

Timesaving techniques for decision of electron–molecule collisions in Monte Carlo simulation of electrical discharges

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Received 9 June 2006; accepted 12 September 2006
Available online 27 October 2006

Abstract

Techniques to reduce the computational load for determination of electron–molecule collisions in Monte Carlo simulations of electrical discharges have been presented. By enhancing the detection efficiency of the no-collision case in the decision scheme of the collisional events, we can decrease the frequency of access to time-consuming subroutines to calculate the electron collision cross sections of the gas molecules for obtaining the collision probability. A benchmark test and an estimation to evaluate the present techniques have shown a practical timesaving efficiency.

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PACS: 52.65.Pp

Keywords: Monte Carlo; Plasma; Electrical discharge; Electron collision; Probability; Time step; Timesaving scheme

1. Introduction

Collision of electrons with gas molecules is one of the key processes which govern the properties of plasmas and electrical discharges used for applications such as material processing and light sources. In Monte Carlo simulations of such phenomena, the occurrence of the electron collision and the choice of the subsequent physical or chemical processes are the very stochastic events determined by random numbers. The collision probability is given from the electron collision cross section q defined for each reaction of a gas molecule. Because q is usually a function of speed v or energy ϵ of the colliding electron, the calculation of $q(v)$, typically consisting of table look-up and interpolation/extrapolation, is often time-consuming. Even with recent progress in the computer technologies, timesaving algorithms are still valuable under an increasing demand on the computational throughput.

Some efficient techniques to reduce the computational load concerned with the decision of the collisional events have been presented. Skullerud [1] introduced an imaginary collision cross section of zero momentum

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transfer in order to make the total collision frequency ν_{total} seemingly constant, with which the free flight time τ of a particle until the succeeding collision can be given simply as $\tau = -\nu_{\text{total}}^{-1} \ln(1 - \xi)$, where ξ is a uniform random number ($0 \leq \xi < 1$). Nanbu [2] proposed a method to decide the occurrence of a collision in a simulation time step Δt and the kind of collision at the same time referring to only one value of ξ . In contrast that the conventional method needs to calculate $q(v)$ for all kinds of collisions under consideration for every Δt , Nanbu’s method needs to calculate only one of them; when the number of the kinds of collision is n , the computational load becomes $\frac{1}{n}$ of the conventional method.

In this paper, we customize Nanbu’s method. We begin with showing an overview of the conventional and Nanbu’s methods. Next, we compare two criteria on the upper limit of Δt . One is Nanbu’s criterion arising from the algorithm of Nanbu’s method itself, and the other is an analytical requirement for the precision in the evaluation of the collision probability. After that, we present three new techniques to reduce the computational load. The first is reduction of the access to the calculation subroutines for $q(v)$. This is applicable to simulations of a gas with a small n (favorably up to 10–20). The second is division of large collision probabilities of a gas with a large n (practically over 50) into some portions to evade Nanbu’s criterion which would require a shortening of Δt leading to an increase in the computational cycles in the simulation. The third is an improvement of the detection efficiency of the no-collision case. This can be combined with both of the first and second techniques. By a benchmark test and an estimation, the efficiency of these techniques is evaluated.

2. Overview of conventional and Nanbu’s methods

The probability P of the occurrence of an electron collision during a simulation time step Δt is given from $q(v)$ as

$$P = \nu \Delta t = Nq(v)v\Delta t, \tag{1}$$

where ν is the collision frequency, and N is the number density of gas molecules. When we need to distinguish the kind of collision, we denote these variables with subscript, hereafter; e.g. “ k ” for the collisions of the k th kind, and “total” for the sum over k ’s.

Fig. 1 shows a comparison between the decision schemes for collisional events by the conventional and Nanbu’s methods.

