Available online at www.sciencedirect.com
ScienceDirect
Journal of Computational Physics 227 (2008) 1663–1675
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

Algorithms for accurate relativistic particle injection

Y. Feng *, H.C. Kim, J.P. Verboncoeur

Department of Nuclear Engineering, University of California, Berkeley, CA 94720-1730, United States

Received 9 March 2007; received in revised form 26 August 2007; accepted 19 September 2007
Available online 19 November 2007

Abstract

In particle-in-cell plasma codes, the second-order leap-frog method is used to push the velocity and position of each particle in the main loop. Once a velocity distribution has been inverted for injection, time-centering of the position and velocity is necessary to maintain second-order accuracy. We have set up non-relativistic time-centering algorithms for particle injection in our PIC code. We further developed relativistic time-centering methods for injection and we added methods to calculate higher order accurate position. Also, the algorithms are expanded to find the position and velocity at any specific time from those at the initial discrete time, which can be used not only in the leap-frog method but also any other algorithms.

Keywords: Relativistic injection leap-frog time-centering

1. Introduction

In particle-in-cell plasma codes, the leap-frog integrator, which is generally second-order accurate [1–3], is widely used to solve the equations of motion for the particles. To update the particle motion, the leap-frog method requires that the position and velocity are offset by one half time step (so called time-centering). Cartwright et al. [4] developed a non-relativistic second-order method for particle loading and injection. The model and error analysis were improved more recently in the non-relativistic limit [5].

Recent advances in high power microwave source technology include relativistic devices such as the relativistic Klystron oscillator [6] and the relativistic magnetron [7]. Either relativistic initial velocity or high acceleration field (many high power microwave devices operate at a relativistic potential greater than 0.5 MeV) require a corresponding relativistic time-centering algorithm. Moreover, some simulations do not include the relativistic cathode–anode acceleration, but instead they start with the beam already accelerated to reduce the computational expense associated with resolving anode–cathode field gradients. Data from a gun code or

DOI of original article: 10.1016/j.jcp.2006.09.026.
* Corresponding author. Tel.: +1 530 220 0010.
E-mail address: yangfeng@berkeley.edu (Y. Feng).

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2007.09.016

similar model may produce an input distribution for a particle model of a beam–circuit interaction, also requiring proper adjustment of the velocities and positions.

In this work, the injection schemes of [5] are extended to the relativistic regime. Algorithms with different order of local error for particle injection are developed, which are more complicated than the corresponding classical cases. Since the injection schemes are designed for pushing particles in the initial fractional time step, it is ambiguous to define their order of global error. Instead, we use the order of local error for classification. In this paper, second-order accuracy means the lowest order term of local error is third order. The accuracy derived from the error analysis will be confirmed by comparing numerically computed values of position and velocity with higher order numerical solutions, since there is no close form analytical solution for relativistic motion even for simplified cases.

2. Standard relativistic leap-frog push

In order to understand the design of an injection scheme required to match the leap-frog method, we first review the relativistic leap-frog scheme for solving the relativistic Newton–Lorentz equations of motion. The continuum relativistic momentum equation is

$$m\frac{\mathrm{d}(\gamma\dot{\mathbf{x}})}{\mathrm{d}t} = q\mathbf{E}(\mathbf{x}(t),t) + q\mathbf{v}(t)\times\mathbf{B}(\mathbf{x}(t),t), \tag{1}$$

where $\dot{\mathbf{x}} = \mathrm{d}\mathbf{x}/\mathrm{d}t = \mathbf{v}(t)$. Setting $\mathbf{e} = q\mathbf{E}/m$, and $\mathbf{b} = q\mathbf{B}/m$, we get

$$\gamma\ddot{\mathbf{x}} + \dot{\gamma}\dot{\mathbf{x}} = \mathbf{e}(\mathbf{x}(t),t) + \mathbf{v}(t)\times\mathbf{b}(\mathbf{x}(t),t). \tag{2}$$

Then the corresponding standard leap-frog integrator for the relativistic case with the magnetic term centered by averaging becomes [1]

$$\gamma_{n+1/2}\mathbf{v}_{n+1/2} - \gamma_{n-1/2}\mathbf{v}_{n-1/2} = \mathbf{e}(\mathbf{x}_n,t_n)\Delta t + \frac{1}{2}(\mathbf{v}_{n-1/2}+\mathbf{v}_{n+1/2})\times\mathbf{b}(\mathbf{x}_n,t_n)\Delta t, \tag{3}$$

and

$$\mathbf{x}_{n+1} - \mathbf{x}_n = \mathbf{v}_{n+1/2}\Delta t, \tag{4}$$

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 time step, assuming that the values at the previous time step are exact.

To get the local truncation error of the velocity, we define $\mathbf{u}(t) = \gamma(t)\mathbf{v}(t)$. $\mathbf{v}(t_{n+1/2})$ and $\mathbf{u}(t_{n+1/2})$ denote the exact solutions, while $\mathbf{v}_{n+1/2}$ and $\mathbf{u}_{n+1/2}$ denote approximate solutions. So when there is an error $\varepsilon_{\mathbf{v},\text{leap-frog}} = \mathbf{v}(t_{n+1/2}) - \mathbf{v}_{n+1/2}$, the corresponding error $\varepsilon_{\mathbf{u},\text{leap-frog}} = \mathbf{u}(t_{n+1/2}) - \mathbf{u}_{n+1/2} \approx (\partial\mathbf{u}/\partial\mathbf{v})\varepsilon_{\mathbf{v},\text{leap-frog}} = \gamma^3\varepsilon_{\mathbf{v},\text{leap-frog}}$. Then Eq. (3) becomes:

$$\mathbf{u}(t_{n+1/2}) - \varepsilon_{\mathbf{u},\text{leap-frog}} - \mathbf{u}_{n-1/2} = \mathbf{e}(\mathbf{x}_n,t_n)\Delta t + \frac{1}{2}(\mathbf{v}_{n-1/2} + \mathbf{v}(t_{n+1/2}) - \varepsilon_{\mathbf{v},\text{leap-frog}})\times\mathbf{b}(\mathbf{x}_n,t_n)\Delta t. \tag{5}$$

