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Weighted Particles in Coulomb Collision Simulations Based on the Theory of a Cumulative Scattering Angle

K. Nanbu[1] and S. Yonemura

Institute of Fluid Science, Tohoku University, Sendai 980-8577, Japan
E-mail: nanbu@ifs.tohoku.ac.jp and yonemura@ifs.tohoku.ac.jp

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A cumulative property of Coulomb collisions in plasmas was formulated by Nanbu. A succession of small-angle binary collisions is grouped into a unique binary collision with a large scattering angle; the law of scattering is given by the exponential cosine function. Proposed here is a Coulomb collision algorithm for weighted particles, based on that work. Three cases of the weight algorithm are considered: (1) the weights of particles are the same; (2) the weights of particles are different from species to species; and (3) the weights are different from particle to particle. Sample calculations demonstrate the accuracy of the weight algorithm.

1. INTRODUCTION

The use of high plasma density and low gas pressure is a recent trend in plasma-assisted materials processing. Plasma sources are changing from radio-frequency discharge to other methods based on inductive coupling, electron cyclotron resonance, helicon waves, or surface waves. Physically, this means that Coulomb collisions play a more important role in processing plasmas. Copious articles have been published on methods to model Coulomb collisions in plasmas. A selection of the published papers are referred to here. (See also the references cited in the following papers.) In Coulomb collisions small-angle collisions are much more important than collisions resulting in large velocity changes. Based on this idea, Rosenbluth, MacDonald, and Judd [1] starting from the Boltzmann equation, derived the Fokker–Planck equation for an arbitrary distribution function. Many articles on Coulomb collision simulations still are influenced by Rosenbluth, MacDonald, and Judd's paper. Takizuka and Abé [2] proposed a binary collision model suited to a Monte Carlo particle simulation of plasma. Birdsall [3] discussed the feasibility of their method in particle-in-cell

[1] Corresponding author.

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codes. Miller and Combi [4] proposed a collision algorithm for weighted particles based on Takizuka and Abé's method. Ma, Sydra, and Dawson [5] extended Takizuka and Abé's method to construct a gyrokinetic particle simulation model. Wang *et al.* [6] made a significant improvement of Takizuka and Abé's method; the relation between a collision operator proposed and the Fokker–Planck operator of the Landau form was defined clearly. Jones *et al.* [7] presented a method to calculate the force acting on a particle from grid quantities in the particle-in-cell codes. Since two collision frequencies in the expression for the force are derived by assuming a drifting Maxwellian distribution, their method cannot be used when deviations from Maxwellian behavior are significant. Manheimer, Lampe, and Joyce [8] improved this point by use of a Fokker–Planck equation to describe an isotropic velocity distribution function. In all of these works small-angle Coulomb collisions are calculated one by one. If many small-angle collisions can be grouped into one large-angle collision, collisions can be calculated more efficiently since the use of a larger time step is possible. In fact, Cranfill, Brackbill, and Goldman [9] used the idea of grouping many small-angle collisions and succeeded in using a large time step in their time-implicit particle-in-cell algorithm. Nanbu [10, 11] proposed a quite different formulation on a cumulative property of Coulomb collisions in plasmas; he determined the probability distribution for a cumulative deflection angle resulting from many small-angle collisions. The idea of grouping is also discussed in the Boltzmann equation analysis of electron–electron collisions [12]. The nature of Nanbu's formulation yields a drastic decrease in computational effort that is realized in the Monte Carlo particle simulation of Coulomb collisions.

In etching of metal or oxide, electronegative gases are usually employed. Let us imagine the particle-in-cell/Monte Carlo collision simulation of plasmas of electronegative gases. First the flow field is divided into small cells. For such gases electron number density is much lower than ion number density. The concept of "weight" is naturally introduced to keep the number of simulated particles in a cell roughly equal among species. (If the weight is W, a particle represents W real particles.) Another example is a high-temperature plasma, in which ions have multiple charges; hence, electron density is much higher than ion density. In the high-temperature plasma case it is preferable to assign a larger weight to electrons. The introduction of weight is a common technique employed in Monte Carlo simulations of neutral molecules [13] and charged particles [4]. In the method proposed we consider elastic collisions between charged particles. The inclusion of weight results in momentum and energy not always being conserved in particle collisions, but it can be shown that macroscopic momentum and energy are conserved on the average. In the present work we propose a Coulomb collision algorithm for weighted particles, based on Nanbu's theory [10] of Coulomb collisions.

2. HOW TO TREAT COULOMB COLLISIONS

In the particle-in-cell simulation of plasmas the computational domain is divided into cells with a dimension of the Debye length λ_D. Since there is no need to consider the Coulomb interaction between two particles separated by λ_D or more, it is an acceptable approximation to model only the Coulomb collisions in a cell and disregard all charged particles in neighboring cells. Therefore let us focus our attention only on the charged particles in a cell. For simplicity we only consider the case when a plasma contains electrons (α) and a single species of ions (β). Then we have only to consider α–α, α–β, and β–β

collisions. The number of real particles in a cell is too large to be simulated even by the use of a supercomputer. Therefore a small number of real particles are randomly sampled and simulated. Such particles are called simulated particles or, simply, particles. Let N_α and N_β be the numbers of simulated particles α and β in a cell, in general, $N_\alpha \neq N_\beta$. The next step is to determine the velocities of all simulated particles after time step Δt. Accomplishing this task requires an explanation of the essence of Nanbu's theory [10].

