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Algorithms for accurate collection, ejection, and loading in particle simulations

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Abstract

Algorithms for accurate collection, ejection, and loading of particles in particle simulations are presented. The algorithm for particle collection finds the position and velocity at any specific time from those at a discrete time. The algorithms for particle ejection and loading find the value at a discrete time from those at a given time. The accuracy of these algorithms is analyzed for general fields and is confirmed by comparing the numerically computed value with its exact solution under a homogeneous magnetic field. In particular, this ejection method can be applied to secondary emission as well as spontaneous emission.

Keywords: Particle simulation; Particle collection; Particle ejection; Particle loading

1. Introduction

In particle simulations, the velocity and position of particles are usually updated at pre-defined discrete times determined by the algorithms employed. However, in many physical applications, it is necessary to obtain them at any specific time. For example, in bounded systems where particles can cross the boundary, the interaction process between particles and boundary material often depends on the velocity and position of the incident particle at the impact time. This impact time is generally arbitrary and does not need to be a pre-defined time. Another common example is the ejection of particles at the boundary at any specific time. In both examples, an additional algorithm is required to connect the velocity and position at the discrete time with those at the specific time.

In particle-in-cell codes, the leap-frog integrator is widely used to solve the equations of motion for the particles [1–3]. The leap-frog method is generally a second-order method. Cartwright et al. [4] found that the accuracy of the velocity and position of particles injected from the boundary has a significant effect on the simulation of a crossed-field diode and developed a second-order method for particle loading and injection.

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However, we find that their analysis of truncation error is inconsistent: their algorithms were based on the error of the derivative of quantities rather than that of quantities themselves. The meaning of the acceleration error is obscure. In the analysis of the error of the velocity, it is contradictory that the finite difference equation for the position is used although the finite difference equation for the velocity does not include the position explicitly. It will be shown that in some cases the real accuracy of their algorithms for particle ejection and loading turns out to be different from that indicated in their paper.

In addition, we emphasize the importance of the accuracy of the velocity and position of particles collected at the boundary. In the secondary electron emission process, the secondary emission yield depends upon the energy and angle of the particle impacting the boundary [5]. Thus, the accuracy of the flux of ejected particles is limited by that of the velocity of the particle impacting the boundary in the secondary emission process. In a two- or three-dimensional simulation of a plasma system with dielectric boundaries, the position where charged particles are accumulated is also important in order to obtain the electric field accurately.

This paper presents zeroth-, first-, and second-order algorithms for particle collection, ejection, and loading. They are applicable to general main schemes (including the main leap-frog algorithm) for integration of the equations of motion. The accuracy derived from the error analysis will be confirmed by comparing numerically computed values (position and velocity) with their exact solutions.

2. Main algorithm

This section shows how the accuracy of the main algorithm is analyzed. The leap-frog method will be analyzed as an example, although the method is more generally applicable.

The Lorentz equation of motion for charged particles can be written as

$$\ddot{\mathbf{x}}(t) = \mathbf{e}(\mathbf{x}(t), t) + \mathbf{v}(t) \times \mathbf{b}(\mathbf{x}(t), t), \tag{1}$$

where $\mathbf{e} = q\mathbf{E}/m$ and $\mathbf{b} = q\mathbf{B}/m$.

The main leap-frog method is given as follows:

$$\mathbf{v}_{n+1/2} = \mathbf{v}_{n-1/2} + \mathbf{e}(\mathbf{x}_n, t_n)\Delta t + \frac{1}{2}(\mathbf{v}_{n-1/2} + \mathbf{v}_{n+1/2}) \times \mathbf{b}(\mathbf{x}_n, t_n)\Delta t \tag{2}$$

and

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{v}_{n+1/2}\Delta t, \tag{3}$$

where n indicates evaluation at $t_n = n\Delta t$, i.e., $\mathbf{x}_{n+1}$ is the approximate solution of the particle position at the time t_{n+1}.

The truncation error is the difference between the exact solution and the approximate solution obtained from the iterative method. The local truncation error is the truncation error incurred during one timestep, assuming that the values at the previous timestep are initially given.

In the main leap-frog method, the local truncation error of the velocity, $\varepsilon_{\mathbf{v},\mathrm{main}}$, is

$$\begin{aligned}
\varepsilon_{\mathbf{v},\mathrm{main}} &= \mathbf{v}(t_{n+1/2}) - \mathbf{v}_{n+1/2} \\
&= \mathbf{v}(t_{n+1/2}) - \mathbf{v}_{n-1/2} - \mathbf{e}(\mathbf{x}_n, t_n)\Delta t \\
&\quad - \frac{1}{2}[\mathbf{v}_{n-1/2} + \mathbf{v}(t_{n+1/2})] \times \mathbf{b}(\mathbf{x}_n, t_n)\Delta t \\
&\quad + \frac{1}{2}\varepsilon_{\mathbf{v},\mathrm{main}} \times \mathbf{b}(\mathbf{x}_n, t_n)\Delta t,
\end{aligned} \tag{4}$$

where $\mathbf{v}(t_{n+1/2})$ and $\mathbf{v}_{n+1/2}$ denote the exact and approximate solutions, respectively. Since the lowest order term in Δt is the focus of our study, the last term of Eq. (4) can be ignored as a one order higher term. $\mathbf{v}_{n-1/2}$ is the same as $\mathbf{v}(t_{n-1/2})$, since it is initially given value in this analysis. With Taylor expansions of $\mathbf{v}(t_{n+1/2})$ and $\mathbf{v}(t_{n-1/2})$, it can be shown that the velocity error is $\mathbf{O}(\Delta t^3)$ as follows:

$$\varepsilon_{\mathbf{v},\mathrm{main}} = \frac{1}{24}\dddot{\mathbf{a}}(t_n)\Delta t^3 - \frac{1}{8}\dot{\mathbf{a}}(t_n) \times \mathbf{b}(t_n)\Delta t^3 + \mathbf{O}(\Delta t^4), \tag{5}$$

which means that the velocity in the main leap-frog method is second-order accurate. Here, $\mathbf{a}(=\dot{\mathbf{v}})$ is the acceleration of the particle as follows:

$$\mathbf{a}(t_n) = \mathbf{e}(t_n) + \mathbf{v}(t_n) \times \mathbf{b}(t_n). \tag{6}$$

The local truncation error of the position, $\varepsilon_{\mathbf{x},\text{main}}$, is $\mathbf{x}(t_{n+1}) - \mathbf{x}_{n+1}$, where $\mathbf{x}(t_{n+1})$ and $\mathbf{x}_{n+1}$ denote the exact and approximate solutions, respectively. $\mathbf{x}_{n-1}$ is the same as $\mathbf{x}(t_{n-1})$. Since the position in Eq. (3) is updated by using the approximate velocity, the position error should include the velocity error term. With Taylor expansions of $\mathbf{x}(t_{n+1})$ and $\mathbf{v}(t_{n+1/2})$, it can be shown that the position error is $\mathbf{O}(\Delta t^3)$ as follows:

$$\begin{aligned}\varepsilon_{\mathbf{x},\text{main}} &= \mathbf{x}(t_{n+1}) - \mathbf{x}_{n+1} \\ &= \mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - [\mathbf{v}(t_{n+1/2}) - \varepsilon_{\mathbf{v},\text{main}}]\Delta t \\ &= \frac{1}{24}\dot{\mathbf{a}}(t_n)\Delta t^3 + \mathbf{O}(\Delta t^4),\end{aligned} \tag{7}$$

which means that the position in the main leap-frog method is second-order accurate.

Although the leap-frog method was analyzed as an example in this section, the following sections (algorithms for particle collection, ejection, and loading) will be applicable not only to the main leap-frog method but also to any general main algorithm. The accuracy of algorithms for particle collection, ejection, and loading depends on that of the main algorithm. In this article, the accuracy of the main algorithm is assumed to be better than first-order so that the error resulting from the main algorithm does not become dominant in following algorithms.