Substitute in the relationship between $\varepsilon_{\mathbf{u},\text{leap-frog}}$ and $\varepsilon_{\mathbf{v},\text{leap-frog}}$

$$\varepsilon_{\mathbf{u},\text{leap-frog}} = \mathbf{u}(t_{n+1/2}) - \mathbf{u}_{n-1/2} - \mathbf{e}(\mathbf{x}_n,t_n)\Delta t - \frac{1}{2}\left(\mathbf{v}_{n-1/2} + \mathbf{v}(t_{n+1/2}) - \frac{\varepsilon_{\mathbf{u},\text{leap-frog}}}{\gamma^3}\right)\times\mathbf{b}(\mathbf{x}_n,t_n)\Delta t. \tag{6}$$

We only focus on the lowest order term in Δt, so the last term of Eq. (6) $\varepsilon_{\mathbf{u},\text{leap-frog}}/(2\gamma^3)\times\mathbf{b}(\mathbf{x}_n,t_n)\Delta t$, can be ignored. $\mathbf{v}_{n-1/2}$ and $\mathbf{u}_{n-1/2}$ are the same as $\mathbf{v}(t_{n-1/2})$ and $\mathbf{u}(t_{n-1/2})$, since they are initially given values in this analysis. With Taylor expansions of $\mathbf{v}(t_{n+1/2})$, $\mathbf{v}(t_{n-1/2})$, $\mathbf{u}(t_{n+1/2})$ and $\mathbf{u}(t_{n-1/2})$ about time t_n, we get

$$\varepsilon_{\mathbf{u},\text{leap-frog}} = \frac{1}{24}\mathrm{d}_{ttt}(\mathbf{u})(t_n)\Delta t^3 - \frac{1}{8}\dot{\mathbf{a}}(t_n)\times\mathbf{b}(t_n)\Delta t^3 + \mathbf{O}(\Delta t^4), \tag{7}$$

where $d_{t\times m}$ is shorthand for $(d/dt)^m$, $\mathbf{O}(\Delta t^k)$ is a vector where the lowest order component is order k, and $\mathbf{a}(=\dot{\mathbf{v}})$ is the acceleration of the particle as follows:

$$\mathbf{a}(t_n) = \mathbf{e}(t_n) + \mathbf{v}(t_n) \times \mathbf{b}(t_n). \tag{8}$$

So the velocity in the leap-frog method is second-order accurate since its error term is of the same order as $\boldsymbol{\varepsilon}_{\mathbf{u},\text{leap-frog}}$.

The local truncation error of the position, $\boldsymbol{\varepsilon}_{\mathbf{x},\text{leap-frog}}$, 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. (4) 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:

$$\boldsymbol{\varepsilon}_{\mathbf{x},\text{leap-frog}} = \mathbf{x}(t_{n+1}) - \mathbf{x}_{n+1} = \mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - [\mathbf{v}(t_{n+1/2}) - \boldsymbol{\varepsilon}_{\mathbf{v},\text{leap-frog}}]\Delta t = \frac{1}{24}\dot{\mathbf{a}}(t_n)\Delta t^3 + \mathbf{O}(\Delta t^4) \tag{9}$$

which means that the position in the leap-frog method is also second-order accurate. The results are slightly different compared to the non-relativistic case. [5]

The leap-frog method requires a half time step offset between velocity and position. In order to generalize our algorithm, we offset the position and velocity by a fractional time step, $s\Delta t$ $(0 \leqslant s < 1)$. The $s = 1/2$ case corresponds to the classic leap-frog method; $s = 0$ corresponds to a method in which $\mathbf{x}$ and $\mathbf{v}$ are synchronous.

3. Relativistic particle injection algorithms

Here, we focus on the injection of particles from the boundary originating from spontaneous emission, such as field and thermionic emission from metals. It is supposed that their velocity ($\mathbf{v}$) and position ($\mathbf{x}$) are given exactly at the time of their emission from the boundary, $t_{n-f} = (n-f)\Delta t$. $(0 < f < 1)$. They need to be time-centered in order to apply the leap-frog method at the next time step. $\mathbf{v}_{n-1/2}$ and $\mathbf{x}_n$ will be obtained as a function of $\mathbf{v}_{n-f}$, $\mathbf{x}_{n-f}$, and the fields. In our PIC code, we store $\mathbf{u}(t) = \gamma(t)\mathbf{v}(t)$ but not $\mathbf{v}(t)$, so we are trying to obtain $\mathbf{u}_{n-1/2}$ directly. The error analysis for $\mathbf{u}_{n-1/2}$ is efficient since it will has the same order error as $\mathbf{v}_{n-1/2}$.

Following each method developed in the following subsections, we give the corresponding numerical verification. Since there is no analytic solution even for the simplest case (constant electric field without magnetic fields) in the relativistic regime, we use a fourth order accurate numerical ordinary differential equation solver as the standard solution to verify the order of accuracy of our methods.

3.1. Simple relativistic injection method

$$\mathbf{x}_n - \mathbf{x}_{n-f} = \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}} f\Delta t, \quad \text{and} \quad \mathbf{u}_{n-s} - \mathbf{u}_{n-f} = \mathbf{e}(\mathbf{x}_{n-f}, n-1)(f-s)\Delta t. \tag{10}$$

The local error of the velocity, $\boldsymbol{\varepsilon}_{\mathbf{u}}$, is $\mathbf{O}(\Delta t)$ as follows:

$$\boldsymbol{\varepsilon}_{\mathbf{u}} = \mathbf{u}(t_{n-s}) - \mathbf{u}_{n-s} = (f-s)\mathbf{v}(t_n) \times \mathbf{b}(t_n)\Delta t + \mathbf{O}(\Delta t^2) \tag{11}$$

which means that the velocity is zeroth-order accurate for general fields.

The local error of the position, $\boldsymbol{\varepsilon}_{\mathbf{x}}$, is

$$\boldsymbol{\varepsilon}_{\mathbf{x}} = \mathbf{x}(t_n) - \mathbf{x}_n = \mathbf{x}(t_n) - \mathbf{x}(t_{n-f}) - f\mathbf{v}(t_{n-f})\Delta t = -\frac{1}{2}f^2\ddot{\mathbf{x}}_n\Delta t^2 + \mathbf{O}(\Delta t^3) \tag{12}$$

which means that the position is first-order accurate. Without magnetic fields, the velocity will also be first-order accurate. We choose $\mathbf{E}(\mathbf{x}, t) = (-1\text{e}10 - 4.49\text{e}13x - 1\text{e}10\sin(1\text{e}12 * t))\hat{\mathbf{x}}$ V/m, $\mathbf{B} = (1 + \sin(1\text{e}12 * t))\hat{\mathbf{z}}$ T as testing fields. Fig. 1a and b show the numerical verification for zero-order accurate velocity and first-order accurate position separately. Fig. 1c shows that the velocity also becomes first-order accurate without magnetic fields.