Let the sets $\{\boldsymbol{v}_{\alpha i};\ i = 1, \ldots, N_\alpha\}$ and $\{\boldsymbol{v}_{\beta j};\ j = 1, \ldots, N_\beta\}$ be the velocities of particles α and velocities of particles β at time t, respectively. Hereafter, $\boldsymbol{v}_{\alpha i}$ is defined as the velocity of particle (αi). Focusing our attention on particle (αi), particle (αi) changes velocity due to α–β and α–α collisions in Δt. Initially we consider α–β collisions in Δt. To explain Nanbu's theory we begin with the case that the force between two particles is short range. In this case the postcollision velocity $\boldsymbol{v}'_{\alpha i}$ is given by [14]

$$\boldsymbol{v}'_{\alpha i} = \boldsymbol{v}_{\alpha i} - \frac{m_\beta}{m_\alpha + m_\beta}[\boldsymbol{g}(1 - \cos\chi) + \boldsymbol{h}\sin\chi], \tag{1a}$$

$$\boldsymbol{v}'_{\beta j} = \boldsymbol{v}_{\beta j} + \frac{m_\alpha}{m_\alpha + m_\beta}[\boldsymbol{g}(1 - \cos\chi) + \boldsymbol{h}\sin\chi]. \tag{1b}$$

Here $\boldsymbol{v}_{\beta j}$ and $\boldsymbol{v}'_{\beta j}$ are the precollision and postcollision velocities of a collision partner (βj). The symbols m_α and m_β are the masses of particles α and β, $\boldsymbol{g}(=\boldsymbol{v}_{\alpha i} - \boldsymbol{v}_{\beta j})$ is the relative velocity, χ is the deflection angle of $\boldsymbol{g}$, and the Cartesian components of vector $\boldsymbol{h}$ are

$$\begin{aligned} h_x &= g_\perp \cos\varepsilon, \\ h_y &= -(g_y g_x \cos\varepsilon + g g_z \sin\varepsilon)/g_\perp, \\ h_z &= -(g_z g_x \cos\varepsilon - g g_y \sin\varepsilon)/g_\perp, \end{aligned}$$

where $g_\perp = (g_y^2 + g_z^2)^{1/2}$ and ε is the azimuthal angle of a collision plane. Equation (1) satisfies the conservation of energy and momentum during a collision. Random samples of (χ, ε) are determined by use of the probability $\sigma(g, \chi)\, d\Omega/\sigma_{\mathrm{T}}(g)$ of finding the postcollision relative velocity $\boldsymbol{g}'(=\boldsymbol{v}'_{\alpha i} - \boldsymbol{v}'_{\beta j})$ in solid angle $d\Omega(=\sin\chi\, d\chi\, d\varepsilon)$ [15]. The symbols σ and σ_{T} are the differential and the total cross section, respectively. Since σ does not depend on ε, $\varepsilon = 2\pi U$, where U is a random number between 0 and 1. The probability of choosing a collision partner (βj) is proportional to $g\sigma_{\mathrm{T}}$.

Let us go back to Coulomb collisions. Charged particles in a plasma undergo many small-angle scatterings; such scatterings can be grouped into a unique binary collision with a large scattering angle [10]. Coulomb collisions can now be treated as if they were short-range collisions; the velocities of particles (αi) and (βj) at the end of time step Δt are given by Eq.(1), where χ is now the cumulative deflection angle of $\boldsymbol{g}$ as a result of many small-angle collisions with particles β. We now describe the method to determine $\boldsymbol{v}_{\beta j}$, ε, and χ in Eq.(1). The velocity of a collision partner (βj) is randomly sampled from the set of velocities of particles β; there is no need to pick up a special partner because particle (αi) undergoes many small-angle collisions with particles β in Δt. The method to pair particles α and β is described in Section 3.1. The angle ε is uniformly distributed, so that $\varepsilon = 2\pi U$. The cumulative property is reflected in the rule to determine χ. First note that χ is an angle between $\boldsymbol{g}(=\boldsymbol{v}_{\alpha i} - \boldsymbol{v}_{\beta j})$ and $\boldsymbol{g}'(=\boldsymbol{v}'_{\alpha i} - \boldsymbol{v}'_{\beta j})$. Let $f(\chi)\, d\Omega$ be defined as the probability of

finding $\boldsymbol{g}'$ in solid angle $d\Omega(=2\pi\ \sin\chi\ d\chi)$. The function $f(\chi)$ is now given by [10].

$$f(\chi) = \frac{A}{4\pi \sinh A} \exp(A\cos\chi). \tag{2}$$

Here the shape factor A depends on the time, Δt, spent by particle (αi) while engaged in the cumulative collision. The factor A is a solution of the nonlinear equation

$$\coth A - A^{-1} = \exp[-s_{\alpha\beta}(\Delta t)], \tag{3}$$

where

$$s_{\alpha\beta}(\Delta t) = \frac{\ln\Lambda_{\alpha\beta}}{4\pi}\left(\frac{q_\alpha q_\beta}{\epsilon_0\mu_{\alpha\beta}}\right)^2 n_\beta g_{\alpha\beta}^{-3}\Delta t. \tag{4}$$

Here q_α and q_β represent the charges of particles α and β, ϵ_0 is the permittivity of free space, $\mu_{\alpha\beta}$ is the reduced mass, n_β is the number density, $g_{\alpha\beta}(=|\boldsymbol{v}_{\alpha i} - \boldsymbol{v}_{\beta j}|)$ is the relative speed, and $\ln\Lambda_{\alpha\beta}$ is the Coulomb logarithm. The solution of Eq.(3) is tabulated in Ref.[9]. In the limit of $\Delta t \to 0$ or $s_{\alpha\beta} \to 0$ we have $A \to 1/s_{\alpha\beta}$; hence we need only consider small χ values in Eq.(2). Using $\cos\chi \simeq 1 - \chi^2/2$, we see that $f(\chi)$ has a Gaussian profile with a narrow width, as in the case of Takizuka and Abé [2]. In the limit of $\Delta t \to \infty$ we have $A \to 0$; hence $f(\chi) \to 1/4\pi$. This limit indicates isotropic scattering occurs as expected. The time step Δt is chosen in such a way that the value of $s_{\alpha\beta}$, which changes from collision to collision, does not exceed 5. Once $\boldsymbol{v}_{\alpha i}$, $\boldsymbol{v}_{\beta j}$, and Δt are given, we can make a random sample of $\cos\chi$ from Eq.(2), represented by

$$\cos\chi = \frac{1}{A}\ln(e^{-A} + 2U\sinh A), \tag{5}$$

where $0 < \chi < \pi$ and U is the random number. Now since we have found $\cos\chi$ and $\sin\chi = +(1 - \cos^2\chi)^{1/2}$ in Eq.(1), the velocities of particles (αi) and (βj) at time $t + \Delta t$ can be obtained.

