A three-step Boris integrator for Lorentz force equation of charged particles

Takayuki Umeda

Institute for Space-Earth Environmental Research, Nagoya University, Nagoya City, Aichi 464-8601, JAPAN

Abstract

This paper provides a numerical procedure for integrating the equations of motion for electrically charged particles in magnetic fields with higher accuracy than the conventional Boris integrator. It is confirmed by both of numerical test and theoretical analysis that the proposed three-step integrator has the same accuracy as the standard (two-step) Boris integrator with a half time step.

Keywords: Boris integrator; Lorentz force equation; Higher accuracy

1. Introduction

The Particle-In-Cell (PIC) method was first developed for plasma physics, but has now become used more widely in various scientific fields. The PIC method includes various educational as well as fundamental numerical schemes [1, 2]. The Boris integrator (or the Boris push) [3] is one of them, which solves the gyration of electrically charged particles by the Lorentz force.

Email address: `taka.umeda@nagoya-u.jp` (Takayuki Umeda)

The acceleration of charged particles by the Coulomb-Lorentz force is expressed by

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\boldsymbol{v}) = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}). \tag{1}$$

The central time difference of Eq.(1) is written as

$$\frac{\boldsymbol{u}^{t+\frac{\Delta t}{2}} - \boldsymbol{u}^{t-\frac{\Delta t}{2}}}{\Delta t} = \frac{q}{m}\left(\boldsymbol{E}^t + \frac{\boldsymbol{u}^{t+\frac{\Delta t}{2}} + \boldsymbol{u}^{t-\frac{\Delta t}{2}}}{2} \times \boldsymbol{B}_\gamma^t\right), \tag{2}$$

where $\boldsymbol{u} = c\boldsymbol{v}/\sqrt{c^2 - |\boldsymbol{v}|^2}$ and $\boldsymbol{B}_\gamma = c\boldsymbol{B}/\sqrt{c^2 + |\boldsymbol{u}|^2}$. Then, the acceleration forces are separated into operators of the electric and magnetic forces as follows [4]:

$$\boldsymbol{u}^- = \boldsymbol{u}^{t-\frac{\Delta t}{2}} + \frac{q}{m}\boldsymbol{E}^t\frac{\Delta t}{2}, \tag{3a}$$

$$\frac{\boldsymbol{u}^+ - \boldsymbol{u}^-}{\Delta t} = \frac{q}{m}\left(\frac{\boldsymbol{u}^+ + \boldsymbol{u}^-}{2} \times \boldsymbol{B}_\gamma^t\right), \tag{3b}$$

$$\boldsymbol{u}^{t+\frac{\Delta t}{2}} = \boldsymbol{u}^+ + \frac{q}{m}\boldsymbol{E}^t\frac{\Delta t}{2}. \tag{3c}$$

This paper deals with the Lorentz force equation (3b) only. For solving this implicit equation, we generally need to perform a complex matrix inversion [5]. On the other hand, Boris found a simple approximation of $(\boldsymbol{u}^+ + \boldsymbol{u}^-)/2$ as follows [3]:

$$\beta = \frac{1}{1 + \left(\frac{q}{m}\left|\boldsymbol{B}_\gamma^t\right|\frac{\Delta t}{2}\right)^2}, \tag{4a}$$

$$\frac{\boldsymbol{u}^+ + \boldsymbol{u}^-}{2} \equiv \boldsymbol{u}^\tau \approx \beta\left\{\boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^- \times \boldsymbol{B}_\gamma^t)\frac{\Delta t}{2}\right\}. \tag{4b}$$

Taking the inner dot product of Eq.(3b) with $\boldsymbol{u}^+ + \boldsymbol{u}^-$, we obtain $|\boldsymbol{u}^+|^2 - |\boldsymbol{u}^-|^2 = 0$. This suggests that the velocity vector moves from $\boldsymbol{u}^-$ to $\boldsymbol{u}^+$ along a segment of the circle satisfying $|\boldsymbol{u}| = \text{const.}$ in the velocity space as shown in Fig.1. Since magnetic fields do not work, the kinetic energy does not change during the gyration in the velocity space. Equation (4a) is the unique solution to the following equation:

$$\left\{2\boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^\tau \times \boldsymbol{B}^t_\gamma)\Delta t\right\} \cdot \left(\boldsymbol{u}^\tau \times \boldsymbol{B}^t_\gamma\right) = 0. \tag{5}$$

The procedures (3) and (4) are also called the Buneman-Boris scheme in some literatures [2, 6], since the time-symmetric equations (3) were first discussed by Buneman [4].[1]