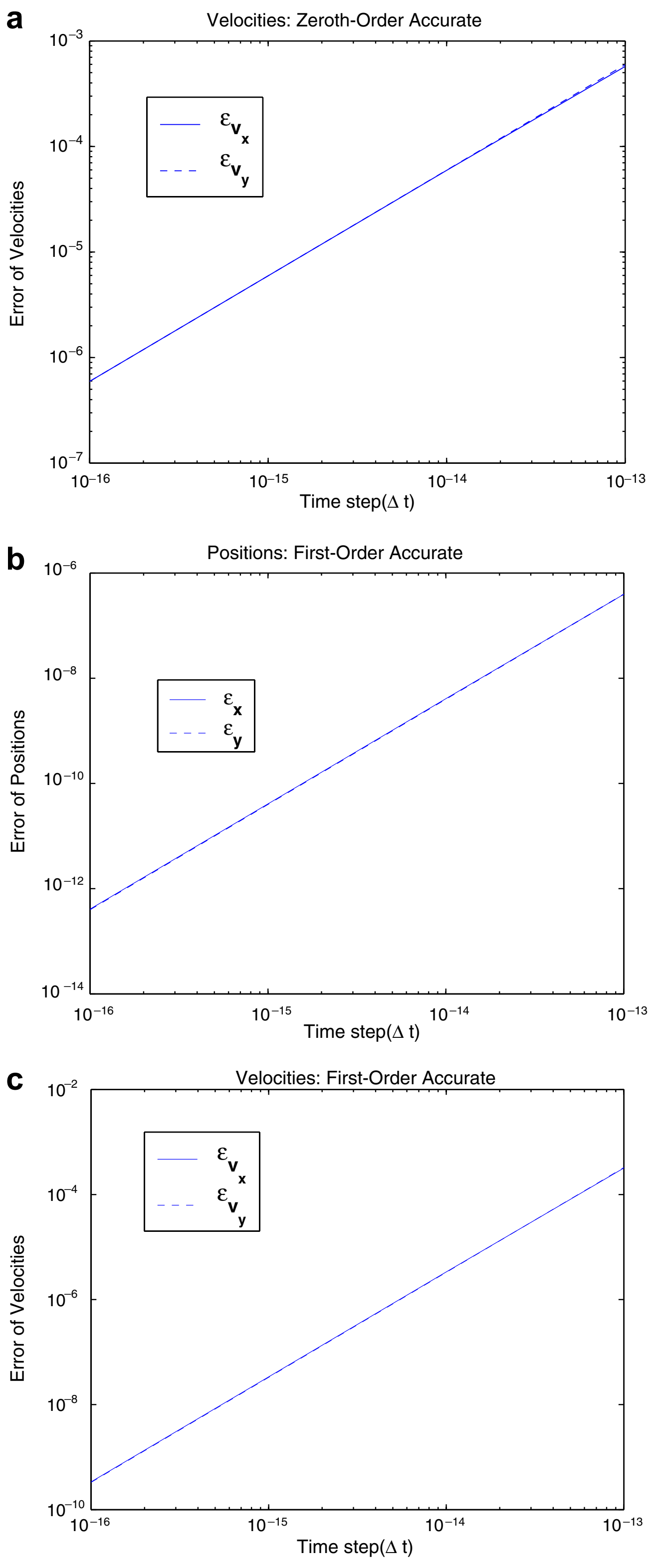

Fig. 1. Test fields: $\mathbf{E}(\mathbf{x}, t) = (-1e10 - 4.49e13x - 1e10\sin(1e12 * t))\hat{\mathbf{x}}$ V/m, $\mathbf{B} = (1 + \sin(1e12 * t))\hat{\mathbf{z}}$ T. (a) The local error of velocity. (b) The local error of position. (c) The local error of velocity when $B = 0$.

3.2. Relativistic fractional time step Boris push

Higher order methods can be obtained by adding terms to the simple relativistic injection method of Eq. (10), considering the lowest order term in the velocity and position errors (Eqs. (11) and (12)). The following is the simple relativistic fractional time step Boris push to obtain the position and velocity of particles at the boundary:

$$\mathbf{u}_{n-s} - \mathbf{u}_{n-f} = (f-s)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t + \frac{f-s}{2}\left(\frac{\mathbf{u}_{n-s}}{\gamma_{n-s}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$

$$\mathbf{u}_{n-f/2} - \mathbf{u}_{n-f} = \frac{f}{2}\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t + \frac{f}{4}\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \text{and}$$

$$\mathbf{x}_n - \mathbf{x}_{n-f} = f\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}}\Delta t. \tag{13}$$

The local error of the velocity, $\boldsymbol{\varepsilon}_{\mathbf{u}}$, is $\mathbf{O}(\Delta t^2)$ as follows:

$$\boldsymbol{\varepsilon}_{\mathbf{u}} = \mathbf{u}(t_{n-s}) - \mathbf{u}_{n-s} = -\frac{1}{2}(f-s)(f+s)[\dot{\mathbf{e}}(t_n) + \mathbf{v}(t_n) \times \dot{\mathbf{b}}(t_n)]\Delta t^2 + (f-s)\left[\frac{\partial \mathbf{e}(t_n)}{\partial t} + f(\mathbf{v}(t_n)\cdot\nabla)\mathbf{e}(t_n)\right]\Delta t^2 + (f-s)\mathbf{v}(t_n) \times \left[\frac{\partial \mathbf{b}(t_n)}{\partial t} + f(\mathbf{v}(t_n)\cdot\nabla)\mathbf{b}(t_n)\right]\Delta t^2 + \mathbf{O}(\Delta t^3) \tag{14}$$

which means that the velocity is first-order accurate for general fields.