In general, the position and velocity in the main algorithm can be defined at different moments of time. In the following sections, the position and velocity are offset by a fractional timestep, $s\Delta t$ ($0 \leqslant s < 1$). For example, for the main leap-frog method, s is 0.5. For the method where the position and velocity are defined at the same moment of time, s is 0.

3. Collection of incident particles

Fig. 1 shows the collection of a particle at the boundary. In the main algorithm, the velocity and position are calculated at t_{n+1-s} and t_{n+1}, respectively. In the collection of particles which exit the system, their velocity ($\mathbf{v}^{\text{p}}$) and position ($\mathbf{x}^{\text{p}}$) need to be obtained in time ($t_{n+f} = t_n + \delta t^{\text{p}} = (n+f)\Delta t$, where $0 < f \leqslant 1$) upon crossing the boundary. $\mathbf{v}^{\text{p}}_{n+f}$ and $\mathbf{x}^{\text{p}}_{n+f}$ will be expressed as a function of $\mathbf{v}^{\text{p}}_{n+1-s}$ and $\mathbf{x}^{\text{p}}_{n+1}$ obtained from the main algorithm. For simplicity, it is assumed that the boundary is normal to the x-direction.

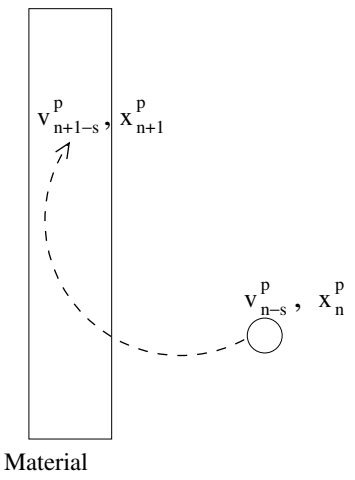

Fig. 1. Collection of a particle at the boundary.

In this section, the fields known at the boundary ($\mathbf{x}^{\mathrm{p}}_{n+f}$) will be used for the collection method instead of the ones at the particle position (either $\mathbf{x}^{\mathrm{p}}_{n}$ or $\mathbf{x}^{\mathrm{p}}_{n+1}$), e.g., $\mathbf{b}(\mathbf{x}^{\mathrm{p}}_{n+f}, t_n)$, $\mathbf{b}(\mathbf{x}^{\mathrm{p}}_{n+f}, t_{n-1})$, and $\mathbf{e}(\mathbf{x}^{\mathrm{p}}_{n+f}, t_{n-1})$. In the error analysis, they will be represented as a first-order Taylor series around $x(t_n)$ and t_n, e.g.

$$\mathbf{b}(\mathbf{x}_{n+f}, t_n) = \mathbf{b}(\mathbf{x}(t_n), t_n) + f(\mathbf{v}(t_n)\cdot\nabla)\mathbf{b}(\mathbf{x}(t_n), t_n)\Delta t - (\varepsilon_{\mathbf{x}}\cdot\nabla)\mathbf{b}(\mathbf{x}(t_n), t_n) + \mathbf{O}(\Delta t^2) \tag{8}$$

and

$$\mathbf{e}(\mathbf{x}_{n+f}, t_{n-1}) = \mathbf{e}(\mathbf{x}(t_n), t_n) + f(\mathbf{v}(t_n)\cdot\nabla)\mathbf{e}(\mathbf{x}(t_n), t_n)\Delta t - \frac{\partial \mathbf{e}(\mathbf{x}(t_n), t_n)}{\partial t}\Delta t - (\varepsilon_{\mathbf{x}}\cdot\nabla)\mathbf{e}(\mathbf{x}(t_n), t_n) + \mathbf{O}(\Delta t^2), \tag{9}$$

where $\varepsilon_{\mathbf{x}} = \mathbf{x}(t_{n+f}) - \mathbf{x}_{n+f}$.

3.1. Zeroth-order method

The following is the simplest way to set the position and velocity of particles at the boundary:

$$\mathbf{x}^{\mathrm{p}}_{n+f} = \mathbf{x}^{\mathrm{p}}_{n+1} \tag{10}$$

and

$$\mathbf{v}^{\mathrm{p}}_{n+f} = \mathbf{v}^{\mathrm{p}}_{n+1-s} \tag{11}$$

The local error of the position, $\varepsilon^{\mathrm{p}}_{\mathbf{x}}$, is $\mathbf{O}(\Delta t)$ as follows:

$$\begin{aligned}\varepsilon^{\mathrm{p}}_{\mathbf{x}} &= \mathbf{x}^{\mathrm{p}}(t_{n+f}) - \mathbf{x}^{\mathrm{p}}_{n+1}\\ &= \mathbf{x}^{\mathrm{p}}(t_{n+f}) - [\mathbf{x}^{\mathrm{p}}(t_{n+1}) - \varepsilon_{\mathbf{x},\mathrm{main}}]\\ &= (f-1)\mathbf{v}^{\mathrm{p}}(t_n)\Delta t + \mathbf{O}(\Delta t^2),\end{aligned} \tag{12}$$

which means that the position is zeroth-order accurate. The local error of the velocity, $\varepsilon^{\mathrm{p}}_{\mathbf{v}}$, is $\mathbf{O}(\Delta t)$ as follows:

$$\begin{aligned}\varepsilon^{\mathrm{p}}_{\mathbf{v}} &= \mathbf{v}^{\mathrm{p}}(t_{n+f}) - \mathbf{v}^{\mathrm{p}}_{n+1-s}\\ &= \mathbf{v}^{\mathrm{p}}(t_{n+f}) - [\mathbf{v}^{\mathrm{p}}(t_{n+1-s}) - \varepsilon_{\mathbf{v},\mathrm{main}}]\\ &= (f-1+s)\mathbf{a}^{\mathrm{p}}(t_n)\Delta t + \mathbf{O}(\Delta t^2),\end{aligned} \tag{13}$$

which means that the velocity is zeroth-order accurate.

3.2. First-order method

The first-order method can be obtained by adding terms to the zeroth-order method of Eqs. (10) and (11), considering the lowest order term in position and velocity errors (Eqs. (12) and (13)). The following is the first-order method to obtain the position and velocity of particles at the boundary:

$$\mathbf{x}^{\mathrm{p}}_{n+f} = \mathbf{x}^{\mathrm{p}}_{n+1} + (f_1 - 1)\mathbf{v}^{\mathrm{p}}_{n+1-s}\Delta t. \tag{14}$$

and

$$\begin{aligned}\mathbf{v}^{\mathrm{p}}_{n+f} = \mathbf{v}^{\mathrm{p}}_{n+1-s} &+ (f_1 - 1 + s)\mathbf{e}(\mathbf{x}^{\mathrm{p}}_{n+f}, t_n)\Delta t\\ &+ \frac{1}{2}(f_1 - 1 + s)(\mathbf{v}^{\mathrm{p}}_{n+1-s} + \mathbf{v}^{\mathrm{p}}_{n+f})\times\mathbf{b}(\mathbf{x}^{\mathrm{p}}_{n+f}, t_n)\Delta t.\end{aligned} \tag{15}$$

Here, $f_1(=\delta t^{\mathrm{p}}_1/\Delta t)$ is the approximate solution of $f(=\delta t^{\mathrm{p}}/\Delta t)$:

$$f_1 = \frac{x_b - x^{\mathrm{p}}_n}{v^{\mathrm{p}}_{x,n+1-s}\Delta t}. \tag{16}$$

$\delta t^{\mathrm{e}}_1(=\Delta t - \delta t^{\mathrm{p}}_1)$ is the approximate time remaining after particle impact, relevant for post-impact phenomena such as secondary emission or sputtering.