There are several recent works showing that the Buneman-Boris scheme follows trajectories of charged particles with more precision than the fourth-order Runge-Kutta scheme even with the second-order (leap-frog) time stepping [7, 8]. The Buneman-Boris scheme has also been widely adopted in PIC simulations for about a half century because of its property of the energy conservation and simpleness of the code implementation. It should be noted, however, that the Boris integrator (4) itself has a numerical error in its gyration angle for one time step. As schematically illustrated in Fig.1b, Eq.(4b) suggests that the gyration angle for one time step $\omega_c \Delta t$ (where $\omega_c = q|\boldsymbol{B}^t_\gamma|/m$) is approximated as

$$\cos^2\left(\frac{\omega_c^* \Delta t}{2}\right) \approx \beta \qquad \text{or} \qquad \omega_c^* \Delta t \approx 2\tan^{-1}\left(\frac{q|\boldsymbol{B}^t_\gamma|\Delta t}{2m}\right). \tag{6}$$

The solid line in Fig.2 shows the approximated gyration angle for one time step $\omega_c^* \Delta t$ and the corresponding error $\varepsilon = (\omega_c - \omega_c^*)/\omega_c$ as a function of

[1] The Boris scheme corresponds to the numerical procedure (4) for the Lorentz force equation only, although many scientists misunderstand that the Boris scheme corresponds the procedures (3) and (4) for the entire Coulomb-Lorentz force equation.

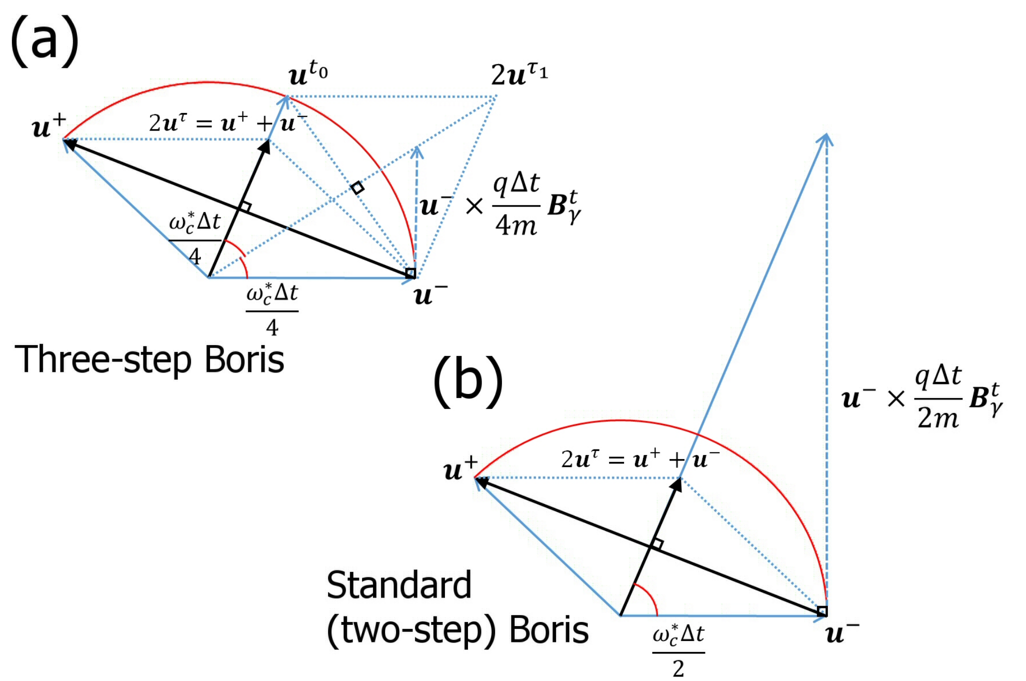

Figure 1: Schematic illustration of the velocity vector change in the Boris integrator. The proposed scheme (three-step Boris integrator) (a) and the standard (two-step) Boris integrator (b).

$\omega_c \Delta t$ for the Boris integrator. For a small time step ($\omega_c \Delta t \ll 1$), the Boris integrator has the second-order accuracy in time. For a larger time step ($\omega_c \Delta t > 1$), on the other hand, the accuracy is nonlinear and is worse. For an example, the gyration angle of $30^\circ(\omega_c \Delta t \sim 0.5236)$ is approximated as $29.34^\circ(\omega_c^* \Delta t \approx 0.5121)$ by the Boris integrator.

The purpose of the present study is to improve the accuracy of the gyration of the Boris integrator for a large time step of $\omega_c \Delta t > 1$. As an extension to the the standard two-step Boris integrator, we develop a three-step integrator.