A remark on forming the Coulomb logarithm may yield some insight into the formulation. Since $\ln\Lambda_{\alpha\beta}$ depends only weakly on $g_{\alpha\beta}$, it is adequate to use the approximation [10]

$$\Lambda_{\alpha\beta} = \frac{2\pi\epsilon_0\mu_{\alpha\beta}\lambda_D\langle g_{\alpha\beta}^2\rangle}{|q_\alpha q_\beta|}.$$

Here the mean square of relative speed is

$$\langle g_{\alpha\beta}^2\rangle = \frac{3kT_\alpha}{m_\alpha} + \frac{3kT_\beta}{m_\beta} + (\langle\boldsymbol{v}_\alpha\rangle - \langle\boldsymbol{v}_\beta\rangle)^2,$$

where k is the Boltzmann constant. This equation is obtained by assuming that the velocity distributions of particles α and β are Maxwellian, T and $\langle\boldsymbol{v}\rangle$ are the temperature and flow

velocity in the distribution. In practical simulations we determine the cell properties such as $\langle \boldsymbol{v}_\alpha \rangle$ and T_α by

$$\langle \boldsymbol{v}_\alpha \rangle = \frac{1}{N_\alpha} \sum_{i=1}^{N_\alpha} \boldsymbol{v}_{\alpha i},$$

$$T_\alpha = \frac{m_\alpha}{3k} \left(\langle v_\alpha^2 \rangle - \langle \boldsymbol{v}_\alpha \rangle^2 \right),$$

where $\langle v_\alpha^2 \rangle$ is the mean of $v_{\alpha 1}^2, v_{\alpha 2}^2, \ldots$.

Now that we have described the method to determine the final velocity of particle (αi) at time $t + \Delta t$ after the cumulative collision with particles β in time Δt, other particles may be calculated in the same way. Repeating the procedure described, we can calculate all α–β, α–α, and β–β collisions in Δt. The order of types of collisions is arbitrary. We may calculate collisions, say, in the order of α–α, α–β, and β–β. The objective of the present work is to present a systematic way to calculate all α–β and α–α (or β–β) collisions in Δt in the case when the weights W_α and W_β for species α and β are different.

3. COLLISIONS BETWEEN UNLIKE PARTICLES

An examination of Eqs.(3) through (5) shows that the cumulative scattering angle χ of particle (αi) in time Δt is calculated by use of $s_{\alpha\beta}(\Delta t)$. The same angle χ appears in Eqs.(1a) and (1b). On the other hand, the scattering angle of particle (βj) should be calculated by use of

$$s_{\beta\alpha}(\Delta t) = \frac{\ln \Lambda_{\alpha\beta}}{4\pi} \left(\frac{q_\alpha q_\beta}{\epsilon_0 \mu_{\alpha\beta}} \right)^2 n_\alpha g_{\alpha\beta}^{-3} \Delta t, \tag{6}$$

where $\Lambda_{\alpha\beta} = \Lambda_{\beta\alpha}$ is assumed. If $s_{\beta\alpha}(\Delta t) = s_{\alpha\beta}(\Delta t)$, then the probability density function for the scattering angle of particle (βj) coincides with that for particle (αi); a common angle χ given by Eq.(5) can be used in determining the postcollision velocities of the pair $(\alpha i, \beta j)$. If $n_\beta = n_\alpha$ then $s_{\beta\alpha}(\Delta t) = s_{\alpha\beta}(\Delta t)$ and the probability density function coincide. In this case Eqs.(1a) and (1b) give the velocities of particles (αi) and (βj) after time increment Δt. In general, $n_\beta \neq n_\alpha$, for example in radio-frequency discharge of electronegative gases the electron density is only a few percentages of the negative ion density. Also, in plasmas containing ions with multiple charges, electron density is several times larger than ion density. We can conclude from Eqs.(4) and (6) that

$$s_{\alpha\beta}(\Delta t) = s_{\beta\alpha}\left(\frac{n_\beta}{n_\alpha} \Delta t \right). \tag{7}$$

This equation means that when using Eqs.(1a) and (1b) the time increment of particle (βj) should be $(n_\beta / n_\alpha)\Delta t$ when particle (αi) is Δt. This time increment concept is developed further in the following section.

3.1. *Equally Weighted Particles*

Let W_α represent the common weight of all particles of species α. Similarly, let W_β represent the weight of all particles β. We consider the simplest case of $W_\alpha = W_\beta (\equiv W)$ in

$\alpha 1-\beta 1$	$\alpha 1-\beta 1$
$\alpha 2-\beta 2$	$\alpha 2-\beta 2$
$\alpha 3-\beta 3$	$\alpha 3-\beta 3$
$\alpha 4-\beta 4$	$\alpha 4-\beta 1'$
$\alpha 5-\beta 5$	$\alpha 5-\beta 2'$
$\alpha 6-\beta 6$	$\alpha 6-\beta 3'$
$\alpha 7-\beta 7$	$\alpha 7-\beta 1''$
(a)	(b)

FIG. 1. Collision pairs for particles of different species: (a) $N_\alpha = N_\beta = 7$; (b) $N_\alpha = 7$, $N_\beta = 3$.

this section. First let us begin the analysis with the case of $N_\alpha = N_\beta (\equiv N)$. Since Coulomb interaction is a long-range force, the velocities of all particles are changed after time Δt. This is best illustrated by defining N pairs of particles α and β and recalling that in Eq.(1) a collision partner of particle (αi) is chosen randomly from the set of all particles β. Figure 1a shows $N(=7)$ pairs $(\alpha i, \beta j)$, where $\beta 1, \beta 2, \ldots$ are sampled randomly without replacement. Note that each particle appears only once in N pairs.

Let us go back to the discussion on Eq.(7). Hereafter we suppose, for simplicity, that all particles are in a cell with unit volume. We then have

$$n_\alpha = W_\alpha N_\alpha, \quad n_\beta = W_\beta N_\beta, \tag{8}$$

where $n_\alpha (= n_\beta)$ is the number of real particles α in the cell. It is important to remember that all pairs $(\alpha i, \beta j)$ change velocities in collision. If Eq.(4) is used to obtain the scattering angle, the time increment of a simulated particle of species α is Δt, which means that the sum of the time increments of W real particles is $W\Delta t$. Since the number of collision is N, the mean time increment per real particle α is $N \times W\Delta t/n_\alpha = \Delta t$. Similarly, the time increment of a simulated particle β is $(n_\beta/n_\alpha)\Delta t = \Delta t$; hence, the time increment per real particle β is also Δt. It should be now understood that for this case the time increment per real particle is the same for two species.