The local error of the fractional time δt_1^{p} (and hence δt_1^{e}), $\varepsilon_{\delta t,1}$, is $O(\Delta t^2)$ as follows:

$$\begin{aligned}\varepsilon_{\delta t,1} &= \delta t^{\mathrm{p}} - \delta t_1^{\mathrm{p}} \\ &= f\Delta t - \frac{x^{\mathrm{p}}(t_{n+f}) - x^{\mathrm{p}}(t_n)}{v_x^{\mathrm{p}}(t_{n+1-s}) - \varepsilon_{v_x,\mathrm{main}}} \\ &= f\left(1 - s - \frac{1}{2}f\right)\frac{a_x^{\mathrm{p}}(t_n)}{v_x^{\mathrm{p}}(t_n)}\Delta t^2 + O(\Delta t^3),\end{aligned} \tag{17}$$

which means that the fractional time is first-order accurate. The local error of the position, $\varepsilon_{\mathbf{x}}^{\mathrm{p}}$, is $\mathbf{O}(\Delta t^2)$ as follows:

$$\begin{aligned}\varepsilon_{\mathbf{x}}^{\mathrm{p}} &= \mathbf{x}^{\mathrm{p}}(t_{n+f}) - \mathbf{x}_{n+f}^{\mathrm{p}} \\ &= \mathbf{x}^{\mathrm{p}}(t_{n+f}) - \mathbf{x}_{n+1}^{\mathrm{p}} + (1-f_1)\mathbf{v}_{n+1-s}^{\mathrm{p}}\Delta t \\ &= \mathbf{x}^{\mathrm{p}}(t_{n+f}) - [\mathbf{x}^{\mathrm{p}}(t_{n+1}) - \varepsilon_{\mathbf{x},\mathrm{main}}] \\ &\quad + (1-f_1)[\mathbf{v}^{\mathrm{p}}(t_{n+1-s}) - \varepsilon_{\mathbf{v},\mathrm{main}}]\Delta t \\ &= \left(\frac{1}{2}(f-1) + s\right)(f-1)\mathbf{a}^{\mathrm{p}}(t_n)\Delta t^2 + \mathbf{v}^{\mathrm{p}}(t_n)\varepsilon_{\delta t,1} + \mathbf{O}(\Delta t^3),\end{aligned} \tag{18}$$

which means that the position is first-order accurate. The local error of the velocity, $\varepsilon_{\mathbf{v}}^{\mathrm{p}}$, is $\mathbf{O}(\Delta t^2)$ as follows:

$$\begin{aligned}\varepsilon_{\mathbf{v}}^{\mathrm{p}} &= \mathbf{v}^{\mathrm{p}}(t_{n+f}) - \mathbf{v}_{n+f}^{\mathrm{p}} \\ &= \frac{1}{2}(f+1-s)(f-1+s)[\dot{\mathbf{e}}(t_n) + \mathbf{v}^{\mathrm{p}}(t_n)\times\dot{\mathbf{b}}(t_n)]\Delta t^2 \\ &\quad - f(f-1+s)(\mathbf{v}^{\mathrm{p}}(t_n)\cdot\nabla)\mathbf{e}(t_n)\Delta t^2 \\ &\quad - f(f-1+s)\mathbf{v}^{\mathrm{p}}(t_n)\times(\mathbf{v}^{\mathrm{p}}(t_n)\cdot\nabla)\mathbf{b}(t_n)\Delta t^2 \\ &\quad + \mathbf{a}^{\mathrm{p}}(t_n)\varepsilon_{\delta t,1} + \mathbf{O}(\Delta t^3),\end{aligned} \tag{19}$$

which means that the velocity is first-order accurate.

3.3. Second-order method

The second-order method can be obtained by adding terms to the first-order method of Eqs. (14) and (15), considering the lowest order terms in position and velocity errors (Eqs. (18) and (19)).

The following is the second-order method to obtain the position and velocity of particles at the boundary:

$$\mathbf{x}_{n+f}^{\mathrm{p}} = \mathbf{x}_{n+1}^{\mathrm{p}} + (f_2-1)\mathbf{v}'_{n+(1+f)/2}\Delta t, \tag{20}$$

and

$$\begin{aligned}\mathbf{v}_{n+f}^{\mathrm{p}} &= \mathbf{v}_{n+1-s}^{\mathrm{p}} + (f_2-1+s)\mathbf{e}_{\mathbf{v}}^{\mathrm{p}}\Delta t \\ &\quad + \frac{1}{2}(f_2-1+s)(\mathbf{v}_{n+1-s}^{\mathrm{p}} + \mathbf{v}_{n+f}^{\mathrm{p}})\times\mathbf{b}_{\mathbf{v}}^{\mathrm{p}}\Delta t\end{aligned} \tag{21}$$

where

$$\mathbf{v}'_{n+(1+f)/2} = \mathbf{v}_{n+1-s}^{\mathrm{p}} + \left(\frac{1}{2}(f_1-1)+s\right)[\mathbf{e}(\mathbf{x}_{n+1}^{\mathrm{p}}, t_n) + \mathbf{v}_{n+1-s}^{\mathrm{p}}\times\mathbf{b}(\mathbf{x}_{n+1}^{\mathrm{p}}, t_n)]\Delta t \tag{22}$$

$$\mathbf{e}_{\mathbf{v}}^{\mathrm{p}} = (1+d^{\mathrm{p}})\mathbf{e}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n) - d^{\mathrm{p}}\mathbf{e}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_{n-1}) + (1-s-d^{\mathrm{p}})(\mathbf{v}_{n+1-s}^{\mathrm{p}}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n)\Delta t \tag{23}$$

$$\mathbf{b}_{\mathbf{v}}^{\mathrm{p}} = (1+d^{\mathrm{p}})\mathbf{b}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n) - d^{\mathrm{p}}\mathbf{b}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_{n-1}) + (1-s-d^{\mathrm{p}})(\mathbf{v}_{n+1-s}^{\mathrm{p}}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n)\Delta t \tag{24}$$

$$d^{\mathrm{p}} = \frac{f_2+1-s}{2} \tag{25}$$

$f_2(=\delta t_2^{\mathrm{p}}/\Delta t)$ is the approximate solution of $f(=\delta t^{\mathrm{p}}/\Delta t)$:

$$f_2 = \frac{x_b - x_n^{\mathrm{p}}}{v'_{x,n+(1+f)/2}\Delta t} = f_1 \frac{v_{x,n+1-s}^{\mathrm{p}}}{v'_{x,n+(1+f)/2}}. \tag{26}$$

$\delta t_2^{\mathrm{e}}(=\Delta t - \delta t_2^{\mathrm{p}})$ is the approximate time remaining after particle impact. In the derivation procedure of the velocity, the terms including Δt^2 in Eq. (19) have been used in the following form:

$$\begin{aligned}
&\frac{1}{2}(f-1+s)\left[(f+1-s)\frac{\partial \mathbf{e}(t_n)}{\partial t} + (1-s-f)(\mathbf{v}^{\mathrm{p}}(t_n)\cdot\nabla)\mathbf{e}(t_n)\right]\Delta t^2 \\
&\quad + \frac{1}{2}(f-1+s)\mathbf{v}^{\mathrm{p}}(t_n) \times \left[(f+1-s)\frac{\partial \mathbf{b}(t_n)}{\partial t} + (1-s-f)(\mathbf{v}^{\mathrm{p}}(t_n)\cdot\nabla)\mathbf{b}(t_n)\right]\Delta t^2 \\
&= (f_2-1+s)\left[d^{\mathrm{p}}\frac{\partial \mathbf{e}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n)}{\partial t} + (1-s-d^{\mathrm{p}})(\mathbf{v}_{n+1-s}^{\mathrm{p}}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n)\right]\Delta t^2 \\
&\quad + (f_2-1+s)\frac{\mathbf{v}_{n+1-s}^{\mathrm{p}} + \mathbf{v}_{n+f}^{\mathrm{p}}}{2} \times \left[d^{\mathrm{p}}\frac{\partial \mathbf{b}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n)}{\partial t} + (1-s-d^{\mathrm{p}})(\mathbf{v}_{n+1-s}^{\mathrm{p}}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n+f}^{\mathrm{p}}, t_n)\right]\Delta t^2 + \mathbf{O}(\Delta t^3)
\end{aligned}$$

Eqs. (23) and (24) show that the fields at t_{n-1} as well as t_n are required because of time-dependence of the fields.