The local error of the position, $\boldsymbol{\varepsilon}_{\mathbf{x}}$, is $\mathbf{O}(\Delta t^3)$ as follows:

$$\boldsymbol{\varepsilon}_{\mathbf{x}} = \mathbf{x}(t_n) - \mathbf{x}_n = \frac{f^3}{24}\dot{\mathbf{a}}(t_n)\Delta t^3 + \mathbf{O}(\Delta t^4) \tag{15}$$

which means that the position is second-order accurate and the lowest error term is similar to the leap-frog position error. Again, with constant fields (electric field and magnetic field are uniform and time-independent),the velocity will be second-order accurate. Fig. 2a and b show the first-order accurate velocity and second-order accurate position separately, and Fig. 2c shows that the velocity will also be second-order accurate under constant fields.

3.3. Modified relativistic fractional time step Boris push

The relativistic fractional time step Boris push method can be modified to be third order accurate in position for constant fields. As the analysis shown above, the velocity is second-order accurate under constant fields. To make the position accuracy one order higher, $\dot{\mathbf{a}}(t_n)$ in Eq. (15) is needed. Take total derivative with respect to t for both sides of Eq. (2):

$$\gamma(\mathrm{d}_{ttt}\mathbf{x}) + 2\dot{\gamma}\ddot{\mathbf{x}} + \ddot{\gamma}\dot{\mathbf{x}} = \dot{\mathbf{v}}(t) \times \mathbf{b}(\mathbf{x}(t), t) + \mathbf{v}(t)\cdot(\nabla\mathbf{e}(\mathbf{x}(t)) + \mathbf{v}(t) \times \nabla\mathbf{b}(\mathbf{x}(t), t)) + \partial_t\mathbf{e}(\mathbf{x}(t), t) + \mathbf{v}(t) \times \partial_t\mathbf{b}(\mathbf{x}(t), t), \tag{16}$$

where $(\mathrm{d}_{ttt}\mathbf{x}) = \dot{\mathbf{a}}(t_n)$.

So for constant fields, we can get

$$\gamma\dot{\mathbf{a}}(t_n) = \dot{\mathbf{v}}(t) \times \mathbf{b}(\mathbf{x}(t), t) - 2\dot{\gamma}\ddot{\mathbf{x}} - \ddot{\gamma}\dot{\mathbf{x}} \tag{17}$$

Note there are two additional terms $-2\dot{\gamma}\ddot{\mathbf{x}} - \ddot{\gamma}\dot{\mathbf{x}}$ to be calculated compared to non-relativistic case, where we need to use one more Boris push to get the $\ddot{\gamma}$ term. So the modified relativistic fractional time step Boris push method is

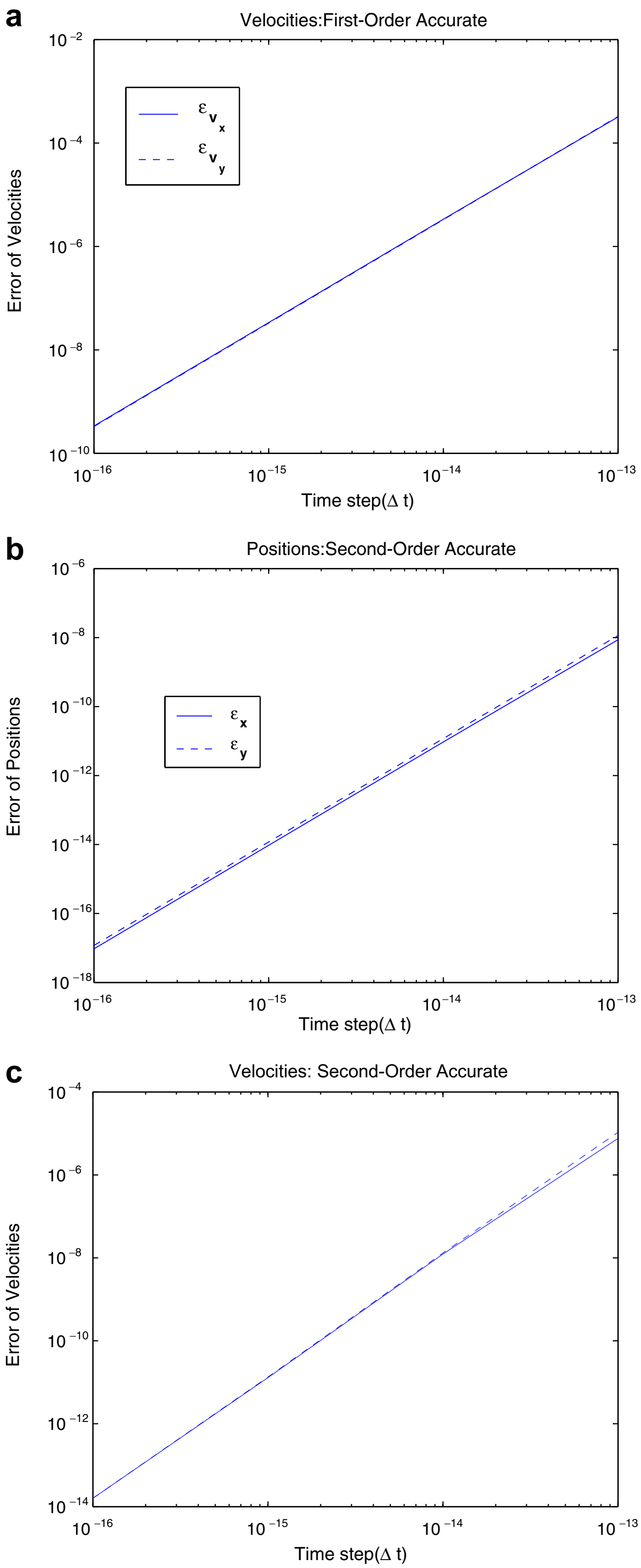

Fig. 2. Test fields: $\mathbf{E}(\mathbf{x},t) = (-1e10 - 4.49e13x - 1e10\sin(1e12 * t))\hat{\mathbf{x}}$ V/m, $\mathbf{B} = (1 + \sin(1e12 * t))\hat{\mathbf{z}}$ T. (a) The local error of velocity. (b) The local error of position. (c) The local error of velocity when the testing fields become constant: $\mathbf{E}(\mathbf{x},t) = -1e10\hat{\mathbf{x}}$ V/m, $\mathbf{B} = 1\hat{\mathbf{z}}$ T.

