could sample the EEDF (or EVDF) and then integrate the appropriate quantity over the distribution. For typical needs, the distribution function contains an abundance of information, which we may not need, and since the EEDF (moreover the EVDF) requires a large number of simulated particles for good resolution, a different route is followed. As electrons are traced in phase space, only the quantity of interest is recorded. The integral over the distribution function (e.g., drift velocity) is calculated by averaging over the finite ensemble as shown in the following example.

III. EXAMPLE APPLICATION: HELIUM DISCHARGE

The Boltzmann equation is solved from the electrons in a helium discharge by using the DMCS technique presented in the preceding section. The external force applied on the electrons is provided by a uniform dc or rf electric field aligned in the z direction. The EVDF is followed in three velocity dimensions, even though the problem configuration allows an axial symmetry around the z axis. No space dependence of the EVDF is considered in this work, owing to the uniform electric field. However, the inclusion of the space coordinates can be handled in a straightforward manner. No differential scattering cross sections $\sigma_{ij}(u,\chi)$ were available so the integral cross sections [11] $\hat{\sigma}_{ij}(u)$ were used. The integral cross sections are defined as the integrals of the corresponding differential cross sections over the solid angle

$$\hat{\sigma}_{ij}(u)=2\pi\int_0^{\pi}\sigma_{ij}(u,\chi)\sin\chi\, d\chi \ . \tag{25}$$

Nevertheless, the lack of differential cross sections allows us to arbitrarily select a distribution $\mathcal{P}_{ij}^{\chi}(\chi/u_0)$ provided that it is normalized over the scattering angle. The scattering-angle distribution may vary from a purely uniform distribution (isotropic scattering) to a distribution that allows for a single scattering angle (e.g., purely forward scattering). In this study $\sigma_{ij}(u,\chi)/\hat{\sigma}_{ij}(u)$ has been approximated, for all electron-impact processes, by the following distribution function [14] at various values of speeds u ($\varepsilon=mu^2/2$) and scattering angles χ:

$$\frac{\sigma_{ij}(u,\chi)}{\hat{\sigma}_{ij}(u)}=\frac{\varepsilon}{4\pi\left[1+\varepsilon\sin^2\frac{\chi}{2}\right]\ln(1+\varepsilon)} \ . \tag{26}$$

The scattering angle χ is found by setting the cumulative distribution function of Eq. (26), equal to a uniform random number, and then solving for χ [1]. For this specific distribution function Eq. (26) the cumulative distribution function is invertible and the inverse method may be used [26]. This distribution Eq. (26) predicts an approximately isotropic scattering at low energies, whereas high energies render the distribution anisotropic. In this sense Eq. (26) can capture the main features of e-n scattering.

The cross sections for the He discharge were provided by Surendra [19] and shown in Table I. The electron collisions considered in this simulation were momentum transfer, excitation, and ionization ($i=3$) and the collision partners are neutral He atoms ($j=1$). The threshold energies for both excitation and ionization collision are relatively high, with $\varepsilon_i=19.8$ and 24.5 eV, respectively. The EEDF $f(\varepsilon)$ denotes the probability that an electron has an energy between ε and $\varepsilon+d\varepsilon$. In the following figures the EEDF is normalized as

$$\int_0^{\infty}\sqrt{\varepsilon}f(\varepsilon)d\varepsilon=1 \ . \tag{27}$$

A semilogarithmic plot of the EEDF $f(\varepsilon)$ against the energy ε is a straight line for a Maxwellian distribution. Hence the EEDF computed in this way can readily be compared to the Maxwellian distribution.

The mean electron energy, as well as the rate coefficients, is computed as the appropriate ensemble averages

$$\langle\cdots\rangle=\frac{1}{N_e}\int(\cdots)f(\mathbf{r},\mathbf{u};t)d\mathbf{u} \ . \tag{28}$$

Hence we can compute the mean electron energy and the rate coefficients by performing the integral Eq. (28) over $\langle\varepsilon\rangle:=\langle mu^2/2\rangle$ and $k_{ij}:=\langle\hat{\sigma}_{ij}(u)u\rangle$, respectively. This approach requires the solution of the time-evolution equation for the distribution function, which in general constitutes a computationally expensive task. However, since our stochastic simulation uses the same underlying stochastic process implied by the time-evolution equation to generate an ensemble of realizations, we can use this ensemble to estimate averages

TABLE I. Most significant processes taking place in the helium discharge.