3.4. Numerical verification

To confirm the error of the methods, the exact solution for two test cases is compared with the numerical one with $s = 0.5$ (leap-frog method).

Under constant fields of $\mathbf{e} = e_x\hat{\mathbf{x}}$ and $\mathbf{b} = \Omega\hat{\mathbf{z}}$, the exact solution is given by

$$v_x(t_f) = \left(v_{y,-1/2} + \frac{e_x}{\Omega}\right)\sin(\Omega t_{f+1/2}) + v_{x,-1/2}\cos(\Omega t_{f+1/2}), \tag{27}$$

$$v_y(t_f) = \left(v_{y,-1/2} + \frac{e_x}{\Omega}\right)\cos(\Omega t_{f+1/2}) - v_{x,-1/2}\sin(\Omega t_{f+1/2}) - \frac{e_x}{\Omega}, \tag{28}$$

$$\begin{aligned}
x(t_f) &= x_0 - \frac{1}{\Omega}\left(v_{y,-1/2} + \frac{e_x}{\Omega}\right)[\cos(\Omega t_{f+1/2}) - \cos(\Omega t_{1/2})] \\
&\quad + \frac{1}{\Omega}v_{x,-1/2}[\sin(\Omega t_{f+1/2}) - \sin(\Omega t_{1/2})],
\end{aligned} \tag{29}$$

$$\begin{aligned}
y(t_f) &= y_0 - \frac{1}{\Omega}\left(v_{y,-1/2} + \frac{e_x}{\Omega}\right)[\sin(\Omega t_{f+1/2}) - \sin(\Omega t_{1/2})] \\
&\quad + \frac{1}{\Omega}v_{x,-1/2}[\cos(\Omega t_{f+1/2}) - \cos(\Omega t_{1/2})] - \frac{e_x}{\Omega}t_f.
\end{aligned} \tag{30}$$

The first-order method of Eqs. (14) and (15) is applied to the case with constant fields of $\mathbf{e} = e_x\hat{\mathbf{x}}$ ($e_x = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$) and initial conditions of $v_{x,-1/2} = v_{y,-1/2} = 0.2$ and $x_0 = y_0 = 1$. The position of the boundary was set to $x_b = x_0 + (x_1 - x_0)/3$. Fig. 2 shows the local error in the first-order method. The local error of the fractional time, $\varepsilon_{\delta t,1}$, is $O(\Delta t^2)$ as expected from Eq. (17). The local error of the velocity of the incident particle, $\varepsilon_{\mathbf{v}}^{\mathrm{p}}$, is $O(\Delta t^2)$ as expected from Eq. (19). The local error of the position of the incident particle, $\varepsilon_{\mathbf{x}}^{\mathrm{p}}$, is $O(\Delta t^2)$ as expected from Eq. (18).

Under fields of $\mathbf{e}(\mathbf{x}, t) = \{e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x + e_x^{\mathrm{rf}}\cos(wt)\}\hat{\mathbf{x}}$ and $\mathbf{b} = \Omega\hat{\mathbf{z}}$, the exact solution is given by

$$v_x(t_f) = v_{x,-1/2} + h\sin(w't_{f+1/2}) + r(\cos(w't_{f+1/2}) - 1) - \frac{e_x^{\mathrm{rf}}w}{w'^2 - w^2}[\sin(wt_f) + \sin(wt_{1/2})] \tag{31}$$

$$v_y(t_f) = v_{y,-1/2} + \frac{\Omega}{w'}[h(\cos(w't_{f+1/2}) - 1) - r\sin(w't_{f+1/2})] - \frac{\Omega}{w'^2 - w^2}[\cos(wt_f) - \cos(wt_{1/2})] \tag{32}$$

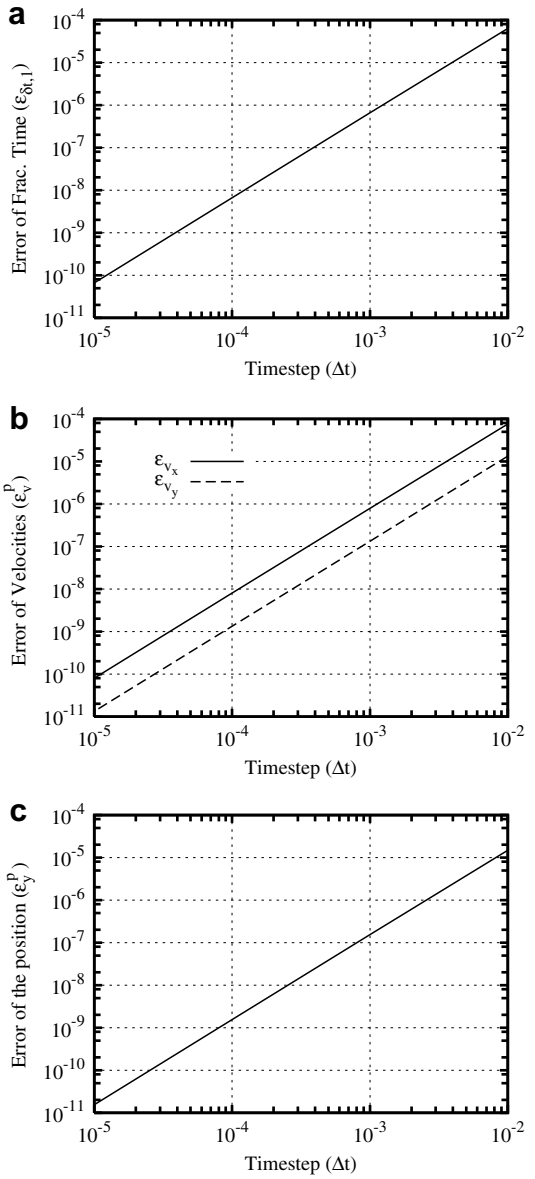

Fig. 2. First-order collection method: the local error of: (a) the fractional time ($\varepsilon_{\delta t,1}$); (b) the velocity of the incident particle (ε_v^p); (c) the position of the incident particle (ε_y^p) under the condition of $\mathbf{e} = e_x\hat{\mathbf{x}}$ ($e_x = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$).

$$x(t_f) = x_0 - \frac{h}{w'}[\cos(w't_{f+1/2}) - \cos(w't_{1/2})] + \frac{r}{w'}[\sin(w't_{f+1/2}) - \sin(w't_{1/2})] + \frac{e_x^{\mathrm{rf}}}{w'^2 - w^2}[\cos(wt_f) - 1] \tag{33}$$

$$y(t_f) = y_0 + \Omega\left[\frac{h}{w'^2}\{\sin(w't_{f+1/2}) - \sin(w't_{1/2})\} + \frac{r}{w'^2}\{\cos(w't_{f+1/2}) - \cos(w't_{1/2})\} - \frac{e_x^{\mathrm{rf}}}{(w'^2 - w^2)w}\sin(wt_f)\right] + \left[v_{y,-1/2} - h\frac{\Omega}{w} + \frac{\Omega e_x^{\mathrm{rf}}}{w'^2 - w^2}\cos(wt_{1/2})\right]t_f, \tag{34}$$

where

$$w'^2 = \Omega^2 - e_x^{\mathrm{dc},1} \tag{35}$$

$$r = v_{x,-1/2} - \frac{e_x^{\mathrm{rf}} w}{w'^2 - w^2} \sin(wt_{1/2}) \tag{36}$$

$$h = \frac{w'\Omega}{\Omega^2 - e_x^{\mathrm{dc},1}\cos(w't_{1/2})}\left[v_{y,-1/2} + \frac{\Omega e_x^{\mathrm{rf}}}{w'^2 - w^2}\cos(wt_{1/2}) + \frac{e_x^{\mathrm{dc},0}}{\Omega} - r\frac{e_x^{\mathrm{dc},1}}{w'\Omega}\sin(w't_{1/2}) - \frac{e_x^{\mathrm{dc},1}}{\Omega}\left(\frac{e_x^{\mathrm{rf}}}{w'^2 - w^2} - x_0\right)\right]. \tag{37}$$