$$\mathbf{u}_{n-s} - \mathbf{u}_{n-f} = (f-s)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t + \frac{f-s}{2}\left(\frac{\mathbf{u}_{n-s}}{\gamma_{n-s}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$

$$\mathbf{u}_{n+1-f} - \mathbf{u}_{n-f} = \mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t + \frac{1}{2}\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$

$$\mathbf{u}_{n-1-f} - \mathbf{u}_{n-f} = -\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t - \frac{1}{2}\left(\frac{\mathbf{u}_{n-1-f}}{\gamma_{n-1-f}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$

$$\mathbf{u}_{\text{add}} = \frac{1}{24}\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} - \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t - \frac{1}{12}(\gamma_{n+1-f} - \gamma_{n-f})\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} - \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)$$
$$- \frac{1}{24}(\gamma_{n+1-f} - 2\gamma_{n-f} + \gamma_{n-1-f})\frac{\mathbf{u}_{n-f}}{\gamma_{n-f}},$$

$$\mathbf{u}_{n-f/2} - \mathbf{u}_{n-f} = \frac{f}{2}\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t + \frac{f}{4}\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \text{and}$$

$$\mathbf{x}_n - \mathbf{x}_{n-f} = f\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{\text{add}}}{\gamma_{n-f}}\right)\Delta t. \tag{18}$$

Fig. 3a and b shows that under constant fields, this method leads to second-order accurate velocity and third-order accurate position separately.

3.4. Field gradient relativistic fractional time step Boris push

This method treats time-independent but spatial varying fields to yield a second-order accurate velocity and third order accurate position. Based on the Modified relativistic Boris push, it added the consideration of field gradient terms. First, the field parameters are modified by the derivatives for the velocity and position integration:

$$\mathbf{b}_v = \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{f-s}{2}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \mathbf{e}_v = \mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{f-s}{2}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$
$$\mathbf{b}_t = \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \mathbf{e}_t = \mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$
$$\mathbf{b}_{t1} = \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) - 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \mathbf{e}_{t1} = \mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) - 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,$$
$$\mathbf{b}_x = \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{f}{4}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \text{and} \quad \mathbf{e}_x = \mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{f}{4}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \tag{19}$$

where $\mathbf{v}_{n-f} = \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}$.

Then based on the modified relativistic Boris push, we only need add the field gradient terms to get

$$\gamma(\mathrm{d}_{ttt}\mathbf{x}) = \dot{\mathbf{v}}(t) \times \mathbf{b}(\mathbf{x}(t), t) - 2\dot{\gamma}\ddot{\mathbf{x}} - \ddot{\gamma}\dot{\mathbf{x}} + \mathbf{v}(t)\cdot(\nabla\mathbf{e}(\mathbf{x}(t)) + \mathbf{v}(t) \times \nabla\mathbf{b}(\mathbf{x}(t), t)). \tag{20}$$

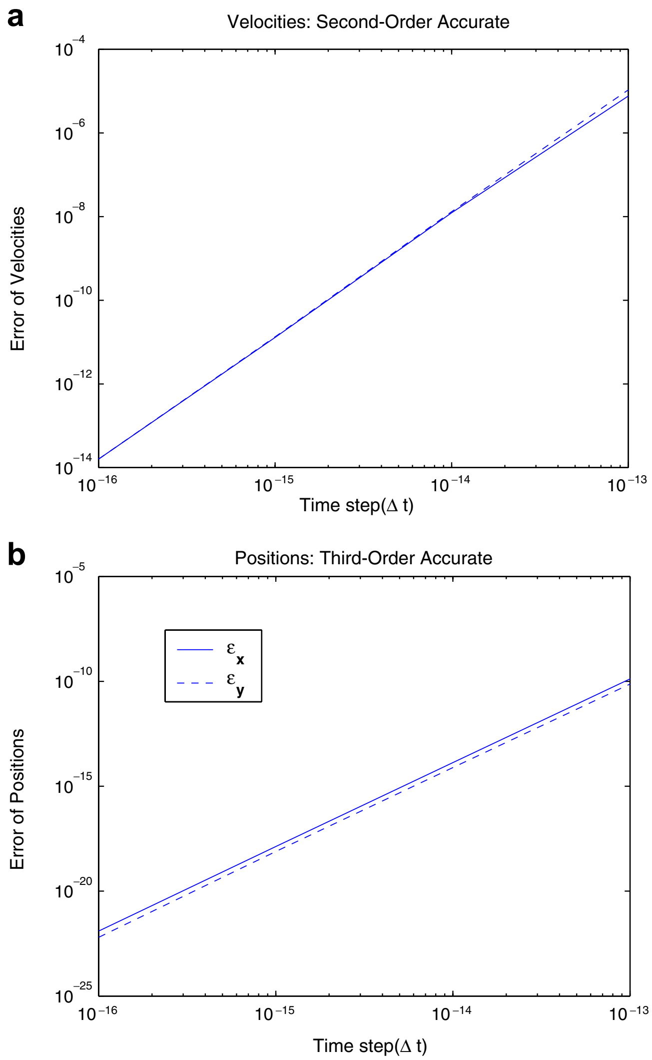

Fig. 3. Test fields: $\mathbf{E}(\mathbf{x},t) = -1\text{e}10\hat{\mathbf{x}}$ V/m, $\mathbf{B} = 1\hat{\mathbf{z}}$ T. (a) The local error of velocity. (b) The local error of position.