Electron–neutral species collision	Cross section $\hat{\sigma}$ (cm^2)		Energy loss ε_{ij} (eV)
elastic	$\hat{\sigma}=8.5\times10^{-15}/(\varepsilon+10)^{1.1}$		0.0
excitation	$\hat{\sigma}=0$	$0\le\varepsilon\le19.8$	
$He+e\rightarrow He^*+e$	$\hat{\sigma}=2.08\times10^{-18}(\varepsilon-19.8)$	$19.8\le\varepsilon\le27.0$	19.8
	$\hat{\sigma}=3.4\times10^{-15}/(\varepsilon+200)$	$27.0\le\varepsilon$	
ionization	$\hat{\sigma}=0$	$0\le\varepsilon\le24.5$	24.5
$He+e\rightarrow He^++2e$	$\hat{\sigma}=1\times10^{-13}(\varepsilon-24.5)/\{(\varepsilon+50)(\varepsilon+300)^{1.2}\}$	$24.5\le\varepsilon$	

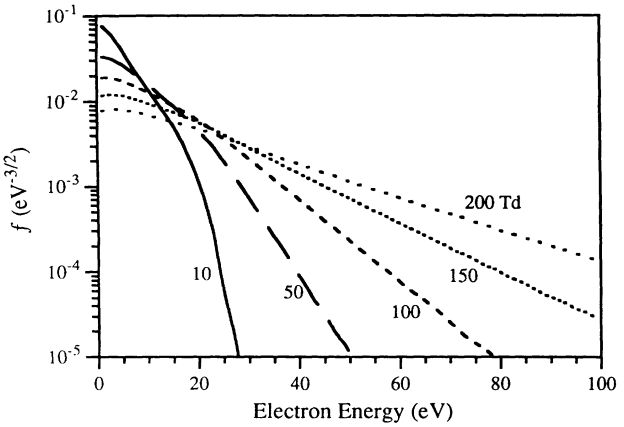

FIG. 1. Steady-state electron energy distribution function for He dc fields of $E/N=10$, 50, 100, 150, and 200 Td.

$$\langle F(\mathbf{u})\rangle \cong \frac{1}{\mathcal{N}_e}\sum_i F(\mathbf{u}_i)\ , \tag{29}$$

where $\mathbf{u}_i$ is the velocity of the ith electron in our ensemble and $\mathcal{N}_e$ is the total number of electrons in the ensemble.

The swarm parameters were calculated for gas number density equal to $N=3.22\times10^{16}$ cm^{-3}, which corresponds to 1 Torr pressure and 300 K gas temperature. Each run required less than 1 min on a Hewlett-Packard 735 workstation. The estimated statistical error for the mean electron energy is $\pm0.2\%$ and the electron-impact rate coefficient is $\pm1\%$. No significant time-discretization error was found by halving the time step.

The EEDF for a dc field with different E/N values is shown in Fig. 1. Clearly, as the applied dc field increases, the EEDF shifts towards higher energies. The tail of the EEDF at $E/N=10$ Td (1 Td$=10^{-17}$ V cm^2) falls off rapidly since the highly energetic electrons are depleted due to the inelastic collisions. However, as E/N increases, the EEDF tends to become more Maxwellian-like by raising the tail of the EEDF. The EVDF for a dc field of 200 Td is shown in Fig. 2. Since the electric field is aligned in the z direction, u_x is isotropically distributed between positive and negative values. However, the u_z velocity component is elongated towards negative values since the electric field points in the positive z direction.

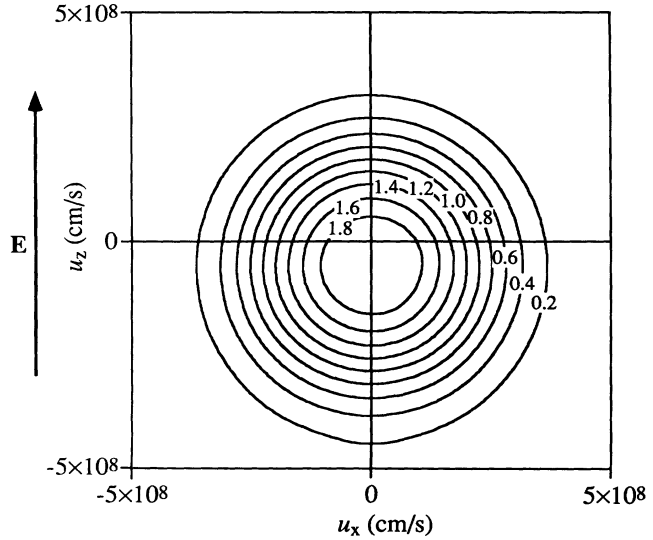

FIG. 2. Contour plot of the steady-state electron velocity distribution function for the He dc field of $E/N=150$ Td. Values shown are multiplied by 4.17×10^{13}.