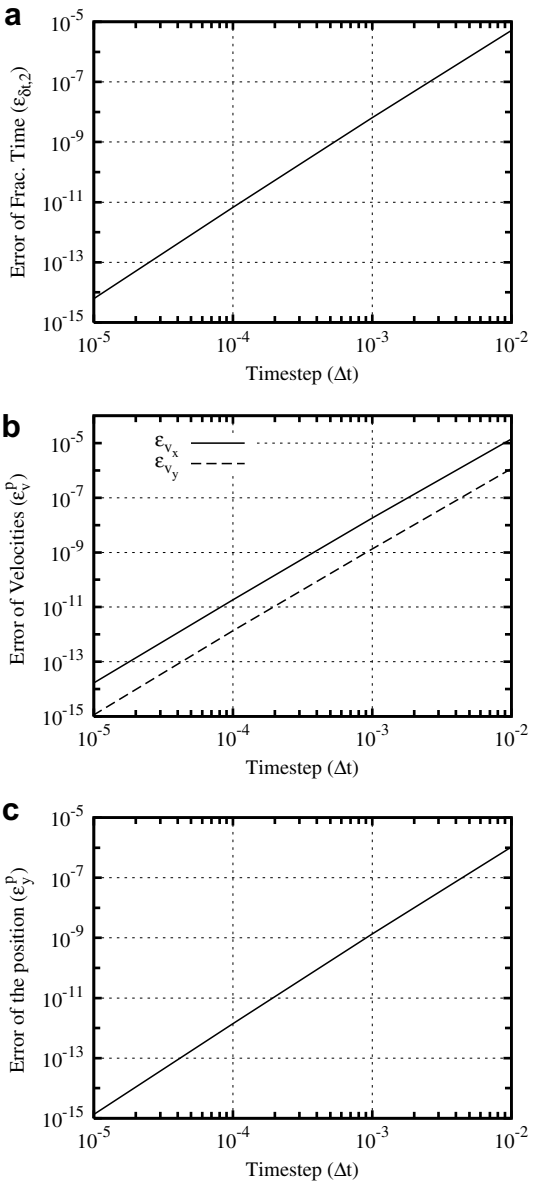

Fig. 3. Second-order collection method: the local error of: (a) the fractional time ($\varepsilon_{\delta t,2}$); (b) the velocity of the incident particle ($\varepsilon_{\mathbf{v}}^{\mathrm{p}}$); (c) the position of the incident particle ($\varepsilon_{\mathbf{y}}^{\mathrm{p}}$) under the condition of $\mathbf{e}(\mathbf{x},t) = \{e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x + e_x^{\mathrm{rf}}\cos(wt)\}\hat{\mathbf{x}}$ ($e_x^{\mathrm{dc},0} = 1, e_x^{\mathrm{dc},1} = 0.5, e_x^{\mathrm{rf}} = 1$, and $w = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$).

The second-order method of Eqs. (20) and (21) is applied to the case with fields of $\mathbf{e}(\mathbf{x},t) = \{e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x + e_x^{\mathrm{rf}}\cos(wt)\}\hat{\mathbf{x}}$ ($e_x^{\mathrm{dc},0} = 1, e_x^{\mathrm{dc},1} = 0.5, e_x^{\mathrm{rf}} = 1$, and $w = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$) and initial conditions of $v_{x,-1/2} = v_{y,-1/2} = 0.2$ and $x_0 = y_0 = 1$. Fig. 3 shows the local error in the second-order method. The error of the fractional time, $\varepsilon_{\delta t,2}$, is $O(\Delta t^3)$. The velocity and position of the incident particle, $\varepsilon_{\mathbf{v}}^{\mathrm{p}}$ and $\varepsilon_{\mathbf{x}}^{\mathrm{p}}$, are second-order accurate.

4. Ejection of particles

The ejection of particles from the boundary originates from either spontaneous emission or secondary emission due to the impact of an incident particle. In the former case, such as field and thermionic emission from metals, it is supposed that their velocity is given exactly at the time of their emission from the boundary. The known value of δt^{e} ($=g\Delta t$) is used so that $\varepsilon_{\delta t} = 0$. In the latter, the time of ejection of the secondary particle depends on the impact time of the incident particle. The approximate value of δt^{e} (i.e., δt_1^{e} and δt_2^{e}) is used as defined in Section 3. For simplicity, it is assumed that particle ejection is instantaneous, following the impact of the incident particle. In both cases, the accuracy of approximate value of δt^{e} is better than zeroth-order.

Fig. 4 shows the ejection of a particle at the boundary. In the ejection of particles from the boundary, their velocity ($\mathbf{v}^{\mathrm{e}}$) and position ($\mathbf{x}^{\mathrm{e}}$) are given at the time of the ejection, t_{n-g}. They need to be advanced forward or backward in time in order to apply the main algorithm at the next timestep. $\mathbf{v}_{n-s}^{\mathrm{e}}$ and $\mathbf{x}_n^{\mathrm{e}}$ will be obtained as a function of $\mathbf{v}_{n-g}^{\mathrm{e}}$, $\mathbf{x}_{n-g}^{\mathrm{e}}$, and the fields. Here, the fields known at the boundary ($\mathbf{x}_{n-g}^{\mathrm{e}}$) will be used for the ejection method instead of the ones at the particle position ($\mathbf{x}_n^{\mathrm{e}}$), e.g., $\mathbf{e}(\mathbf{x}_{n-g}^{\mathrm{e}})$.

4.1. Zeroth-order method

The following is the simplest way to set the velocity and position of particles ejected from the boundary:

$$\mathbf{v}_{n-s}^{\mathrm{e}} = \mathbf{v}_{n-g}^{\mathrm{e}} \tag{38}$$

and

$$\mathbf{x}_n^{\mathrm{e}} = \mathbf{x}_{n-g}^{\mathrm{e}} \tag{39}$$

The local error of the velocity, $\varepsilon_{\mathbf{v}}^{\mathrm{e}}$, is $\mathbf{O}(\Delta t)$ as follows:

$$\begin{aligned}\varepsilon_{\mathbf{v}}^{\mathrm{e}} &= \mathbf{v}^{\mathrm{e}}(t_{n-s}) - \mathbf{v}^{\mathrm{e}}(t_{n-g}) \\ &= (g-s)\mathbf{a}^{\mathrm{e}}(t_n)\Delta t + \mathbf{O}(\Delta t^2),\end{aligned} \tag{40}$$

which means that the velocity is zeroth-order accurate. The local error of the position, $\varepsilon_{\mathbf{x}}^{\mathrm{e}}$, is

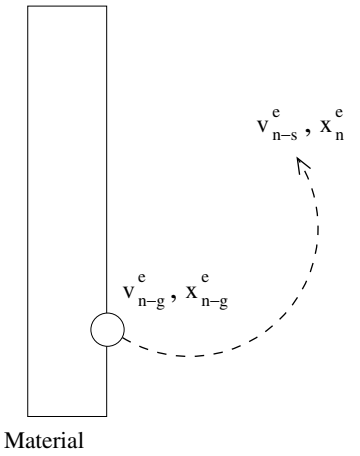

Fig. 4. Ejection of a particle at the boundary.

$$\begin{aligned}\varepsilon_{\mathbf{x}}^{\mathrm{e}} &= \mathbf{x}^{\mathrm{e}}(t_n) - \mathbf{x}^{\mathrm{e}}(t_{n-g}) \\ &= g\mathbf{v}^{\mathrm{e}}(t_n)\Delta t + \mathbf{O}(\Delta t^2),\end{aligned} \tag{41}$$

which means that the position is zeroth-order accurate.