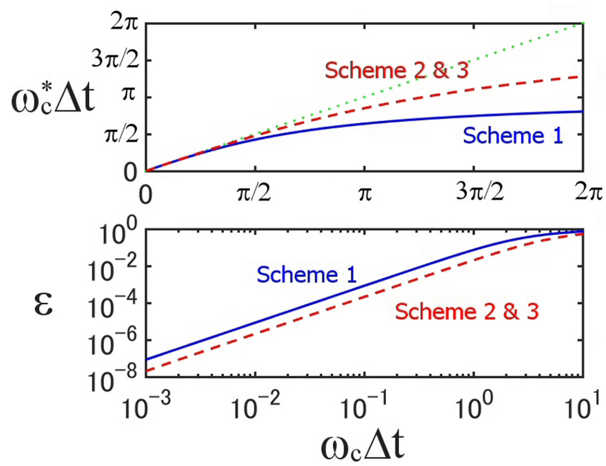

Figure 2: Approximated gyration angle for one time step $\omega_c^* \Delta t$ as a function of $\omega_c \Delta t$ and the corresponding error $\varepsilon = (\omega_c - \omega_c^*)/\omega_c$. The "scheme 1" corresponds to the standard (two-step) Boris integrator. The "scheme 2" corresponds to the standard Boris integrator twice with a half time step. The "scheme 3" corresponds to the proposed three-step integrator. The dotted line in the top panel shows $\omega_c^* = \omega_c$.

2. Numerical procedures

In the present study, we compare the following three integrators. The first scheme corresponds to the standard (two-step) Boris integrator,

$$B_1^2 = \left(\frac{q}{m} \left| \boldsymbol{B}^\gamma \right| \frac{\Delta t}{2} \right)^2, \qquad \beta_1 = \frac{1}{1 + B_1^2},$$

$$\boldsymbol{u}^\tau = \beta_1 \left\{ \boldsymbol{u}^- + \frac{q}{m} (\boldsymbol{u}^- \times \boldsymbol{B}^\gamma) \frac{\Delta t}{2} \right\}, \tag{7a}$$

$$\boldsymbol{u}^+ = \boldsymbol{u}^- + \frac{q}{m} (\boldsymbol{u}^\tau \times \boldsymbol{B}^\gamma) \Delta t. \tag{7b}$$

The second scheme uses the standard Boris integrator twice with a half time step as follows,

$$B_2^2 = \left(\frac{q}{m} \left| \boldsymbol{B}^\gamma \right| \frac{\Delta t}{4} \right)^2, \qquad \beta_2 = \frac{1}{1 + B_2^2},$$

$$\boldsymbol{u}^{\tau_1} = \beta_2 \left\{ \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^- \times \boldsymbol{B}^\gamma)\frac{\Delta t}{4} \right\}, \tag{8a}$$

$$\boldsymbol{u}^{t_0} = \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^{\tau_1} \times \boldsymbol{B}^\gamma)\frac{\Delta t}{2}, \tag{8b}$$

$$\boldsymbol{u}^{\tau_2} = \beta_2 \left\{ \boldsymbol{u}^{t_0} + \frac{q}{m}(\boldsymbol{u}^{t_0} \times \boldsymbol{B}^\gamma)\frac{\Delta t}{4} \right\}, \tag{8c}$$

$$\boldsymbol{u}^+ = \boldsymbol{u}^{t_0} + \frac{q}{m}(\boldsymbol{u}^{\tau_2} \times \boldsymbol{B}^\gamma)\frac{\Delta t}{2}. \tag{8d}$$

The third scheme corresponds to a three-step Boris integrator proposed in the present study.

$$B_2^2 = \left(\frac{q}{m}\left|\boldsymbol{B}^\gamma\right|\frac{\Delta t}{4}\right)^2, \qquad \beta_2 = \frac{1}{1+B_2^2}, \qquad \alpha = \frac{\beta_2}{\left(1-2\beta_2 B_2^2\right)^2 + 4\beta_2^2 B_2^2} = \beta_2, \tag{9a}$$

$$\boldsymbol{u}^{\tau_1} = \beta_2 \left\{ \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^- \times \boldsymbol{B}^\gamma)\frac{\Delta t}{4} \right\}, \tag{9b}$$

$$\boldsymbol{u}^{\tau} = \alpha \left\{ \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^{\tau_1} \times \boldsymbol{B}^\gamma)\frac{\Delta t}{2} \right\}, \tag{9c}$$

$$\boldsymbol{u}^+ = \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^{\tau} \times \boldsymbol{B}^\gamma)\Delta t. \tag{9d}$$