Next let us consider the case of $N_\alpha \neq N_\beta$ and $W_\alpha = W_\beta (= W)$; note that this implies $n_\alpha \neq n_\beta$. We will discuss the case of $N_\alpha > N_\beta$ since the opposite case can be treated similarly. Figure 1b shows the case of $N_\alpha = 7$ and $N_\beta = 3$. The array of $\beta 1, \beta 2, \beta 3$ is random. Since $N_\beta < N_\alpha$, certain particles β must collide two or three times. The single prime indicates a second collision and the double prime a third collision. We calculate the scattering angle by using Eq.(4) and, hence, the simulated particle (αi) time is advanced by Δt. Now let us evaluate the time increment per real particle. For species α the time increment is $N_\alpha \times W\Delta t/n_\alpha = \Delta t$. For species β the time increment per simulated particle is $(n_\beta/n_\alpha)\Delta t$, the number of collision is N_α, and the number of real particles is n_β; hence, the mean time increment per real particle is $N_\alpha \times W \times (n_\beta/n_\alpha)\Delta t/n_\beta = \Delta t$, which coincides with the mean time increment per real particle α, as expected.

Note that we have advanced the time of a larger set α by Δt through the use of Eq.(4). If we use $s_{\beta\alpha}(\Delta t)$ to evaluate the scattering angle, the time of a smaller set β is advanced by Δt. Equation (6) can be rewritten as

$$s_{\beta\alpha}(\Delta t) = s_{\alpha\beta}\left(\frac{n_\alpha}{n_\beta}\Delta t\right). \tag{9}$$

Let us calculate the time increment per real particle from Fig.1b. For species β the time increment is $N_\alpha \times W \times \Delta t/n_\beta = (n_\alpha/n_\beta)\Delta t$ and for species α it is $N_\alpha \times W \times (n_\alpha/n_\beta)\Delta t/n_\alpha = (n_\alpha/n_\beta)\Delta t$. We therefore have the same time increment. However, the time increment changes from cell to cell if n_α and n_β are spatially nonuniform, which is inconvenient. We want to use a common time increment $\Delta t'$ for all cells. A common time increment is found by choosing $\Delta t = (n_\beta/n_\alpha)\Delta t'$. Note that Δt changes from cell to cell.

It is simpler to have the time of a larger set α advance by Δt through the use of $s_{\alpha\beta}(\Delta t)$. In Fig.1b, the sum of the time increments for particle $\beta 1$ is $3 \times (3/7)\Delta t$, and the sum for particle $\beta 2$ and the sum for particle $\beta 3$ are equal to $2 \times (3/7)\Delta t$. The mean of the three sums is Δt, which corresponds with the time increment per real particle. A common time increment is defined by assigning such a mean time increment to a set of particles in simulating a time-evolving physical system; the mean time increment may be called the time increment of a system.

Thus far we have considered the case of $N_\alpha > N_\beta$. In the case of $N_\beta > N_\alpha$, let us advance the time of a larger set β by Δt through the use of $s_{\beta\alpha}(\Delta t)$. The time increment per real particle β is $N_\beta \times W\Delta t/n_\beta = \Delta t$ and the time increment per real particle α is $N_\beta \times W(n_\alpha/n_\beta)\Delta t/n_\alpha = \Delta t$. Now a general rule can be stated: Advance the time of a larger set by Δt and then the time of a system of particles is advanced by the same time increment.

3.2. *Different Weights for Different Species*

Macroscopic properties such as flow velocity and temperature obtained from an average of simulated particles show larger fluctuations for smaller numbers of particles. Therefore, it is better to employ a nearly equal number of simulated particles for each species even if there is a large difference among species number densities. This requires the introduction of different weighting factors to each species. The case of $W_\alpha \neq W_\beta$ is now considered. First let us examine the meaning of a collision between a simulated particle α with weight W_α and a simulated particle β with W_β. The α–β collision for $W_\alpha = 3$ and $W_\beta = 5$ and that for $W_\alpha = 5$ and $W_\beta = 3$ are shown in Fig.2, where the numbers designate the names of *real* particles. Since we consider collisions in pairs, only three real particles of species β undergo collisions in Fig.2a. This can be described through probability theory; simulated particle α undergoes a collision with probability $W_\beta/\max(W_\alpha, W_\beta)[=1]$ and simulated particle β does with probability $W_\alpha/\max(W_\alpha, W_\beta)[=3/5]$. This rule is also applicable to case (b) in Fig.2, where the collision probabilities of particles α and β are now exchanged.

α	β	α	β
1	1	1	1
2	2	2	2
3	3	3	3
	4	4	
	5	5	
(a)		(b)	

FIG. 2. Collision pairs of real particles: (a) $W_\alpha = 3$, $W_\beta = 5$; (b) $W_\alpha = 5$, $W_\beta = 3$.

This methodology is a common Monte Carlo simulation technique [4, 13], which conserves average momentum and energy. The postcollision velocities $\boldsymbol{v}^*_{\alpha i}$ and $\boldsymbol{v}^*_{\beta j}$ of particles (αi) and (βj) are given by

$$\boldsymbol{v}^*_{\alpha i} = (1 - Z_\alpha)\boldsymbol{v}_{\alpha i} + Z_\alpha \boldsymbol{v}'_{\alpha i}, \tag{10a}$$

$$\boldsymbol{v}^*_{\beta j} = (1 - Z_\beta)\boldsymbol{v}_{\beta j} + Z_\beta \boldsymbol{v}'_{\beta j}, \tag{10b}$$

where $\boldsymbol{v}'_{\alpha i}$ and $\boldsymbol{v}'_{\beta j}$ are given by Eqs.(1a) and (1b), and

$$\begin{aligned}
\text{Prob}[Z_\alpha = 1] &= W_\beta / \max(W_\alpha, W_\beta), \\
\text{Prob}[Z_\alpha = 0] &= 1 - \text{Prob}[Z_\alpha = 1], \\
\text{Prob}[Z_\beta = 1] &= W_\alpha / \max(W_\alpha, W_\beta), \\
\text{Prob}[Z_\beta = 0] &= 1 - \text{Prob}[Z_\beta = 1].
\end{aligned}$$

Here Prob[ ] denotes probability.