4.2. First-order method

The first-order method can be obtained by adding terms to the zeroth-order method of Eqs. (38) and (39), considering the lowest order term in velocity and position errors (Eqs. (40) and (41)). The following is the first-order method to obtain the velocity and position of particles ejected from the boundary:

$$\begin{aligned}\mathbf{v}_{n-s}^{\mathrm{e}} &= \mathbf{v}_{n-g}^{\mathrm{e}} + (g' - s)\mathbf{e}(\mathbf{x}_{n-g}^{\mathrm{e}}, t_{n-1})\Delta t \\ &\quad + \frac{1}{2}(g' - s)(\mathbf{v}_{n-s}^{\mathrm{e}} + \mathbf{v}_{n-g}^{\mathrm{e}}) \times \mathbf{b}(\mathbf{x}_{n-g}^{\mathrm{e}}, t_{n-1})\Delta t\end{aligned} \tag{42}$$

and

$$\mathbf{x}_n^{\mathrm{e}} = \mathbf{x}_{n-g}^{\mathrm{e}} + g'\mathbf{v}_{n-g}^{\mathrm{e}}\Delta t. \tag{43}$$

Here, g' is either $\delta t^{\mathrm{e}}/\Delta t$ ($\varepsilon_{\delta t} = 0$) for spontaneous emission or $\delta t_1^{\mathrm{e}}/\Delta t$ ($\varepsilon_{\delta t} = \varepsilon_{\delta t,1}$) for secondary emission.

The local error of the velocity, $\varepsilon_{\mathbf{v}}^{\mathrm{e}}$, is $\mathbf{O}(\Delta t^2)$ as follows:

$$\varepsilon_{\mathbf{v}}^{\mathrm{e}} = \mathbf{v}^{\mathrm{e}}(t_{n-s}) - \mathbf{v}_{n-s}^{\mathrm{e}} \tag{44}$$

$$\begin{aligned}&= -\frac{1}{2}(g - s)(g + s)[\dot{\mathbf{e}}(t_n) + \mathbf{v}^{\mathrm{e}}(t_n) \times \dot{\mathbf{b}}(t_n)]\Delta t^2 \\ &\quad + (g - s)\left[\frac{\partial \mathbf{e}(t_n)}{\partial t} + g(\mathbf{v}^{\mathrm{e}}(t_n) \cdot \nabla)\mathbf{e}(t_n)\right]\Delta t^2 \\ &\quad + (g - s)\mathbf{v}^{\mathrm{e}}(t_n) \times \left[\frac{\partial \mathbf{b}(t_n)}{\partial t} + g(\mathbf{v}^{\mathrm{e}}(t_n) \cdot \nabla)\mathbf{b}(t_n)\right]\Delta t^2 \\ &\quad + \mathbf{a}^{\mathrm{e}}(t_n)\varepsilon_{\delta t} + \mathbf{O}(\Delta t^3),\end{aligned} \tag{45}$$

which means that the velocity is first-order accurate since the order of $\varepsilon_{\delta t}$ is higher than Δt. In Eq. (45), the second and third terms arise since the fields at $\mathbf{x}_{n-g}^{\mathrm{e}}$ and t_{n-1} were used in Eq. (42) instead of those at $\mathbf{x}_n^{\mathrm{e}}$ and t_n. The local error of the position, $\varepsilon_{\mathbf{x}}^{\mathrm{e}}$, is $\mathbf{O}(\Delta t^2)$ as follows:

$$\begin{aligned}\varepsilon_{\mathbf{x}}^{\mathrm{e}} &= \mathbf{x}^{\mathrm{e}}(t_n) - \mathbf{x}_n^{\mathrm{e}} \\ &= \mathbf{x}^{\mathrm{e}}(t_n) - \mathbf{x}^{\mathrm{e}}(t_{n-g}) - g'\mathbf{v}^{\mathrm{e}}(t_{n-g})\Delta t \\ &= \frac{1}{2}g^2\mathbf{a}^{\mathrm{e}}(t_n)\Delta t^2 + \mathbf{v}^{\mathrm{e}}(t_n)\varepsilon_{\delta t} + \mathbf{O}(\Delta t^3),\end{aligned} \tag{46}$$

which means that the position is first-order accurate.

In the case of spontaneous emission under constant fields, the velocity error of Eq. (45) becomes third-order so that the velocity of Eq. (42) is second-order accurate. It is contradictory to the result in [4] that Eq. (42) with $s = 0.5$ (called the simple Boris push) is referred to as a first-order method under constant fields. Equation (43) (called the simple push) is also referred to as zeroth-order method in [4], which is contradictory to our result of being first-order accurate. Our result will be confirmed by comparing the numerically computed value with its exact solution in Section 4.4.

4.3. Second-order method

The second-order method can be obtained by adding terms to the first-order method of Eqs. (42) and (43), considering the lowest order term in velocity and position errors (Eqs. (45) and (46)).

The following is the second-order method to obtain the velocity and position of particles ejected from the boundary:

$$\mathbf{v}^{\mathrm{e}}_{n-s} = \mathbf{v}^{\mathrm{e}}_{n-g} + (g'' - s)\mathbf{e}^{\mathrm{e}}_{\mathbf{v}}\Delta t + \frac{1}{2}(g'' - s)(\mathbf{v}^{\mathrm{e}}_{n-s} + \mathbf{v}^{\mathrm{e}}_{n-g}) \times \mathbf{b}^{\mathrm{e}}_{\mathbf{v}}\Delta t \tag{47}$$

and

$$\mathbf{x}^{\mathrm{e}}_{n} = \mathbf{x}^{\mathrm{e}}_{n-g} + g''\mathbf{v}'_{n-g/2}\Delta t, \tag{48}$$

where

$$\mathbf{e}^{\mathrm{e}}_{\mathbf{v}} = (1 - d^{\mathrm{e}})\mathbf{e}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1}) + d^{\mathrm{e}}\mathbf{e}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-2}) + (d^{\mathrm{e}} + 1 - s)(\mathbf{v}^{\mathrm{e}}_{n-g} \cdot \nabla)\mathbf{e}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})\Delta t \tag{49}$$

$$\mathbf{b}^{\mathrm{e}}_{\mathbf{v}} = (1 - d^{\mathrm{e}})\mathbf{b}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1}) + d^{\mathrm{e}}\mathbf{b}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-2}) + (d^{\mathrm{e}} + 1 - s)(\mathbf{v}^{\mathrm{e}}_{n-g} \cdot \nabla)\mathbf{b}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})\Delta t \tag{50}$$

$$d^{\mathrm{e}} = \frac{g'' + s}{2} - 1 \tag{51}$$

$$\mathbf{v}'_{n-g/2} = \mathbf{v}^{\mathrm{e}}_{n-g} + \frac{1}{2}g''[\mathbf{e}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1}) + \mathbf{v}^{\mathrm{e}}_{n-g} \times \mathbf{b}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})]\Delta t \tag{52}$$