The procedure of this scheme is schematically illustrated in Fig.1a. The first and second step correspond to the standard Boris integrator with a half time step, in which $\boldsymbol{u}^{\tau_1} = (\boldsymbol{u}^- + \boldsymbol{u}^{t_0})/2$ is computed in the first step and $\boldsymbol{u}^\tau = \alpha\boldsymbol{u}^{t_0} = (\boldsymbol{u}^- + \boldsymbol{u}^+)/2$ is computed in the second step, where $|\boldsymbol{u}^-|^2 = |\boldsymbol{u}^{t_0}|^2 = |\boldsymbol{u}^+|^2$. In this scheme, an approximation of $(\boldsymbol{u}^+ + \boldsymbol{u}^-)/2$ is given by Eq.(9c). We find the unique solution $\alpha = \beta_2$ in Eq.(9a) by inserting Eqs.(9b) and (9c) into Eq.(5).

Equations (9b) and (9c) suggest that the gyration angle for one time step $\omega_c \Delta t$ is approximated as

$$\cos^2\left(\frac{\omega_c^* \Delta t}{4}\right) \approx \alpha \qquad \text{or} \qquad \omega_c^* \Delta t \approx 4\tan^{-1}\left(\frac{q|\boldsymbol{B}_\gamma^t|\Delta t}{4m}\right). \tag{10}$$

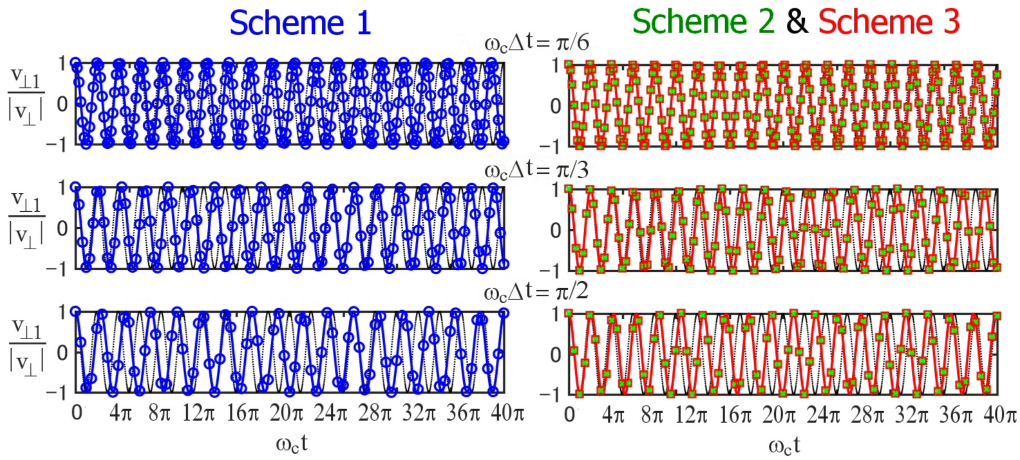

Figure 3: Numerical solutions to the Lorentz force equation by Schemes 1–3 with $\omega_c \Delta t = \pi/6$, $\pi/3$, and $\pi/2$. The circle, cross, and square marks correspond to the result with Scheme 1 (standard two-step Boris), Scheme 2 (standard Boris twice with a half time step), and Scheme 3 (three-step Boris), respectively. The solid lines show the theoretical trajectories given by $\cos \omega_c^* t$. The exact trajectory given by $\cos \omega_c t$ is also shown by the dotted lines as a reference.

The approximated gyration angle for one time step $\omega_c^* \Delta t$ as a function of $\omega_c \Delta t$ and the corresponding error $\varepsilon = (\omega_c - \omega_c^*)/\omega_c$ for the proposed scheme is shown in Fig.2. Both of the standard two-step Boris integrator and the proposed three-step integrator have the second-order accuracy in time for a small time step ($\omega_c \Delta t \ll 1$) due to the central time difference in Eq.(3b). For a larger time step ($\omega_c \Delta t > 1$), the numerical error of the proposed scheme is smaller than that of the standard Boris scheme. One can also see that Schemes 2 and 3 have the same accuracy theoretically.

3. Numerical Test and Discussion

In the present study, we check the consistency between the numerical procedures shown in Eq.(9) and the theoretical approximation shown in Eq.(10) by a simple numerical test as follows. We use a constant (i.e., time-independent) magnetic field $\boldsymbol{B}$ given by random numbers ($0 \le R \le 1$). Then, the magnitude of the magnetic field is normalized to unity. We also initiate the velocity vector $\boldsymbol{v}$ by a different set of random numbers. We define one of velocity components perpendicular to the magnetic field as,

$$\boldsymbol{v}_{\perp 1}^{t=0} \equiv \boldsymbol{v}^{t=0} - \left(\boldsymbol{v}^{t=0} \cdot \frac{\boldsymbol{B}}{|\boldsymbol{B}|}\right) \frac{\boldsymbol{B}}{|\boldsymbol{B}|}, \tag{11}$$

where $|\boldsymbol{B}| = 1$ in the present numerical test.