Let us now examine the case of $N_\alpha \geq N_\beta$; see Fig.1. We use $s_{\alpha\beta}(\Delta t)$ of Eq.(4) to calculate the scattering angle and advance the time of particle (αi) by Δt. In Fig.1b the particles $\beta 1'$, $\beta 2'$, $\beta 3'$, and $\beta 1''$ are renamed $\beta 4$, $\beta 5$, $\beta 6$, and $\beta 7$. Then for each collision of particles (αi) and (βi) $(i = 1, 2, \ldots, N_\alpha)$, the number of real particles α that have collided is $W_\alpha \times W_\beta / \max(W_\alpha, W_\beta)$ and the sum of the time increments of these real particles α is $\Delta t \times W_\alpha W_\beta / \max(W_\alpha, W_\beta)$. The total number of real particles is $n_\alpha (= W_\alpha N_\alpha)$. Now we can obtain the mean time increment per real particle α. Note that the mean is calculated for the total number n_α, including real particles that have and have not undergone a collision. Since the number of pairs is N_α, the mean is

$$N_\alpha \times \Delta t \times \frac{W_\alpha W_\beta}{\max(W_\alpha, W_\beta)} \times \frac{1}{n_\alpha} = \frac{W_\beta}{\max(W_\alpha, W_\beta)} \Delta t (\equiv \Delta t').$$

Similarly, the time increment per real particle β is

$$N_\alpha \times \frac{n_\beta}{n_\alpha} \Delta t \times \frac{W_\beta W_\alpha}{\max(W_\alpha, W_\beta)} \times \frac{1}{n_\beta} = \frac{W_\beta}{\max(W_\alpha, W_\beta)} \Delta t (\equiv \Delta t').$$

The two increments agree, although some real particles do not undergo a collision. Statistically, however, we can interpret this as all real particles have collided and their times are advanced by $\Delta t'$. As before, it is better to choose Δt as

$$\Delta t = \frac{\max(W_\alpha, W_\beta)}{W_\beta} \Delta t' \tag{11a}$$

for a given time step $\Delta t'$. Of course, $\Delta t'$ is the time increment of a physical system.

Let us next consider the case of $N_\beta > N_\alpha$ and $W_\alpha \neq W_\beta$. Exchanging α and β in Fig.1b, the case can be studied. We advance the time of a larger set β by Δt through the use of $s_{\beta\alpha}(\Delta t)$. The time increment $\Delta t'$ per real particle β becomes

$$\frac{W_\alpha}{\max(W_\alpha, W_\beta)} \Delta t (\equiv \Delta t').$$

This agrees with the time increment per real particle α. For this case we choose

$$\Delta t = \frac{\max(W_\alpha, W_\beta)}{W_\alpha}\Delta t' \tag{11b}$$

in the expression for $s_{\beta\alpha}(\Delta t)$, $\Delta t'$ being the given time step.

3.3. *Different Weights for Different Particles*

Let us imagine a uniform plasma in a cylinder. We divide the domain inside the cylinder into cells by equal radial spacing Δr with the Debye length. The number of particles in the cell between r and $r + \Delta r$ is proportional to $2\pi r \Delta r$, where r is the radial distance. If we assign the same weight to all simulated particles, the number of particles in a cell near the axis of the cylinder is very small. This results in a large statistical fluctuation of sampled data. If the number of simulated particles in a cell could be nearly uniform for all cells, it is convenient computationally. This idea results in the introduction of a larger weight for a particle with a larger radius.

Let $W_{\alpha i}$ $(i = 1, \ldots, N_\alpha)$ and $W_{\beta j}$ $(j = 1, \ldots, N_\beta)$ be the weights of particles (αi) and (βj) in a cell. First we consider the case of $N_\alpha \geq N_\beta$, see Fig.1b. Since the cell is assumed to have the unit volume, the number densities are given by

$$n_\alpha = \sum_{i=1}^{N_\alpha} W_{\alpha i}, \quad n_\beta = \sum_{j=1}^{N_\beta} W_{\beta j}.$$

Let us advance the time of a larger set α by Δt by use of $s_{\alpha\beta}(\Delta t)$. In Fig.1b the particles $\beta 1'$, $\beta 2'$, $\beta 3'$, and $\beta 1''$ are renamed $\beta 4$, $\beta 5$, $\beta 6$, and $\beta 7$; the collision pairs are $(\alpha i, \beta i)$ for $i = 1, \ldots, N_\alpha$. Considering $\alpha i - \beta i$ collision, the number of real particles α that have collided is $W_{\alpha i} \times W_{\beta i}/\max(W_{\alpha i}, W_{\beta i})$. The sum of the time increments of these real particles is $\Delta t W_{\alpha i} W_{\beta i}/\max(W_{\alpha i}, W_{\beta i})$. The number of real particles α is n_α. For N_α collisions the time increment per real particle α is given by

$$\frac{n_{\alpha\beta}}{n_\alpha}\Delta t (\equiv \Delta t'), \tag{12}$$

where

$$n_{\alpha\beta} = \sum_{i=1}^{N_\alpha} \frac{W_{\alpha i} W_{\beta i}}{\max(W_{\alpha i}, W_{\beta i})}.$$

The expression is the same for real particle β. Therefore, for a given time step $\Delta t'$ we have only to set $\Delta t = (n_\alpha/n_{\alpha\beta})\Delta t'$ in the equation for $s_{\alpha\beta}(\Delta t)$ to have the system time increment be common to all cells.

In case of $N_\beta > N_\alpha$ the time of a larger set β is advanced by Δt, i.e., the scattering angle is obtained by use of $s_{\beta\alpha}(\Delta t)$. The particles α which have already collided once, twice, ... are renamed in order as in the case of $N_\alpha > N_\beta$. The time increment per real particle α and that for particle β become $(n_{\alpha\beta}/n_\beta)\Delta t$, where $n_{\alpha\beta}$ is given by Eq.(12) with the upper limit replaced by N_β. In this case for a given time step $\Delta t'$ we choose Δt as

$$\Delta t = \frac{n_\beta}{n_{\alpha\beta}}\Delta t'.$$

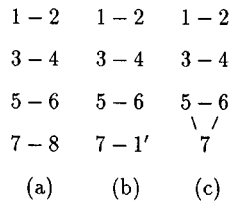

FIG. 3. Collision pairs for particles of the same species: (a) even N_α; (b) odd N_α; (c) odd N_α (Ref.[2]).