In the conventional method, the occurrence of a collision is firstly decided by a comparison between ξ and P_{total} . If $\xi < P_{\text{total}}$ then a collision is deemed to occur. After that, the kind of collision is chosen by another

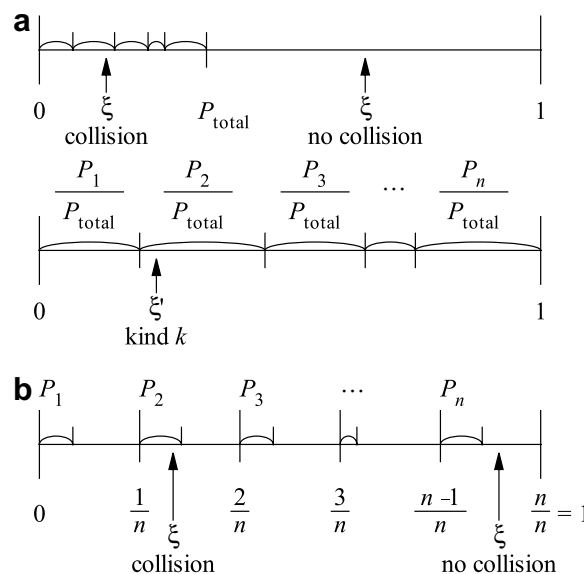


Fig. 1. Decision of collisional events using a uniform random number ξ ($0 \leq \xi < 1$) by (a) conventional and (b) Nanbu’s methods.

random number ξ' , being proportional to the ratios P_k/P_{total} ($k = 1, 2, \dots, n$). Because the conventional method requires calculations of $q_k(v)$ for all k 's to obtain P_{total} , the scheme is time-consuming.

Nanbu's method chooses a k from among numbers 1 to n first by taking the integer part of the value $(n\xi + 1)$. After that, the occurrence of collision k is decided if $\xi - \frac{k-1}{n} < P_k$. Because each P_k is arranged in a segment with a width $W = \frac{1}{n}$ assigned to each of n collisional processes, this scheme requires the calculation of $q_k(v)$ to obtain P_k only for the chosen k . Instead, a criterion $P_k < \frac{1}{n} = W$ (let us call this Nanbu's criterion) must be satisfied for all k 's and v [2]. Otherwise, the occurrence of such a collision k that $P_k > W$ is underestimated.

3. Criteria on time step

Nanbu's method requires

$$P_{k,\text{max}} = v_{k,\text{max}}\Delta t < \frac{1}{n} \quad (1 \leq k \leq n). \quad (\text{Nanbu's criterion}). \quad (2)$$

This is an algorithmic requirement particular to Nanbu's method. On the other hand, being independent of Nanbu's criterion, Δt must be shorter enough than the electron mean free time v_{total}^{-1} in order to allow the following approximations for the probability P of the number of collisions X during Δt ; (i) $P(X \geq 1)$ can be represented simply as $P_{\text{total}} = v_{\text{total}}\Delta t$; and (ii) $P(X \geq 2)$ is negligible. As shown in Eqs. (A.2) and (A.3) in Appendix, both of the principal error terms in these approximations are commonly $\frac{1}{2}(v_{\text{total}}\Delta t)^2$. Therefore, when we adopt a precision of P_{total} for example higher than 99%, we need to set Δt to satisfy $P_{\text{total,max}} = v_{\text{total,max}}\Delta t < \frac{1}{50}$ (cf. early Monte Carlo simulations practically adopted $P_{\text{total}} < \frac{1}{10}$ [3,4]). Let us denote this analytical criterion as

$$P_{\text{total,max}} = v_{\text{total,max}}\Delta t < \frac{1}{a} \quad (\text{analytical criterion}) \quad (3)$$

with an integer a introduced for a correspondence to Nanbu's criterion. Hereafter, we assume that Δt has already been chosen to satisfy the analytical criterion (typically $a = 50$ for a 99% precision for P_{total}) to guarantee the validity of the physical aspect in the simulation result, under which Nanbu's method is customized.

4. Customization 1: introduction of null collision (for $n < a$)

When $n < a$, i.e. the requirement on Δt from the analytical criterion is tighter than that from Nanbu's criterion, we may add the following "null collision" as the $(n + 1)$ th collisional process to the n real processes, without changing any physical aspect. The null collision is an imaginary process which induces nothing and its probability is zero. Therefore, only the number of the kinds of collisions increases from n to $n + 1$. When Nanbu's method is applied to the $n + 1$ collisional processes, the probability of the event that the null collision is chosen is $\frac{1}{n+1}$. If the null collision is chosen, no calculation is required. The average computational load to calculate $q(v)$ can be lightened from $\frac{n}{n}$ to $\frac{n}{n+1}$ by the introduction of the null collision.