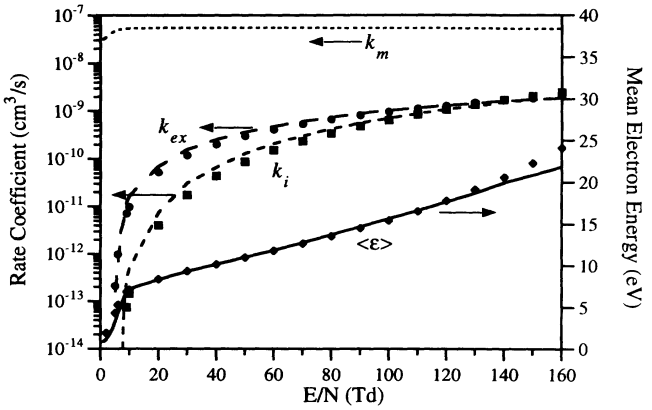

FIG. 3. Steady-state values of momentum k_m, ionization k_i, excitation k_{ex}, rate coefficients, and mean electron energy $\langle\varepsilon\rangle$ as a function of dc E/N in He. Results by using the two-term approximation of the EVDF (Morgan and Penetrante [4]) are shown as points.

Figure 3 shows the mean electron energy $\langle\varepsilon\rangle$, momentum k_m, excitation k_{ex}, and ionization k_i rate coefficient as a function of the applied dc field E/N. Both excitation and ionization rate coefficients increase as E/N increases. Above $E/N=150$ Td the ionization rate becomes more significant even though the ionization threshold energy is greater than the excitation energy. The momentum transfer rate coefficient decreases slightly as E/N increases. Results by using the two-term spherical harmonic expansion [4] of the EVDF are shown as points. Good agreement occurs since the elastic collision cross section is much higher than the inelastic collision cross sections. This induces small perturbations to the

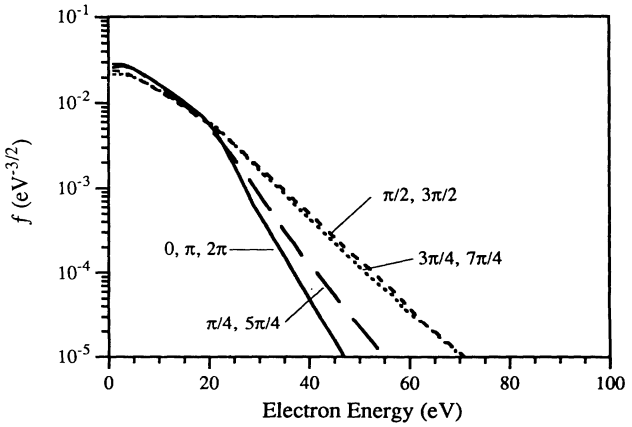

FIG. 4. Harmonic steady-state electron energy distribution function for different fractions of the rf cycle for the He rf field of $E/N=100$ Td and frequency 13.56 MHz.

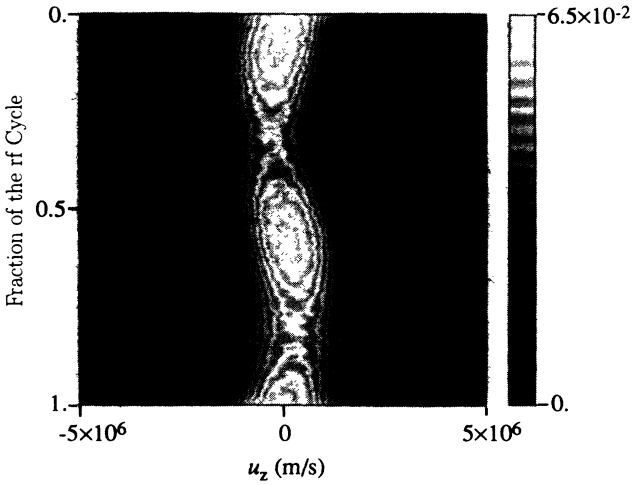

FIG. 5. Distribution function of the z component of the electron velocity for different fractions of the rf cycle for the He rf field of $E/N = 100$ Td and frequency 13.56 MHz.