4. COLLISIONS BETWEEN LIKE PARTICLES

When $\beta = \alpha$ Eq.(4) takes the form

$$s_{\alpha\alpha}(\Delta t) = \frac{\ln \Lambda_{\alpha\alpha}}{\pi}\left(\frac{q_\alpha^2}{\epsilon_0 m_\alpha}\right)^2 n_\alpha g_{\alpha\alpha}^{-3}\Delta t. \tag{13}$$

We should then form a random array of simulated particles α. The particles in this array are named 1, 2, ..., N_α. The array is formed by picking up two by two particles to make pairs. Figure 3a shows the case of $N_\alpha = 8$. If N_α is an odd number, we make the last pair as shown in Fig.3b, where the precollision velocity of particle $1'$ is the postcollision velocity of particle 1. Let us rename particle $1'$ particle 8 (or $N_\alpha + 1$) when N_α is an odd number. Figure 3c shows the method of pairing by Takizuka and Abé [2] which has been simplified in the proposed method. In Takizuka and Abé's method particles 5, 6, and 7 must collide twice.

4.1. *Equally Weighted Particles*

Let weight W_α be defined as common to all particles. In reference to Figs.3a and b let us define the number of pairs N; $N = N_\alpha/2$ for even N_α and $N = (N_\alpha + 1)/2$ for odd N_α. We obtain the scattering angle through Eq.(13); the time of particles is advanced by Δt. The sum of the time increments of all particles (including particle $1'$ in Fig.3b) is $N \times 2\Delta t$. The number of particles is N_α. The mean time increment of a particle, which is equal to the increment per real particle, is

$$\frac{2N}{N_\alpha}\Delta t (\equiv \Delta t'),$$

where $\Delta t'$ is a given time step for a physical system. The choice of Δt in Eq.(13) is

$$\Delta t = \frac{N_\alpha}{2N}\Delta t'.$$

Note that $\Delta t = \Delta t'$ for even N_α but $\Delta t = [N_\alpha/(N_\alpha + 1)]\Delta t'$ for odd N_α. Since an additional collision is calculated for odd N_α, such a correction of Δt is necessary. Note that we have $N = (N_\alpha + 3)/2$ for odd N_α in Takizuka and Abé's method. That is, if we set $\Delta t = [N_\alpha/(N_\alpha + 3)]\Delta t'$, we can use their method of pairing. However, one additional collision should always be calculated.

4.2. *Different Weights for Different Particles*

Let W_i be the weight of particle i. There are N_α particles in a cell with unit volume. The number of real particles is

$$n_\alpha = \sum_{i=1}^{N_\alpha} W_i.$$

We define pairs of particles as indicated in Fig.3a or b. In case of an odd N_α, particle $1'$ in Fig.3b is renamed particle $N_\alpha + 1$. The deflection angle is calculated by using $s_{\alpha\alpha}(\Delta t)$, and hence, the time of each particle is advanced by Δt. The number of collision pairs, N, is $N_\alpha/2$ for even N_α and $(N_\alpha + 1)/2$ for odd N_α. For the first pair 1–2, particle 1 undergoes a collision with probability $W_2/\max(W_1, W_2)$ and particle 2 does with probability $W_1/\max(W_1, W_2)$. The number of real particles that have collided is $W_1 \times W_2/\max(W_1, W_2) + W_2 \times W_1/\max(W_1, W_2)$, and hence, the sum of the time increments of real particles is $\Delta t \times 2W_1W_2/\max(W_1, W_2)$. The mean time increment per real particle can be obtained by dividing the whole sum over N pairs by the number of real particles n_α. It is $(n_{\alpha\alpha}/n_\alpha)\Delta t$, where

$$n_{\alpha\alpha} = 2\sum_{i=1}^{N} \frac{W_{2i-1}W_{2i}}{\max(W_{2i-1}, W_{2i})}.$$

For a given time step $\Delta t'$ of a physical system, Δt in the expression of $s_{\alpha\alpha}(\Delta t)$ is chosen as

$$\Delta t = \frac{n_\alpha}{n_{\alpha\alpha}}\Delta t'. \tag{14}$$

5. SAMPLE CALCULATIONS

We consider the relaxation of temperatures and flow velocities of electrons (1) and ions (2) due to 1–2, 1–1, and 2–2 collisions. Initially electrons are assumed to be in equilibrium with temperature T_{10} and flow velocity V_{10}. Ions are also assumed to be in equilibrium with temperature T_{20} and flow velocity V_{20}. The following values are selected

$$kT_{10} = 1\,\text{keV}, \quad kT_{20} = 100\,\text{eV},$$
$$V_{10} = \sqrt{kT_{10}/m_1}, \quad V_{20} = 0.$$

It should be noted that the present algorithm is not limited to temporal Maxwellian distributions [16]. Initial velocities of electrons and ions are sampled from the Maxwellian distribution for each species. The purpose of this section is to show the validity of the proposed weight algorithms. Therefore we consider ions with imaginary mass of $m_2 = 5m_1$, which makes the relaxation rate of ions comparable to that of electrons and, hence, greatly shortens the computation time. We also introduce the simplification that the Coulomb logarithm is common to 1–2, 1–1, 2–2 collisions and equal to 15.9. This value corresponds to that of an equilibrium plasma with electron and ion temperatures of 1 keV and density 10^{21} m^{-3} [10]. We assume that plasma is electrically neutral,

$$n_1 = Zn_2, \tag{15}$$

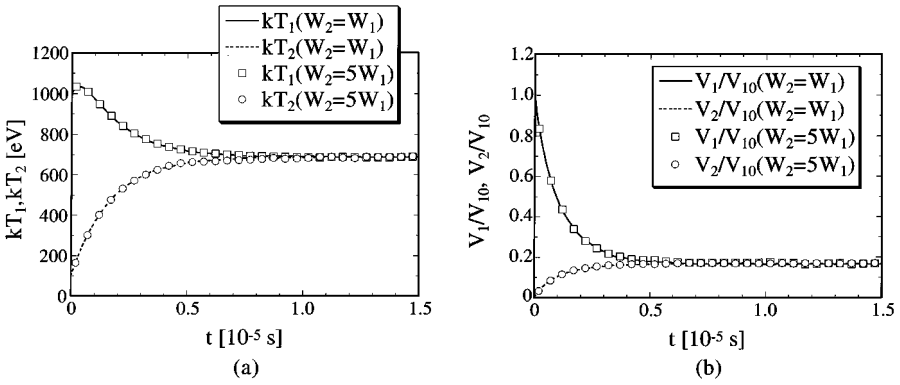

FIG. 4. Relaxation of electron (1) and ion (2) properties (Z = 1): (a) temperatures; (b) flow velocities.

where $+eZ$ is the charge of ion, although charge neutrality is not essential in applying the present theory. The ion density n_2 is fixed at 10^{21} m^{-3} for any Z.