The corresponding injection method becomes:

$$\mathbf{u}_{n-s} - \mathbf{u}_{n-f} = (f-s)\mathbf{e}_v\Delta t + \frac{f-s}{2}\left(\frac{\mathbf{u}_{n-s}}{\gamma_{n-s}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}_v\Delta t,$$

$$\mathbf{u}_{n+1-f} - \mathbf{u}_{n-f} = \mathbf{e}_t\Delta t + \frac{1}{2}\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}_t\Delta t,$$

$$\mathbf{u}_{n-1-f} - \mathbf{u}_{n-f} = -\mathbf{e}_{t1}\Delta t - \frac{1}{2}\left(\frac{\mathbf{u}_{n-1-f}}{\gamma_{n-1-f}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}_{t1}\Delta t,$$

$$\mathbf{u}_{\text{add}} = \frac{1}{24}\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} - \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t - \frac{1}{12}(\gamma_{n+1-f} - \gamma_{n-f})\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} - \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)$$
$$- \frac{1}{24}(\gamma_{n+1-f} - 2\gamma_{n-f} + \gamma_{n-1-f})\frac{\mathbf{u}_{n-f}}{\gamma_{n-f}} + \frac{1}{24}\frac{\mathbf{u}_{n-f}}{\gamma_{n-f}} \cdot \left(\nabla\mathbf{e} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}} \times \nabla\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t\right),$$

$$\mathbf{u}_{n-f/2} - \mathbf{u}_{n-f} = \frac{f}{2}\mathbf{e}_x\Delta t + \frac{f}{4}\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right) \times \mathbf{b}_x\Delta t, \quad \text{and}$$
$$\mathbf{x}_n - \mathbf{x}_{n-f} = f\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{\text{add}}}{\gamma_{n-f}}\right)\Delta t. \tag{21}$$

Fig. 4a and b confirms that under time-independent but spatial varying testing fields, this method leads to second-order accurate velocity and third-order accurate position separately.

3.5. Relativistic general second-order method

This method achieves second-order accurate velocity and third order accurate position for general spatially and temporally varying fields. Based on the field gradient relativistic Boris push, it added the consideration of time dependent terms. First, the fields parameters are modified by the time derivatives using the previous time step field values for the velocity and position integration:

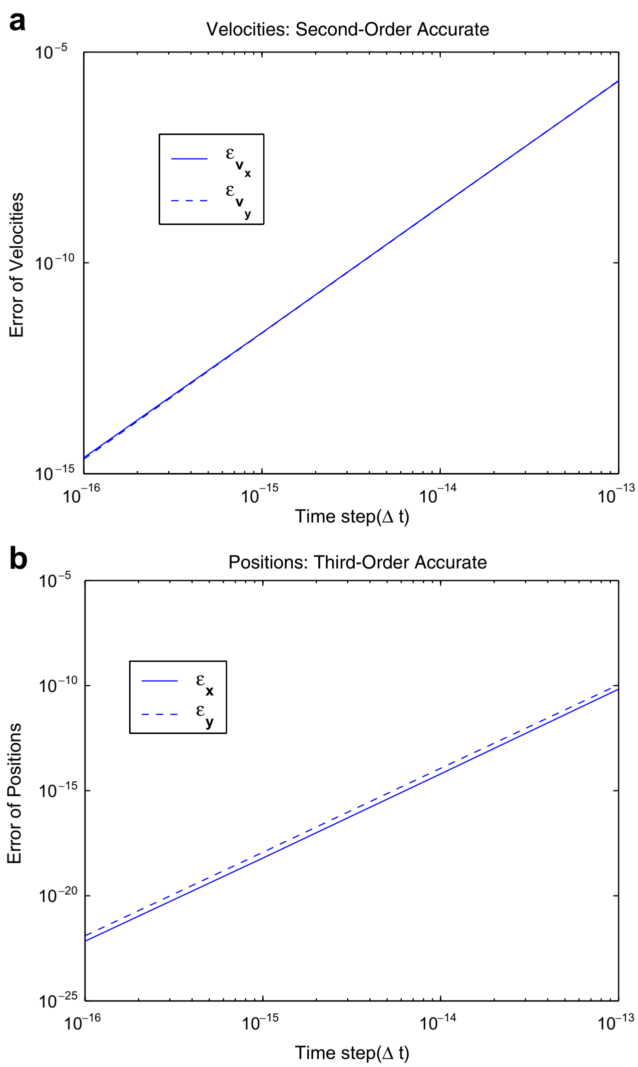

Fig. 4. Test fields: $\mathbf{E}(\mathbf{x},t) = (-1\text{e}10 - 4.49\text{e}13x)\hat{\mathbf{x}}$ V/m, $\mathbf{B} = 1\hat{\mathbf{z}}$ T. (a) The local error of velocity. (b) The local error of position.

$$
\begin{aligned}
\mathbf{b}_v &= \left(1 - \frac{f+s-2}{2}\right)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{f+s-2}{2}\mathbf{b}(\mathbf{x}_{n-f}, t_{n-2}) + \frac{f-s}{2}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,\\
\mathbf{e}_v &= \left(1 - \frac{f+s-2}{2}\right)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{f+s-2}{2}\mathbf{e}(\mathbf{x}_{n-f}, t_{n-2}) + \frac{f-s}{2}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,\\
\mathbf{b}_t &= \left(1 - \frac{2f-3}{2}\right)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{2f-3}{2}\mathbf{b}(\mathbf{x}_{n-f}, t_{n-2}) + 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,\\
\mathbf{e}_t &= \left(1 - \frac{2f-3}{2}\right)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{2f-3}{2}\mathbf{e}(\mathbf{x}_{n-f}, t_{n-2}) + 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,\\
\mathbf{b}_{t1} &= \left(1 - \frac{2f-1}{2}\right)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{2f-1}{2}\mathbf{b}(\mathbf{x}_{n-f}, t_{n-2}) - 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,\\
\mathbf{e}_{t1} &= \left(1 - \frac{2f-1}{2}\right)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{2f-1}{2}\mathbf{e}(\mathbf{x}_{n-f}, t_{n-2}) - 0.5(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,\\
\mathbf{b}_x &= \left(1 - \frac{3f-4}{4}\right)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{3f-4}{4}\mathbf{b}(\mathbf{x}_{n-f}, t_{n-2}) + \frac{f}{4}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t, \quad \text{and}\\
\mathbf{e}_x &= \left(1 - \frac{3f-4}{4}\right)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) + \frac{3f-4}{4}\mathbf{e}(\mathbf{x}_{n-f}, t_{n-2}) + \frac{f}{4}(\mathbf{v}_{n-f}\cdot\nabla)\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1})\Delta t,
\end{aligned}
\tag{22}
$$

where $\mathbf{v}_{n-f} = \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}$.

