The Particle Pushers for Electromagnetic Fields

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Outline

Classic Boris Pusher
Analytic Boris Pusher
Exact Analytic Pusher

One of the most important and long-lived algorithms in plasma physics is the Boris algorithm for solving the relativistic equations of motion for charged particles in electromagnetic fields. It has been in use in Particle-in-Cell (PIC) simulations for more than 50 years. It solves the equations:

$$\frac{d\mathbf{u}}{dt} = \frac{q}{m}\left[\mathbf{E} + \mathbf{v} \times \frac{\mathbf{B}}{c}\right] \text{ and } \frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{1.}$$

where:

$$\mathbf{u} = \gamma\mathbf{v} \text{ and } \gamma = \sqrt{1 + \mathbf{u}\cdot\mathbf{u}/c^2} \tag{2.}$$

Boris algorithm approximates eqn (1) with a finite-difference form:

$$\frac{\mathbf{u}(\Delta t) - \mathbf{u}(0)}{\Delta t} = \tilde{\mathbf{E}} + \left[\frac{\mathbf{v}(\Delta t) + \mathbf{v}(0)}{2}\right] \times \mathbf{\Omega} \tag{3.}$$

where:

$$\tilde{\mathbf{E}} = \frac{q\mathbf{E}}{m} \text{ and } \mathbf{\Omega} = \frac{q\mathbf{B}}{mc} \tag{4.}$$

This is an implicit equation.

The Boris algorithm assumes that γ and the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ are constant during a time step Δt.

J. P. Boris, 4th Conf. Numerical Simulation of Plasmas, 1970
O. Buneman, J. Computational Phys. 1, 517 (1967)

The Boris solution uses a time-splitting scheme with 4 parts:

First, the particle is accelerated half a time step with the electric field $\tilde{\mathbf{E}}$ only:

$$\mathbf{u1} = \mathbf{u}(0) + \tilde{\mathbf{E}}\frac{\Delta \mathrm{t}}{2} \tag{5.}$$

Second, the γ factor is calculated:

$$\gamma_\mathrm{B} = \sqrt{1 + \mathbf{u1} \cdot \mathbf{u1}/\mathrm{c}^{\mathbf{2}}} \tag{6.}$$

Third, the particle is rotated with the magnetic field $\mathbf{B}$ only using the equation:

$$\mathbf{u2} = \mathbf{u1} + \frac{\Delta \mathrm{t}}{2\gamma_\mathrm{B}}(\mathbf{u1} + \mathbf{u2}) \times \boldsymbol{\Omega} \tag{7.}$$

This implicit equation can be solved for **u2** by inverting a 3x3 matrix. The result can be written in the following vector form:

$$\mathbf{u2} = \left\{\mathbf{u1}\left[\mathbf{1} - \left(\frac{\Omega \Delta \mathrm{t}}{2\gamma_\mathrm{B}}\right)^{\mathbf{2}}\right] + \frac{\mathbf{u1} \times \boldsymbol{\Omega}\Delta \mathrm{t}}{\gamma_\mathrm{B}} + \frac{1}{2}\left(\frac{\Delta \mathrm{t}}{\gamma_\mathrm{B}}\right)^2 (\mathbf{u1} \cdot \boldsymbol{\Omega})\boldsymbol{\Omega}\right\} \Big/ \left[\mathbf{1} + \left(\frac{\Omega \Delta \mathrm{t}}{2\gamma_\mathrm{B}}\right)^{\mathbf{2}}\right] \tag{8.}$$

Finally, the particle is accelerated another half a time step with the electric field $\tilde{\mathbf{E}}$ only:

$$\mathbf{u}(\Delta \mathrm{t}) = \mathbf{u2} + \tilde{\mathbf{E}}\frac{\Delta \mathrm{t}}{2} \tag{9.}$$

The rotation can be made more exact by replacing

$$\frac{\Delta \mathrm{t}}{2} \rightarrow \frac{\gamma_\mathrm{B}}{\Omega}\tan\left(\frac{\Omega \Delta \mathrm{t}}{2\gamma_\mathrm{B}}\right) \tag{10.}$$

This replacement improves the accuracy of the rotation, it does not improve the overall accuracy very much and is rarely used.

One reason the Boris algorithm has been so successful is that it is area preserving and therefore energy errors are bounded. But it does have flaws.

One such flaw occurs when the initial velocity is the **ExB** drift.

If $\mathbf{v} = \mathbf{v_E} = \frac{\tilde{\mathbf{E}}\times\mathbf{\Omega}}{\Omega^2}$ and $\tilde{\mathbf{E}} \cdot \mathbf{\Omega} = 0$ then $\mathbf{v_E} \times \mathbf{\Omega} = -\tilde{\mathbf{E}}$ and eqn (1) results in $\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} = 0$.

The particle should move with constant velocity without rotation. The Boris pusher does not give the correct result in this case.

The source of the error: calculation of γ_{B} neglects magnetic forces. In this special case, the electric and magnetic forces cancel each other out.

A number of solutions have been proposed to correct this flaw.