The addition of the null collision can be repeated at least $a - n$ times. Furthermore, because the analytical criterion applies to $P_{\text{total,max}}$, there is a possibility that all $P_{k,\text{max}}$'s ($\leq P_{\text{total,max}}$) can accept extra addition of null collisions. When an integer $b > 0$ satisfies $\max(P_{1,\text{max}}, P_{2,\text{max}}, \dots, P_{n,\text{max}}) \leq \frac{1}{a+b}$, the extra addition is allowed for b times. Fig. 2 shows a result of m times of the addition. The null collision is chosen with a ratio of $\frac{m}{n+m}$ on average; thus, $\frac{m}{n+m}$ of the computational load to calculate $q(v)$ is freed.

5. Customization 2: division of large probability (for $n > a$)

Nanbu's criterion becomes tighter as n increases. Some collision cross section sets include more than 10 cross sections; e.g. n is 19 for CHF_3 [5], 20 for Xe [6], 27 or 31 for Ar [2,7,8], 31 for He [6] and 32 for N_2 [9]. Under tendencies that electronic excitation levels and vibrational excitation modes are identified in detail and that the dissociation processes of molecular gases are distinguished by the product species, n would increase more and more. Especially, n of mixed gases could easily exceed a given a .

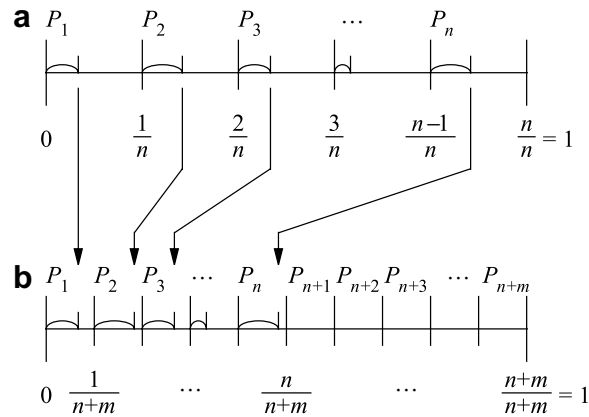


Fig. 2. Arrangement of collision probabilities (1): (a) Nanbu's method and (b) result of introduction of m null collisions. Calculation of $q_k(v)$ is not necessary when a k for the null collision ($n + 1 \leq k \leq n + m$) is chosen.

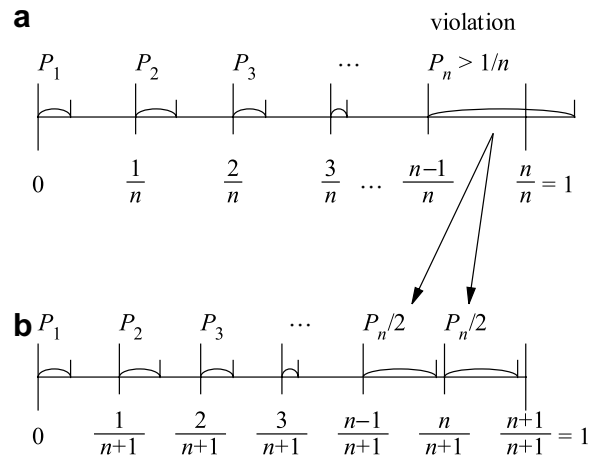


Fig. 3. Arrangement of collision probabilities (2): (a) violation of Nanbu's criterion and (b) division of large probability.

In case $n > a$, some P might violate Nanbu's criterion if Δt is set at the maximum value based on the analytical criterion. In such a case, Nanbu's criterion would require a shorter Δt than allowed by the analytical criterion, and the computation cycles would increase inversely proportional to Δt .

Here, let us consider a case that P_{total} satisfies the analytical criterion but P_n violates Nanbu's criterion. We can evade the shortening of Δt required by Nanbu's criterion, when $\frac{P_n}{m} < \frac{1}{n+m-1}$ for an integer $m \geq 2$. We may divide P_n into m equal portions and may count them as m different kinds of collisions (although the physical processes for the divided P_n are identical). Fig. 3 shows a schematic of this division made for P_n to satisfy Nanbu's criterion. The segment width W is shortened from $\frac{1}{n}$ to $\frac{1}{n+m-1}$; however, it is likely that P_k 's ($k \neq n$) still satisfy $P_k < W$ especially when P_n is solely large as that of elastic collision be in many gases. The division of P_n increases the number of the kinds of collisions, but adds no new computational load. By satisfying Nanbu's criterion formally, we can evade the shortening of Δt . If there are other P 's violating Nanbu's criterion, this division can be applied also to them unless the shortening of W induces other new violations.