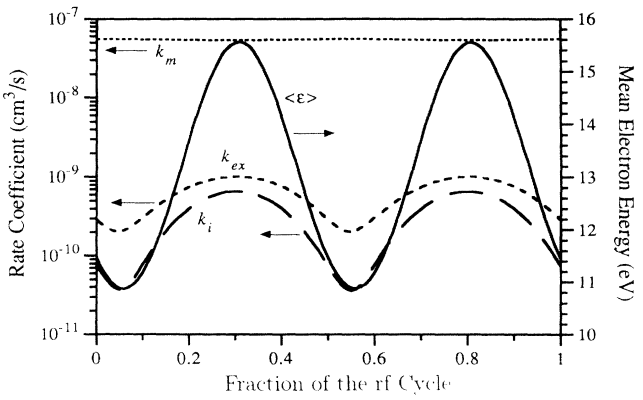

FIG. 6. Harmonic steady-state values of momentum k_m, ionization k_i excitation k_{ex}, rate coefficients, and mean electron energy $\langle \varepsilon \rangle$ as a function of the fraction of the rf cycle for the He rf field of $E/N = 100$ Td and frequency 13.56 MHz.

isotropic part of the EVDF rendering the two-term approximation valid. However, at high E/N ratios, where ionization dominates over the other inelastic processes, significant differences occur. This agreement verifies that the stochastic simulation indeed solves the Boltzmann equation.

The time-dependent EEDF for a sinusoidally varying field with peak $E/N = 100$ Td and a frequency $\omega = 13.56$ MHz is shown in Fig. 4 for different fractions of the rf cycle. The EEDF modulates rather strongly within the rf cycle and with twice the applied frequency. The EVDF represented by the z component of the electron velocity is shown in Fig. 5 as a function of the fraction of the rf cycle. The EVDF has been normalized at each time level of the cycle. Clearly, the EVDF contracts and expands depending on the temporal electric field. When the electric field is at its positive peak ($\tau = \omega t = 0.25$) the EVDF expands and is elongated toward negative velocities, whereas when the electric field is at its negative peak ($\tau = \omega t = 0.75$) the EVDF is elongated toward positive velocities. For the same rf conditions the swarm parameters are plotted against the fraction of the rf period in Fig. 6. The momentum rate coefficient does not modulate strongly; however, both the excitation and the ionization rate coefficient modulate significantly due to the mean electron energy variation within the cycle.

IV. CONCLUDING REMARKS

A method, referred to as the DMCS technique, has been developed for the solution of the Boltzmann equation describing partially ionized gases, via the generation of realizations of the underlying stochastic process. In contrast to the DSMC and the NCMC methods, DMCS does not require the assumption of the free-flight-time distribution. Since the free-flight-time distribution is not an input, the stochastic quantities evolve in time step by step, with a time step selected in such a way as to ensure accuracy in the results, as dictated by the derivation of the DMCS algorithm. Usually, in the DSMC and NCMC methods, the fastest electrons must freeze in real time until the slowest electrons can catch up, in order to record statistics. A constant time step renders the process of collecting statistics with the DMCS straightforward, since there is no need to keep track of the time level in which each electron is located. In the DMCS technique all electrons are at the same point in real time. Most commonly, in the DSMC and the NCMC methods a collision occurs when a random number is less than a computed quantity. Then, if a collision does take place, an additional random number determines the type of the collision. In the DMCS method a single random number determines whether the electron continues its trajectory unhindered or if the electron suffers a collision of a specific type. Although we studied a helium discharge under the influence of a homogeneous electric field, the DMCS technique can easily be extended to handle more complex systems under the influence of inhomogeneous electromagnetic fields to describe spatially varying plasma behavior.

ACKNOWLEDGMENTS

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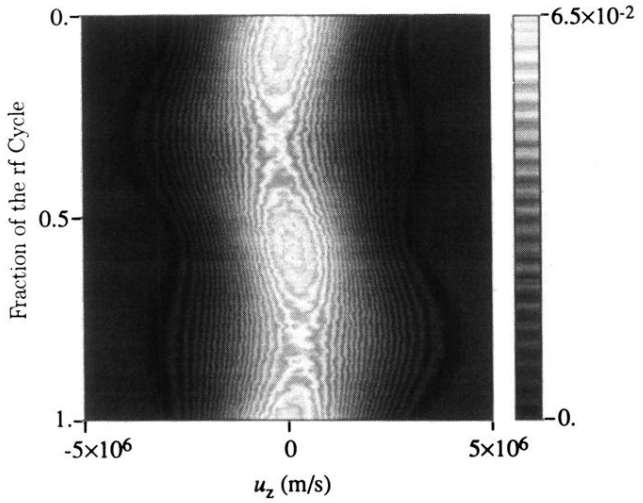

FIG. 5. Distribution function of the z component of the electron velocity for different fractions of the rf cycle for the He rf field of $E/N = 100$ Td and frequency 13.56 MHz.