For general fields, rearranging Eq. (16), we can get

$$
\begin{aligned}
\gamma(\mathrm{d}_{ttt}\mathbf{x}) = &-2\dot{\gamma}\ddot{\mathbf{x}} - \ddot{\gamma}\dot{\mathbf{x}} + \dot{\mathbf{v}}(t)\times\mathbf{b}(\mathbf{x}(t),t) + \mathbf{v}(t)\cdot(\nabla\mathbf{e}(\mathbf{x}(t)) + \mathbf{v}(t)\times\nabla\mathbf{b}(\mathbf{x}(t),t)) + \partial_t\mathbf{e}(\mathbf{x}(t),t)\\
&+ \mathbf{v}(t)\times\partial_t\mathbf{b}(\mathbf{x}(t),t).
\end{aligned}
\tag{23}
$$

So the corresponding general injection method becomes:

$$
\begin{aligned}
&\mathbf{u}_{n-s} - \mathbf{u}_{n-f} = (f-s)\mathbf{e}_v\Delta t + \frac{f-s}{2}\left(\frac{\mathbf{u}_{n-s}}{\gamma_{n-s}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)\times\mathbf{b}_v\Delta t,\\
&\mathbf{u}_{n+1-f} - \mathbf{u}_{n-f} = \mathbf{e}_t\Delta t + \frac{1}{2}\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)\times\mathbf{b}_t\Delta t,\\
&\mathbf{u}_{n-1-f} - \mathbf{u}_{n-f} = -\mathbf{e}_{t1}\Delta t - \frac{1}{2}\left(\frac{\mathbf{u}_{n-1-f}}{\gamma_{n-1-f}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)\times\mathbf{b}_{t1}\Delta t,\\
&\mathbf{u}_{\mathrm{add}} = \frac{1}{24}\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} - \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)\times\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\Delta t - \frac{1}{12}(\gamma_{n+1-f} - \gamma_{n-f})\left(\frac{\mathbf{u}_{n+1-f}}{\gamma_{n+1-f}} - \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)\\
&\qquad - \frac{1}{24}(\gamma_{n+1-f} - 2\gamma_{n-f} + \gamma_{n-1-f})\frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\\
&\qquad + \frac{1}{24}\frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\cdot\left(\nabla\mathbf{e} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\times\nabla\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1})\right)\\
&\qquad + \frac{1}{24}\left(\mathbf{e}(\mathbf{x}_{n-f}, t_{n-1}) - \mathbf{e}(\mathbf{x}_{n-f}, t_{n-2}) + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\times(\mathbf{b}(\mathbf{x}_{n-f}, t_{n-1}) - \mathbf{b}(\mathbf{x}_{n-f}, t_{n-2}))\right),\\
&\mathbf{u}_{n-f/2} - \mathbf{u}_{n-f} = \frac{f}{2}\mathbf{e}_x\Delta t + \frac{f}{4}\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{n-f}}{\gamma_{n-f}}\right)\times\mathbf{b}_x\Delta t, \quad \text{and} \quad \mathbf{x}_n - \mathbf{x}_{n-f} = f\left(\frac{\mathbf{u}_{n-f/2}}{\gamma_{n-f/2}} + \frac{\mathbf{u}_{\mathrm{add}}}{\gamma_{n-f}}\right)\Delta t.
\end{aligned}
\tag{24}
$$

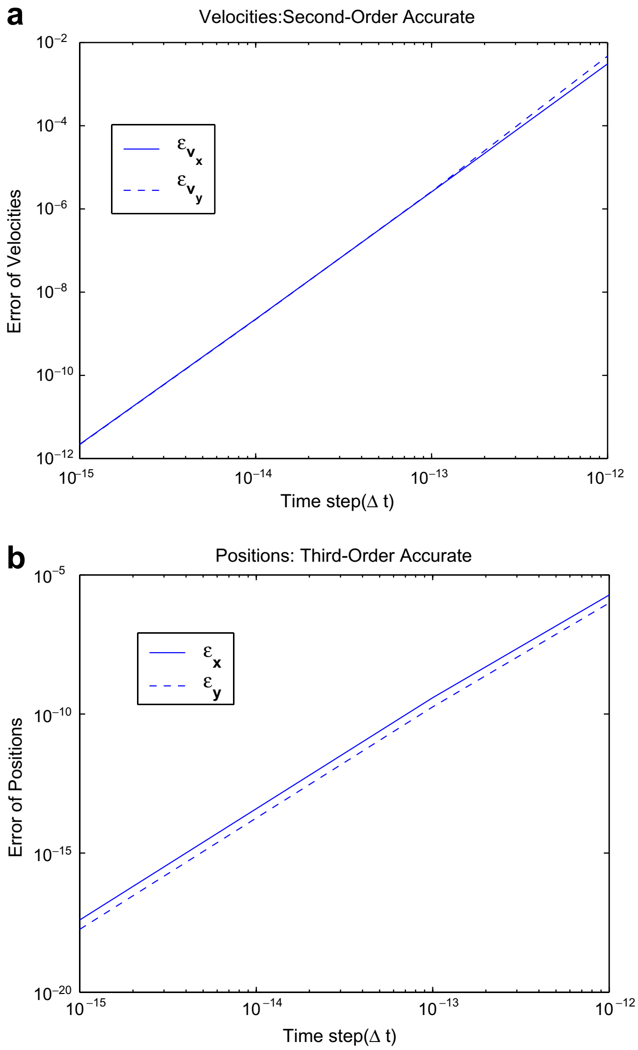

Fig. 5. Test fields: $\mathbf{E}(\mathbf{x},t) = (-1\text{e}10 - 4.49\text{e}13x - 1\text{e}10\sin(1\text{e}12 * t))\hat{\mathbf{x}}$ V/m, $\mathbf{B} = (1 + \sin(1\text{e}12 * t))\hat{\mathbf{z}}$ T. (a) The local error of velocity. (b) The local error of position.

Fig. 5a and b confirms that under general spatially and temporally varying fields, this method leads to second-order accurate velocity and third-order accurate position separately.

4. Comparison with previous methods

Suppose we are tracking the kinetic energy of particles at a specific time after their injection. For simplicity, we assume the fields are constant, $E = 1\text{e}10$ V/m, and $B = 1$ T. Particles are injected with a fixed initial velocity $v_x = v_y = 2.11\text{e}8$ V/m^2. The injected current is so small that we can ignore the space charge.

We choose the leap-frog method as the main loop algorithm ($s = \frac{1}{2}$. To illustrate the importance of the above relativistic algorithms, we compare the error order of particle energy for three different cases: case 1 using the classical algorithm at the injecting time $t = 0$; case 2 without any algorithm at $t = 0$; case 3 using our relativistic algorithm at $t = 0$.