6. Customization 3: reference to the maximum value of P_k

The access to the subroutine for calculation of $q_k(v)$ can be reduced furthermore when $P_{k,\text{max}} < W$. This condition is expected to hold for most of k 's usually. Because $P_{k,\text{max}}$ is a constant for each k , we can make

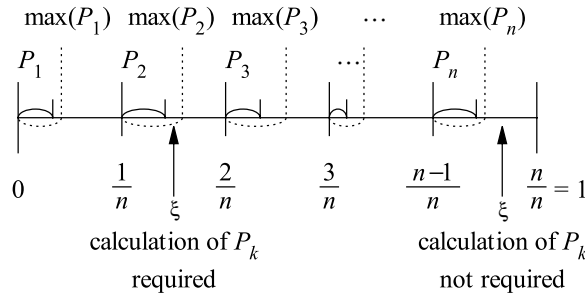


Fig. 4. Omission of calculation of P_k . When $\xi - \frac{k-1}{n} > P_{k,\max}$ for the chosen k , it is obvious that collision k never occurs; at that time, calculation of P_k (subroutine call for $q(v)$) is not necessary.

a table of $P_{k,\max}$ for all k 's in a preprocess before the simulation. After a k is chosen, $P_{k,\max}$ is referred to. We do not need to calculate $q_k(v)$ if $\xi - \frac{k-1}{n} > P_{k,\max}$, because collision does not occur obviously at that time (see Fig. 4); we need to compare $\xi - \frac{k-1}{n}$ and P_k only when $\xi - \frac{k-1}{n} < P_{k,\max}$. This reference to $P_{k,\max}$ can be combined with either of customizations 1 and 2.

7. Examples

In order to evaluate the efficiency of customization 1 for a gas with a small n , a benchmark test using a Monte Carlo simulation of electron swarms in CF_4 (an etching gas) has been performed. At an electric field $E = 100 \text{ V cm}^{-1}$ and $N = 3.54 \times 10^{16} \text{ cm}^{-3}$ (133 Pa at 273 K), 10^8 electrons have been traced for 50 ns to derive electron transport parameters in CF_4 . The results have been verified by those of a previous analysis [10]. The collision cross section set of CF_4 adopted for this test includes seven processes [11]. We have let $\Delta t = 1 \text{ ps}$ under $v_{\text{total,max}} = 2.0 \times 10^{10} \text{ s}^{-1}$. This condition satisfies the analytical criterion at $a = 50$, which enables us to add $a - n = 43$ null collisions, and $\max(v_{1,\max}, v_{2,\max}, \dots, v_{7,\max}) = 1.3 \times 10^{10} \text{ s}^{-1}$ allows us $b = 25$ for the extra addition of null collisions. We have introduced $(a - n) + b = 68$ null collisions, and customization 3 has also been applied to the seven real processes. As a result, the computational time required by a C++ program run on a workstation with a CPU of AMD Opteron 252 (2.6 GHz) has been reduced from 58.5 h to 14.4 h; about 75% of the CPU time has been saved.

Another example is for a gas with a large n : an analysis of electrical discharges in a tertiary mixed gas Xe/Ar/He [8] (a medium for plasma displays). The model considered 82 cross sections in total including those for stepwise ionizations from excited species. A condition assumed in the analysis was a mixture ratio of Xe:Ar:He = 5:50:45 and $N = 1.41 \times 10^{19} \text{ cm}^{-3}$ (53.2 kPa at 273 K). If we would perform a Monte Carlo simulation for this mixed gas, the analytical criterion $v_{\text{total,max}} \Delta t < \frac{1}{50}$ requires $\Delta t < 6.3 \text{ fs}$ under $v_{\text{total,max}} = 3.2 \times 10^{12} \text{ s}^{-1}$ for $\epsilon \leq 200 \text{ eV}$. On the other hand, Nanbu's criterion $v_{k,\max} \Delta t < \frac{1}{82}$ requires $\Delta t < 5.1 \text{ fs}$ under $v_{\text{Ar,elastic,max}} = 2.4 \times 10^{12} \text{ s}^{-1}$ for the elastic collision of Ar. Nanbu's criterion is about 20% tighter than the analytical criterion. After dividing $P_{\text{Ar,elastic}}$ into the halves, no other P 's violates Nanbu's criterion $v_{k,\max} \Delta t < \frac{1}{82+1}$ even at $\Delta t = 6.3 \text{ fs}$. Owing to customization 2, we can evade about 20% increase in the computational cycles in this case. In addition, P of 70 kinds of collisions among $82 + 1$ kinds are less than $\frac{1}{100}$ of $W = \frac{1}{82+1}$; more than 99% of the access to the subroutines to calculate $q(v)$ of the 70 collisions can be omitted by customization 3.