5.1. *Ion with a Single Charge*

We begin with the case of $Z = 1$. The time step $\Delta t'$ of the system is chosen to be 10^{-7} s. First we obtained the standard data by use of the same weight for two species, i.e., $W_1 = W_2$ and $N_1 = N_2 = 10^5$, where W_i is the weight and N_i is the number of particles. Next we assign a different weight to each species. The first case is $W_2 = 5W_1$, and $N_1 = 10^5$ and $N_2 = 2 \times 10^4$. Note that the charge neutrality condition (15) requires $N_1 W_1 = N_2 W_2$. The condition gives $W_1 < W_2$ for $N_1 > N_2$, and hence Eq.(11a) for $\alpha = 1$ and $\beta = 2$ becomes $\Delta t = \Delta t'$, where Δt is the time step in $s_{12}(\Delta t)$. The relaxation of temperatures and flow velocities is shown in Figs.4a and b. The solid and dashed lines represent the standard data for $W_1 = W_2$. The electron temperature T_1 shows a small peak in the early stage of relaxation. We see that the results for $W_2 = 5W_1$ agree well with the standard data. The use of the different weights reduced the computation time by 40%. Next the opposite case is considered: $W_1 = 5W_2$, and $N_1 = 2 \times 10^4$ and $N_2 = 10^5$; since $N_2 > N_1$, Eq.(11b) for $\beta = 2$ and $\alpha = 1$ becomes $\Delta t = \Delta t'$. Figures 5a and b show the comparison of the obtained data

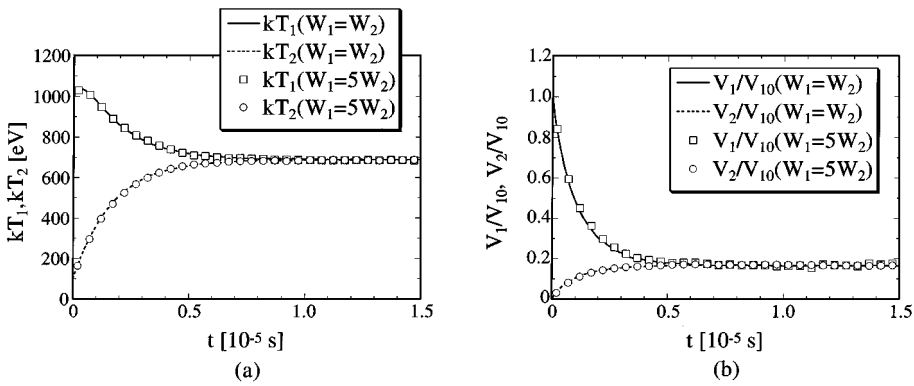

FIG. 5. Relaxation of electron (1) and ion (2) properties (Z = 1): (a) temperatures; (b) flow velocities.

with the standard data for $W_1 = W_2$. We again see almost an exact match between the two sets of data.

5.2. *Ion with Multiple Charges*

We now consider the case of $Z = 3$. Equation (4) shows that there is a large difference among s_{11}, s_{12}, and s_{22} because of the factor Z. That is,

$$s_{12}(\Delta t) = \frac{\ln \Lambda}{4\pi}\left(\frac{e^2}{\epsilon_0 \mu_{12}}\right)^2 n_2 g_{12}^{-3} \cdot Z^2 \Delta t, \tag{16a}$$

$$s_{11}(\Delta t) = \frac{\ln \Lambda}{4\pi}\left(\frac{e^2}{\epsilon_0 \mu_{11}}\right)^2 n_2 g_{11}^{-3} \cdot Z \Delta t, \tag{16b}$$

$$s_{22}(\Delta t) = \frac{\ln \Lambda}{4\pi}\left(\frac{e^2}{\epsilon_0 \mu_{22}}\right)^2 n_2 g_{22}^{-3} \cdot Z^4 \Delta t, \tag{16c}$$

where $\ln \Lambda$ is assumed to be independent of a collision pair, as stated before, and the relation $n_1 = Z n_2$ is used in obtaining Eq.(16b). First we consider the standard case of $W_1 = W_2$. Equation (15) requires $N_1 = Z N_2$. Our choice is $N_1 = 15 \times 10^4$ and $N_2 = 5 \times 10^4$. Equation (11a) for $\alpha = 1$ and $\beta = 2$ shows that Δt in Eq.(16a) agrees with the system time increment $\Delta t'$. Also, Δt's in Eqs.(16b) and (16c) agree with $\Delta t'$ since N_1 and N_2 are even numbers. Since N_2 is 1/3 of N_1, in time Δt each ion collides three times, whereas each electron collides only once. Because of a large factor of $Z^4 (=81)$ in Eq.(16c) our choice of $\Delta t (= \Delta t')$ is $10^{-7}/80$ s$(=1.25 \times 10^{-9}$ s). The obtained data is shown by the solid and dashed lines in Figs. 6a and b.