Fig. 6a shows the error of energy generated just after first time-step. As we expected, the classical time-centering totally fails since our fields and initial velocity are in the relativistic regime. If we do not use any time-

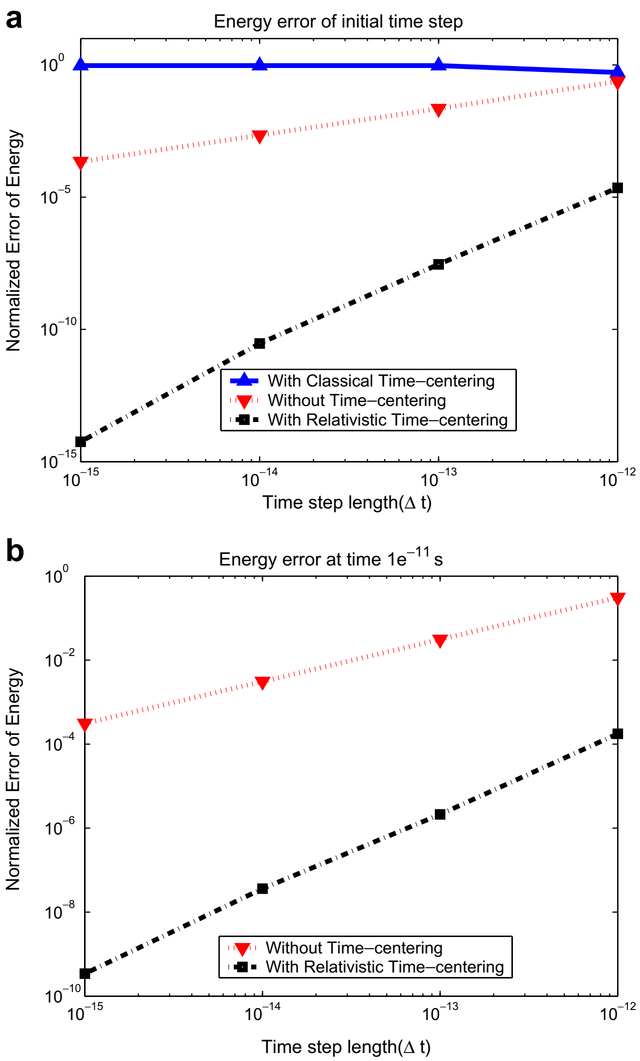

Fig. 6. Test fields: $\mathbf{E}(\mathbf{x}) = -1e10$ V/m, $\mathbf{B} = 1\hat{\mathbf{z}}$ T. (a) The normalized local error of particle kinetic energy at the initial injecting step. (b) The global error of particle kinetic energy at a specific time.

centering, the error term generated in this time step will be first-order. With relativistic time-centering, the error term will be third-order.

Fig. 6b shows the error of energy at the specified time $t = 1e{-}11$ s. For time step $\Delta t = 1e{-}12$ s, we run 9 time step using leap-frog to push particles; for $\Delta t = 1e{-}13$ s, we run 99 time steps following; for $\Delta t = 1e{-}14$ s, we run 999 time steps; and for $\Delta t = 1e{-}15$ s, we run 9999 time steps following the initial time step. We showed that the leap-frog is a second-order accurate algorithm, which expects the global error term to be second-order; however, the order of the error term is determined by the initial time step algorithm. Only when we use the algorithms at the initial injecting time step correctly, can we get the expected accurate result.

5. Conclusions and discussions

We have described five methods with different orders of local error for relativistic particle injection, which are used to calculate the injected particle position and velocity at the initial discrete time. The accuracy of each relativistic method is determined and numerically verified with the following test cases: constant electric fields, spatially varying electric fields and time-dependent electric fields in a homogeneous or time-dependent magnetic field. In addition, we have generalized our algorithm by offsetting the position and velocity by a fractional time step, $s\Delta t$ ($0 \leqslant s < 1$). The $s = 1/2$ case corresponds to the classic leap-frog method; $s = 0$ corresponds to a method in which $\mathbf{x}$ and $\mathbf{v}$ are synchronous.

Now we discuss the global error for the general case. Suppose we choose a first-order accurate (local error: $c_1\Delta t^2 + \mathbf{O}(\Delta t^3)$) velocity injection algorithm from above, and choose a second-order accurate (local error: $c_2\Delta t^3 + \mathbf{O}(\Delta t^4)$) velocity algorithm in the main loop. After a fixed simulated time τ, the global error will be $c_1\Delta t^2 + \mathbf{O}(\Delta t^3) + \tau/\Delta t * (c_2\Delta t^3 + \mathbf{O}(\Delta t^4)) = (c_1 + \tau c_2)\Delta t^2 + \mathbf{O}(\Delta t^3)$ which is in the second-order. So choosing an initial injection algorithm one order lower than the main loop algorithm will be efficient.

Acknowledgments

This work was supported in part by AFOSR Cathodes and Breakdown MURI04 grant FA9550-04-1-0369, AFOSR STTR Phase II contract FA9550-04-C-0069, and the Air Force Research Laboratory – Kirtland.

References

[1] C.K. Birdsall, A.B. Langdon, Plasma Physics via Computer Simulation, Hilger, New York, 1991.
[2] C.K. Birdsall, IEEE Trans. Plasma Sci. 19 (1991) 65.
[3] J.P. Verboncoeur, Plasma Phys. Contr. Fusion 47 (2005) A231.
[4] K.L. Cartwright, J.P. Verboncoeur, C.K. Birdsall, J. Comput. Phys. 162 (2000) 483.
[5] H.C. Kim, Y. Feng, J.P. Verboncoeur, J. Comput. Phys. 223 (2007) 629.
[6] K.J. Hendricks, P.D. Coleman, R.W. Lemke, M.J. Arman, L. Bowers, Phys. Rev. Lett. 76 (1996) 154.
[7] M. Lopez, R.M. Gilgenbach, D.W. Jordan, S.A. Anderson, M.D. Johnston, M.W. Keyser, H. Miyake, C.W. Peters, M.C. Jones, V.B. Neculaes, Y.Y. Lau, T.A. Spencer, J.W. Luginsland, M.D. Haworth, R.W. Lemke, D. Price, IEEE Trans. Plasma Sci. 30 (June) (2002) 947–955.