8. Conclusion

We have proposed three timesaving customization techniques for Nanbu's method to decide electron-molecule collisional events in Monte Carlo simulations of electrical discharges.

The first is introduction of null collisions. This is applicable to simulations of a gas with a small number n of the kinds of collisions. We can reduce the frequency of the access to time-consuming subroutines for calculation of the electron collision cross section q by increasing n virtually.

The second is a solution to violation of Nanbu's criterion on the simulation time step Δt . This violation is likely to occur for a gas with a large n , and requires shortening of Δt , which results in an increase in the computational cycles. However, under a certain condition, we can evade the requirement on Δt from Nanbu's criterion by dividing large q 's into some portions.

The third is an improvement of detection efficiency for the no-collision case. By referring to the maximum value of the collision probability P of a chosen process, the access to the subroutines for q can be reduced. This technique can be combined with either of the first and second techniques.

A benchmark test and an estimation to evaluate the present techniques have shown a satisfactory timesaving effect.

Acknowledgments

This work was in part supported by a Grant-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology, Japan. The authors wish to thank Professor Satoshi Uchida of Tokyo Metropolitan University for valuable information on the analysis of tertiary mixed gases.

Appendix A. Precision of approximation on collision probabilities

At a collision frequency ν , the probability $P(X = x)$ of the event that electron collisions with gas molecules occur x times during Δt is represented as follows (Poisson's distribution):

$$P(X = x) = \lim_{m \rightarrow \infty} {}_m C_x \left(1 - \nu \frac{\Delta t}{m}\right)^{m-x} \left(\nu \frac{\Delta t}{m}\right)^x = \exp(-\nu \Delta t) \frac{1}{x!} (\nu \Delta t)^x. \quad (\text{A.1})$$

The absolute error of an approximation for the probability of the occurrence of collision during Δt , $P(X \geq 1) = 1 - P(X = 0)$, by $P = \nu \Delta t$ is

$$\begin{aligned} P - P(X \geq 1) &= \nu \Delta t - [1 - \exp(-\nu \Delta t)] \\ &= \nu \Delta t - \left\{ 1 - \left[1 - \nu \Delta t + \frac{1}{2!} (\nu \Delta t)^2 - \frac{1}{3!} (\nu \Delta t)^3 + \frac{1}{4!} (\nu \Delta t)^4 - \dots \right] \right\} \\ &= \frac{1}{2!} (\nu \Delta t)^2 - \frac{1}{3!} (\nu \Delta t)^3 + \frac{1}{4!} (\nu \Delta t)^4 - \dots \end{aligned} \quad (\text{A.2})$$

When it is assumed that the number of collisions within Δt is at most one, the neglected probability of plural collisions, $P(X \geq 2) = 1 - P(X = 0) - P(X = 1)$, is

$$\begin{aligned} P(X \geq 2) &= 1 - \exp(-\nu \Delta t) - \exp(-\nu \Delta t) \nu \Delta t \\ &= 1 - \left[1 - \nu \Delta t + \frac{1}{2!} (\nu \Delta t)^2 - \frac{1}{3!} (\nu \Delta t)^3 + \frac{1}{4!} (\nu \Delta t)^4 - \dots \right] \\ &\quad - \left[\nu \Delta t - (\nu \Delta t)^2 + \frac{1}{2!} (\nu \Delta t)^3 - \frac{1}{3!} (\nu \Delta t)^4 + \dots \right] \\ &= \frac{1}{2!} (\nu \Delta t)^2 - \frac{2}{3!} (\nu \Delta t)^3 + \frac{3}{4!} (\nu \Delta t)^4 - \dots \end{aligned} \quad (\text{A.3})$$

In both of Eqs. (A.2) and (A.3), the principal terms which determine the precision of the approximations are $\frac{1}{2} (\nu \Delta t)^2$.

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