Figure 3 shows the time evolution of one of the perpendicular velocity components $v_{\perp 1}^{t}$ calculated by $v_{\perp 1}^{t} = \boldsymbol{v}_{\perp 1}^{t=0} \cdot \boldsymbol{v}^{t}/|\boldsymbol{v}^{t}|$. We change the time step as $\omega_c \Delta t = \pi/6$, $\pi/3$, and $\pi/2$, which correspond to the gyration angle for one time step of 30°, 60°, and 90°, respectively, in the velocity space. The circle, cross, and square marks correspond to the result with Scheme 1 (standard two-step Boris), Scheme 2 (standard Boris twice with a half time step), and Scheme 3 (three-step Boris), respectively. The solid lines show the theoretical trajectories given by $\cos \omega_c^* t$. The exact trajectory given by $\cos \omega_c t$ is also shown by the dotted lines as a reference. The result shows that the marks are well on the solid lines, suggesting that the numerical solutions to the Lorentz force equations are in excellent agreement with the theoretical time development of the velocity component. The numerical test also confirmed that Scheme 3 gives the exactly same result as Scheme 2.

Proof. Inserting Eqs.(8b) and (8c) into Eq.(8d), we obtain

$$\boldsymbol{u}^+ = \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^{\tau_1} \times \boldsymbol{B}^\gamma)\frac{\Delta t}{2} + \frac{q}{m}\beta_2(\boldsymbol{u}^{t_0} \times \boldsymbol{B}^\gamma)\frac{\Delta t}{2} + \frac{q^2}{m^2}\beta_2 \left\{(\boldsymbol{u}^{t_0} \times \boldsymbol{B}^\gamma) \times \boldsymbol{B}^\gamma\right\} \frac{\Delta t^2}{8}$$

$$= \boldsymbol{u}^- + \frac{q}{m}(\boldsymbol{u}^\tau \times \boldsymbol{B}^\gamma)\Delta t + \frac{q^2}{m^2}\beta_2 \left[\left\{\left(\frac{\boldsymbol{u}^-}{2} + \frac{\boldsymbol{u}^{t_0}}{2} - \boldsymbol{u}^{\tau_1}\right) \times \boldsymbol{B}^\gamma\right\} \times \boldsymbol{B}^\gamma\right] \frac{\Delta t^2}{4} \tag{12}$$

It is obvious from Fig.1 that $2\boldsymbol{u}^{\tau_1} = \boldsymbol{u}^- + \boldsymbol{u}^{t_0}$. Hence, Eq.(12) corresponds to Eq.(9d).

We also measured the computational time. We solved the Lorentz force equation with 10,000 particles and 10,000 time steps on a single core of an Intel Xeon E5-2697 v4 processor. The elapse times with Schemes 1, 2, and 3 are 0.13684 sec, 0.26598 sec, and 0.17131 sec, respectively. Hence, the speed up from Scheme 2 to Scheme 3 is a factor of 1.55.

4. Conclusion

We have developed a three-step Boris integrator for solving the Lorentz force equation of charged particle motion. The proposed scheme solves the Lorentz force equation with a higher accuracy than the standard Boris integrator for a large $\omega_c\Delta t > 1$, although the proposed scheme has the same second-order accuracy in time with the standard one for a small $\omega_c\Delta t \ll 1$. It is confirmed by both of numerical test and theoretical analysis that the proposed three-step scheme has the same accuracy as the standard (two-step) Boris integrator with a half time step. The computational cost of the proposed scheme is about 65% cheaper than that of the standard Boris integrator.

It should be noted that hybrid PIC simulations use a typical time step of $\omega_{ci}\Delta t \sim 0.1$, whose accuracy of the standard Boris integrator is high enough (with an error of 0.1%) and the benefit of the proposed scheme is small. Full PIC simulations also use a typical time step of $\omega_{pe}\Delta t \sim 0.1$. The proposed scheme may has a merit for strongly magnetized plasma of $\omega_{ce} \gg \omega_{pe}$.

In conclusion, this paper gives an idea to improve the accuracy of the Boris integrator for the Lorentz force equation by increasing the number of steps. The development of Boris integrators with more steps is left as a future study.

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