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

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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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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 ($0 \leqslant \xi < 1$). 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 kth 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

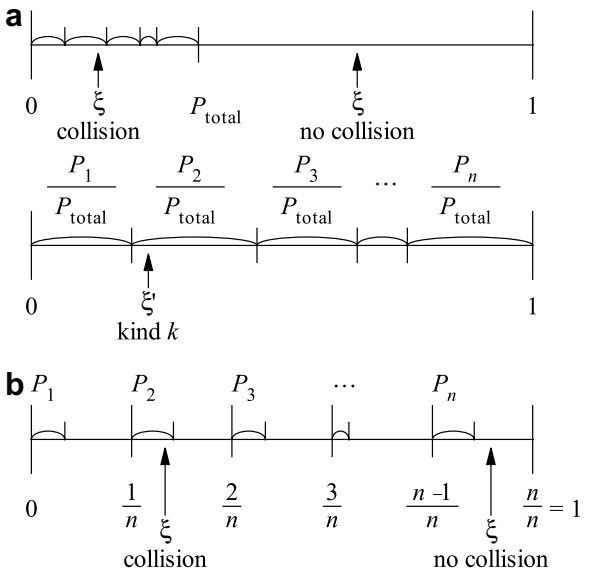

Fig. 1. Decision of collisional events using a uniform random number ξ ($0 \leqslant \xi < 1$) by (a) conventional and (b) Nanbu's methods.