Next we consider the case of $W_1 = Z W_2$; Eq.(15) gives $N_1 = N_2$. Our choice is $N_1 = 5 \times 10^4$. For this case it is more convenient to use the same $\Delta t (= 1.25 \times 10^{-9}$ s) in Eqs.(16a), (16b), and (16c). We use Eq.(16a) to calculate 1–2 collisions. Then Eq.(11a) for $\alpha = 1$ and $\beta = 2$ gives $\Delta t = Z(\Delta t')_{12}$, where $(\Delta t')_{12} (= \Delta t / Z)$ is the system time increment due to 1–2 collisions. Similarly we have $(\Delta t')_{11} = (\Delta t')_{22} = \Delta t$ from Section 4.1. The system time increment due to 1–2 collisions is $1/Z$ of that due to 1–1 and 2–2 collisions. How do we advance the time of the system? The solution of this question is as follows: We calculate 1–2 collisions Z times by use of Eq.(16a) and, hence, advance the system time

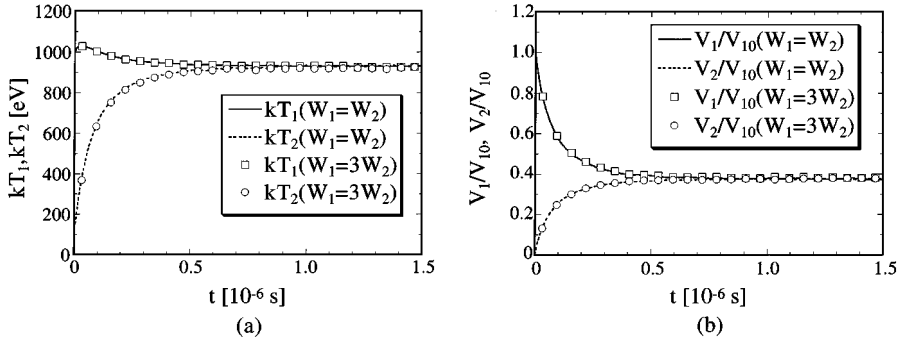

FIG. 6. Relaxation of electron (1) and ion (2) properties (Z = 3): (a) temperatures; (b) flow velocities.

by $\Delta t(=Z \times \Delta t/Z)$, and then 1–1 collisions once by the use of Eq.(16b), and lastly 2–2 collisions once by the use of Eq.(16c). Clearly, the system time is advanced by Δt after this procedure. The results obtained are compared in Figs.6a and b with the standard data for $W_1 = W_2$. The data for $W_1 = ZW_2$ agree well with those for $W_1 = W_2$. The computation time is reduced by 30% by introducing $W_1 = ZW_2$.

We have solved the same problem by assigning a different weight to each particle to check the weight algorithm in Sections 3.3 and 4.2. The weight W_{2i} of ion i is chosen to be

$$W_{2i} = C\left[1 + (a-1)\frac{i-1}{N_2 - 1}\right] \quad (i = 1, 2, \ldots, N_2),$$

where $a = 10$. W_{2i} changes from C to $10C$. The constant C is determined from

$$n_2 = \sum_{i=1}^{N_2} W_{2i} = \frac{a+1}{2} N_2 C.$$

We choose the weight W_{1i} for electron i as

$$W_{1i} = ZW_{2i}.$$

We set $N_1 = N_2$, then Eq.(15) is satisfied and W_{1i} changes from ZC to $10ZC$.

First let us consider 1–2 collisions based on Eq.(16a). Equation (12) yields Δt in Eq.(16a) as $\Delta t = (n_1/n_{12})(\Delta t')_{12}$. We chose the system time increment $(\Delta t')_{12}$ to be $(\Delta t')_{12} = \Delta t'/Z$, where $\Delta t' = 1.25 \times 10^{-9}$ s. Note the $\Delta t'$ is the (given) system time and $(\Delta t')_{12}$ is its subinterval. Choosing the subinterval is arbitrary. Note also that n_{12} should be calculated at each time step $(\Delta t')_{12}$ because $N_1(=N_2)$ pairs are chosen randomly without replacement at each time step. We repeat Z times a set of 1–2 collision calculations and advance the system time by $\Delta t'[=Z \times (\Delta t')_{12}]$. Next we consider 1–1 collisions by setting the system time increment to $\Delta t'$. The time step Δt in Eq.(16b) is given by $\Delta t = (n_1/n_{11})\Delta t'$, where n_{11} should also be calculated at each time step $\Delta t'$. Similarly, we calculate 2–2 collisions by use of Eq.(16c), where $\Delta t = (n_2/n_{22})\Delta t'$. The data obtained for $N_1 = N_2 = 5 \times 10^4$ is shown in Figs.7a and b in comparison with the standard data for $W_1 = W_2$. Note that in

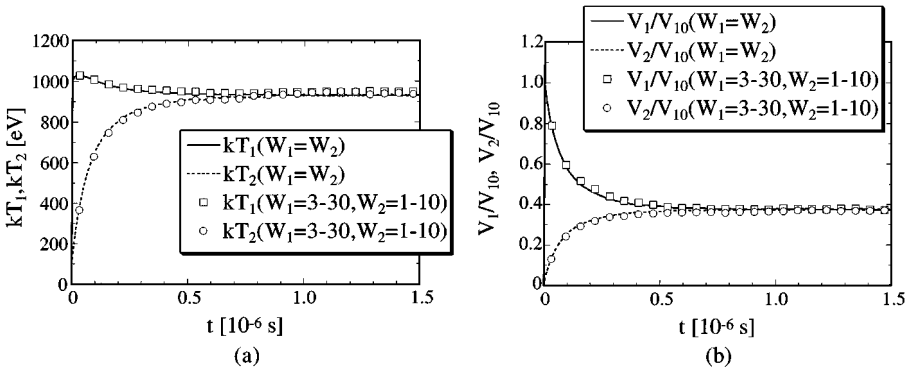

FIG. 7. Relaxation of electron (1) and ion (2) properties (Z = 3): (a) temperatures; (b) flow velocities.

Fig.7 the factor C in the equations of the weights is omitted. We see that the two data sets show almost an exact match supporting the proposed method's validity.

6. CONCLUSION

Proposed is an algorithm applying Nanbu's theory of Coulomb collision to weighted particles. Three cases are demonstrated:

(1) All particles in different species have the same weight.

(2) The weight is different for different species but it is the same for all particles in a species.

(3) The weight is different for each particle.

In order to show the validity of the proposed weight algorithm and explain the details of the method, some sample calculations are performed on the temporal relaxation of temperatures and flows of electrons and ions. All cases studied supported the validity of the present weight algorithm. Applications of the proposed method include modeling high density low temperature plasma, fusion plasma, intense beams, and X-ray laser source plasma.

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