Here, g'' is either $\delta t^{\mathrm{e}}/\Delta t$ ($\varepsilon_{\delta t} = 0$) for spontaneous emission or $\delta t^{\mathrm{e}}_2/\Delta t$ ($\varepsilon_{\delta t} = \varepsilon_{\delta t,2}$) for secondary emission. In the derivation procedure of the velocity, the following terms including Δt^2 in Eq. (45) have been used:

$$\begin{aligned}
&(g - s)\left[\left(1 - \frac{g + s}{2}\right)\frac{\partial \mathbf{e}(t_n)}{\partial t} + \frac{g - s}{2}(\mathbf{v}^{\mathrm{e}}(t_n) \cdot \nabla)\mathbf{e}(t_n)\right]\Delta t^2 \\
&\quad + (g - s)\mathbf{v}^{\mathrm{e}}(t_n) \times \left[\left(1 - \frac{g + s}{2}\right)\frac{\partial \mathbf{b}(t_n)}{\partial t} + \frac{g - s}{2}(\mathbf{v}^{\mathrm{e}}(t_n) \cdot \nabla)\mathbf{b}(t_n)\right]\Delta t^2 \\
&= (g'' - s)\left[-d^{\mathrm{e}}\frac{\partial \mathbf{e}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})}{\partial t} + (d^{\mathrm{e}} + 1 - s)(\mathbf{v}^{\mathrm{e}}_{n-g} \cdot \nabla)\mathbf{e}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})\right]\Delta t^2 \\
&\quad + (g'' - s)\frac{\mathbf{v}^{\mathrm{e}}_{n-s} + \mathbf{v}^{\mathrm{e}}_{n-g}}{2} \times \left[-d^{\mathrm{e}}\frac{\partial \mathbf{b}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})}{\partial t} + (d^{\mathrm{e}} + 1 - s)(\mathbf{v}^{\mathrm{e}}_{n-g} \cdot \nabla)\mathbf{b}(\mathbf{x}^{\mathrm{e}}_{n-g}, t_{n-1})\right]\Delta t^2 \\
&\quad + \mathbf{O}(\Delta t^3)
\end{aligned}$$

Under constant fields, replacing g'' by g', the velocity equation, Eq. (47), becomes the velocity equation in the first-order method, Eq. (42). The position equation, Eq. (48) (called the simple Boris push) is referred to as a second-order method only for constant fields in [4], which is contradictory to our result of being second-order accurate for general fields.

4.4. Numerical verification

To confirm the error of the methods, the exact solution for two test cases is compared with the numerical one with $s = 0.5$ (leap-frog method). In this calculation, to simplify the analytic solution, the time was advanced by the amount of t_g so that the ejection time is t_n.

Under constant fields of $\mathbf{e} = e_x\hat{\mathbf{x}}$ and $\mathbf{b} = \Omega\hat{\mathbf{z}}$, the exact solution is given by

$$v_x(t_{g-1/2}) = \left(v_{y,0} + \frac{e_x}{\Omega}\right)\sin(\Omega t_{g-1/2}) + v_{x,0}\cos(\Omega t_{g-1/2}), \tag{53}$$

$$v_y(t_{g-1/2}) = \left(v_{y,0} + \frac{e_x}{\Omega}\right)\cos(\Omega t_{g-1/2}) - v_{x,0}\sin(\Omega t_{g-1/2}) - \frac{e_x}{\Omega}, \tag{54}$$

$$x(t_g) = x_0 + \frac{1}{\Omega}\left(v_{y,0} + \frac{e_x}{\Omega}\right)[1 - \cos(\Omega t_g)] + \frac{1}{\Omega}v_{x,0}\sin(\Omega t_g), \tag{55}$$

$$y(t_g) = y_0 + \frac{1}{\Omega}\left(v_{y,0} + \frac{e_x}{\Omega}\right)\sin(\Omega t_g) + \frac{1}{\Omega}v_{x,0}[\cos(\Omega t_g) - 1] - \frac{e_x}{\Omega}t_g. \tag{56}$$

The first-order method of Eqs. (42) and (43) for secondary emission is used for the case with constant fields of $\mathbf{e} = e_x\hat{\mathbf{x}}$ ($e_x = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$) and initial conditions of $v_{x,0} = v_{y,0} = 0.2$ and $x_0 = y_0 = 1$. In the numerical calculation, δt^{p}_1 obtained from the first test case of Section 3.4 is used for $g'(= \delta t^{\mathrm{e}}_1/\Delta t)$. Fig. 5 shows the local error in the first-order method for secondary emission. The local error of the velocity of the ejected particle, $\varepsilon^{\mathrm{e}}_{\mathbf{v}}$, is $O(\Delta t^2)$ as expected from Eq. (45). The local error of the position of the ejected particle, $\varepsilon^{\mathrm{e}}_{\mathbf{x}}$, is $O(\Delta t^2)$ as expected from Eq. (46).

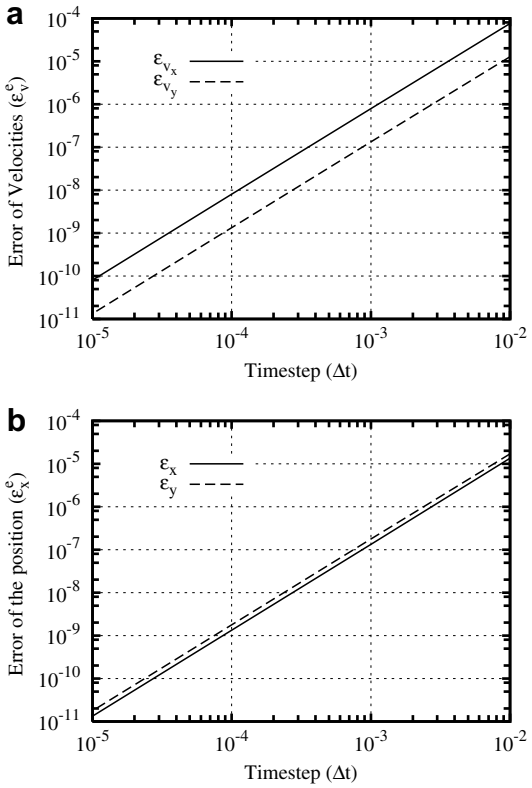

Fig. 5. First-order ejection method for secondary emission: the local error of (a) the velocity of the ejected particle ($\varepsilon_{\mathbf{v}}^e$) and (b) the position of the ejected particle ($\varepsilon_{\mathbf{x}}^e$) under the condition of $\mathbf{e} = e_x\hat{\mathbf{x}}$ ($e_x = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$).

Fig. 6 shows the local error in the first-order method for spontaneous emission under constant fields. In this particular case, the local error of the velocity of the ejected particle, $\varepsilon_{\mathbf{v}}^e$, is $O(\Delta t^3)$ as mentioned in Section 4.2.

Under fields of $\mathbf{e}(\mathbf{x}, t) = \{e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x + e_x^{\mathrm{rf}}\cos(wt)\}\hat{\mathbf{x}}$ and $\mathbf{b} = \Omega\hat{\mathbf{z}}$, the exact solution is given by

$$v_x(t_{g-1/2}) = v_{x,0}\cos(w't_{g-1/2}) + u\sin(w't_{g-1/2}) - \frac{e_x^{\mathrm{rf}}w}{w'^2 - w^2}\sin(wt_{g-1/2}) \tag{57}$$

$$v_y(t_{g-1/2}) = v_{y,0} + \frac{\Omega}{w'}[u(\cos(w't_{g-1/2}) - 1) - v_{x,0}\sin(w't_{g-1/2})] - \frac{\Omega}{w'^2 - w^2}[\cos(wt_{g-1/2}) - 1] \tag{58}$$

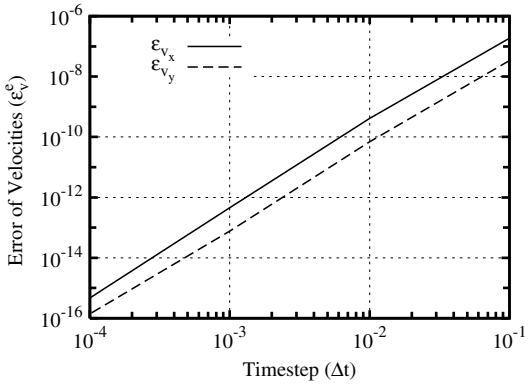

Fig. 6. First-order ejection method for spontaneous emission under constant fields: the local error of the velocity of the ejected particle ($\varepsilon_{\mathbf{v}}^e$) under the condition of $\mathbf{e} = e_x\hat{\mathbf{x}}$ ($e_x = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$).

$$x(t_g) = x_0 - \frac{u}{w'}[\cos(w't_g) - 1] + \frac{v_{x,0}}{w'}\sin(w't_g) + \frac{e_x^{\mathrm{rf}}}{w'^2 - w^2}[\cos(wt_g) - 1] \tag{59}$$

$$y(t_g) = y_0 + \Omega\left[\frac{u}{w'^2}\{\sin(w't_g)\} + \frac{v_{x,0}}{w'^2}\{\cos(w't_g) - 1\} - \frac{e_x^{\mathrm{rf}}}{(w'^2 - w^2)w}\sin(wt_g)\right] + \left[v_{y,0} - u\frac{\Omega}{w} + \frac{\Omega e_x^{\mathrm{rf}}}{w'^2 - w^2}\right]t_g, \tag{60}$$

where

$$u = \frac{1}{w'}\left[\Omega v_{y,0} + e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x_0 + \frac{w'^2 e_x^{\mathrm{rf}}}{w'^2 - w^2}\right]. \tag{61}$$

The second-order method of Eqs. (47) and (48) for secondary emission is used for the case with fields of $\mathbf{e}(\mathbf{x},t) = \{e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x + e_x^{\mathrm{rf}}\cos(wt)\}\hat{\mathbf{x}}$ ($e_x^{\mathrm{dc},0} = 1, e_x^{\mathrm{dc},1} = 0.5, e_x^{\mathrm{rf}} = 1$, and $w = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$) and initial conditions of $v_{x,0} = v_{y,0} = 0.2$ and $x_0 = y_0 = 1$. In the numerical calculation, δt_2^{p} obtained from the second test case of Section 3.4 is used for $g''(=\delta t_2^{\mathrm{e}}/\Delta t)$. Fig. 7 shows the local error in the second-order method for secondary emission. The velocity and position of the ejected particle, $\varepsilon_{\mathbf{v}}^{\mathrm{e}}$ and $\varepsilon_{\mathbf{x}}^{\mathrm{e}}$, are second-order accurate.

5. Loading of particles

When particles are initially loaded into the system, it is usual that their velocity and position are given at the same time. To use the main algorithm with nonzero offset, the velocity need to be retreated in advance. Particle loading is a particular case of particle ejection, with $g = g' = g'' = 0$. In this section, the fields at the particle position ($\mathbf{x}_n^{\mathrm{l}}$) will be used. The zeroth-order method is the same as Eq. (38) with $g = 0$.

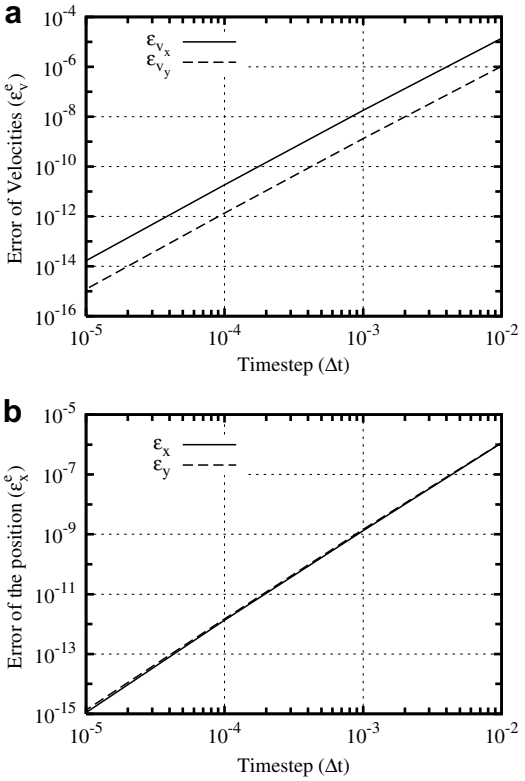

Fig. 7. Second-order ejection method for secondary emission: the local error of (a) the velocity of the ejected particle ($\varepsilon_{\mathbf{v}}^{\mathrm{e}}$) and (b) the position of the ejected particle ($\varepsilon_{\mathbf{x}}^{\mathrm{e}}$) under the condition of $\mathbf{e}(\mathbf{x},t) = \{e_x^{\mathrm{dc},0} + e_x^{\mathrm{dc},1}x + e_x^{\mathrm{rf}}\cos(wt)\}\hat{\mathbf{x}}$ ($e_x^{\mathrm{dc},0} = 1, e_x^{\mathrm{dc},1} = 0.5, e_x^{\mathrm{rf}} = 1$, and $w = 1$) and $\mathbf{b} = \Omega\hat{\mathbf{z}}$ ($\Omega = 1$).

5.1. First-order method

The following is the first-order method to obtain the velocity of the loaded particles:

$$\mathbf{v}^{\mathrm{l}}_{n-s} = \mathbf{v}^{\mathrm{l}}_{n} - s\mathbf{e}(\mathbf{x}^{\mathrm{l}}_{n}, t_n)\Delta t - \frac{1}{2}s(\mathbf{v}^{\mathrm{l}}_{n-s} + \mathbf{v}^{\mathrm{l}}_{n}) \times \mathbf{b}(\mathbf{x}^{\mathrm{l}}_{n}, t_n)\Delta t. \tag{62}$$

5.2. Second-order method

The second-order loading method can be built following the ejection method, except that the second and third terms in Eq. (45) should be excluded. The following is the second-order method to obtain the velocity of the loaded particles:

$$\mathbf{v}^{\mathrm{l}}_{n-s} = \mathbf{v}^{\mathrm{l}}_{n} - s\mathbf{e}^{\mathrm{l}}_{\mathbf{v}}\Delta t - \frac{1}{2}s(\mathbf{v}^{\mathrm{l}}_{n-s} + \mathbf{v}^{\mathrm{l}}_{n}) \times \mathbf{b}^{\mathrm{l}}_{\mathbf{v}}\Delta t, \tag{63}$$

where

$$\mathbf{e}^{\mathrm{l}}_{\mathbf{v}} = \mathbf{e}(\mathbf{x}^{\mathrm{l}}_{n}, t_n) - \frac{s}{2}\left[\frac{\partial \mathbf{e}(\mathbf{x}^{\mathrm{l}}_{n}, t_n)}{\partial t} + (\mathbf{v}^{\mathrm{l}}_{n} \cdot \nabla)\mathbf{e}(\mathbf{x}^{\mathrm{l}}_{n}, t_n)\right]\Delta t \tag{64}$$

$$\mathbf{b}^{\mathrm{l}}_{\mathbf{v}} = \mathbf{b}(\mathbf{x}^{\mathrm{l}}_{n}, t_n) - \frac{s}{2}\left[\frac{\partial \mathbf{b}(\mathbf{x}^{\mathrm{l}}_{n}, t_n)}{\partial t} + (\mathbf{v}^{\mathrm{l}}_{n} \cdot \nabla)\mathbf{b}(\mathbf{x}^{\mathrm{l}}_{n}, t_n)\right]\Delta t. \tag{65}$$

6. Summary and conclusion

We have presented zeroth-, first-, and second-order algorithms for collection, ejection, and loading of particles in particle simulations. The algorithm for particle collection finds the position and velocity at any specific time from those at a discrete time. The algorithms for particle ejection (including both secondary emission and spontaneous emission) and loading find the value at a discrete time from those at a given time. The accuracy of these methods was analyzed for general fields and confirmed by comparing the numerically computed value with its exact solution under a homogeneous magnetic field. These algorithms are easy to implement and can improve overall simulation fidelity at little computational expense. Since our collection and ejection methods do not presume that the physical boundary is located on some specific spatial grid, they are applicable to cut cell simulations where physical boundaries may not reside on the computational spatial grid [6,7]. Although our algorithms have been obtained for time stepping, they can also be used for beam physics simulations with spatial stepping [8] instead of time stepping. The values at any specific location can be obtained simply by exchanging temporal and spatial variables in the algorithms.

Acknowledgements

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