A. V. Higuera and J. R. Cary, Physics of Plasmas, 24, 052104 (2017)

The equation of motion where γ and $\mathbf{E}$ and $\mathbf{B}$ are constant can be described by the approximate equation:

$$\frac{d\mathbf{u}}{dt} = \tilde{\mathbf{E}} + \mathbf{u} \times \frac{\boldsymbol{\Omega}}{\gamma_a} \tag{11.}$$

where the symbol γ_a represents some average value of γ to be determined later.

Separating eqn (11) into components parallel and perpendicular to $\boldsymbol{\Omega}$, one obtains:

$$\frac{d\mathbf{u}_{\parallel}}{dt} = \tilde{\mathbf{E}}_{\parallel} \tag{12.}$$

where $\tilde{\mathbf{E}}_{\parallel} = (\tilde{\mathbf{E}} \cdot \widehat{\Omega})\widehat{\Omega}$ and $\mathbf{u}_{\parallel} = (\mathbf{u} \cdot \widehat{\Omega})\widehat{\Omega}$ and $\widehat{\Omega} = \frac{\boldsymbol{\Omega}}{\Omega}$,

$$\frac{d\mathbf{u}_{\perp}}{dt} = \tilde{\mathbf{E}}_{\perp} + \mathbf{u} \times \frac{\boldsymbol{\Omega}}{\gamma_a} \tag{13.}$$

where $\mathbf{E}_{\perp} = \mathbf{E} - \mathbf{E}_{\parallel}$ and $\mathbf{u}_{\perp} = \mathbf{u} - \mathbf{u}_{\parallel}$.

The analytic solutions are:

$$\mathbf{u}_{\parallel}(t) = \mathbf{u}_{\parallel}(0) + \tilde{\mathbf{E}}_{\parallel} t \tag{14.}$$

$$\mathbf{u}_{\perp}(t) = [\mathbf{u}_{\perp}(0) - \gamma_a \mathbf{v}_E]\cos\left(\frac{\Omega t}{\gamma_a}\right) + \frac{1}{\Omega}[\mathbf{u}_{\perp}(0) \times \boldsymbol{\Omega} + \gamma_a \tilde{\mathbf{E}}_{\perp}]\sin\left(\frac{\Omega t}{\gamma_a}\right) + \gamma_a \mathbf{v}_E \tag{15.}$$

This solution can be verified by substituting these expressions into the equation of motion (eqn 11). It is valid only if the change in γ_a between two time steps is small.

V. K. Decyk, W. B. Mori, and F. Li, Computer Physics Comm. 282, 108559 (2023)

The average value of γ we need is given by:

$$\frac{1}{\gamma_a} = \frac{1}{\Delta t}\int_0^{\Delta t} \frac{dt'}{\gamma(t')} \tag{16.}$$

This is related to the definition of proper time τ

$$\frac{d\tau}{dt} = \frac{1}{\gamma} \Rightarrow \Delta\tau = \int_0^{\Delta t} \frac{dt'}{\gamma(t')} \Rightarrow \frac{1}{\gamma_a} = \frac{\Delta\tau}{\Delta t} \tag{17.}$$

An expression for γ can be found by substituting the solution of the equations of motion eqns (14-15) into eqn (18):

$$\gamma^2 = 1 + \mathbf{u}\cdot\mathbf{u}/c^2 \tag{18.}$$

Since $\mathbf{u}$ depends on γ_a, one needs to iterate to find the roots of eqn (19):

$$\frac{1}{\gamma_a} - \frac{1}{\Delta t}\int_0^{\Delta t} \frac{dt'}{\sqrt{\gamma^2(t')}} = 0 \tag{19.}$$

Calculating γ_a exactly is difficult, but may not be necessary, since eqn (11) is already an approximation. I will discuss an approximate scheme to calculate γ_a later.

One can express this analytic solution as a split-time scheme:

First, calculate γ_a by averaging $\gamma(t)$ as described later, a significant change from the classic Boris algorithm.

Second, accelerate the particle a half time step as follows:

$$\mathbf{u1}' = \mathbf{u(0)} + \tilde{\mathbf{E}}_{\parallel}\frac{\Delta t}{2} + \frac{\gamma_a}{\Omega}\tilde{\mathbf{E}}_{\perp}\tan\left(\frac{\Omega\Delta t}{2\gamma_a}\right) \qquad (20.)$$

Third, rotate the particle with the magnetic field **B** using the equation:

$$\mathbf{u2}' = \mathbf{u1}'\cos\left(\frac{\Omega\Delta t}{\gamma_a}\right) + \frac{\mathbf{u1}'\times\mathbf{\Omega}}{\Omega}\sin\left(\frac{\Omega\Delta t}{\gamma_a}\right) + \left[1-\cos\left(\frac{\Omega\Delta t}{\gamma_a}\right)\right]\frac{(\mathbf{u1}'\cdot\mathbf{\Omega})\mathbf{\Omega}}{\Omega^2} \qquad (21.)$$

Finally, the particle is accelerated another half time step:

$$\mathbf{u}(\Delta t) = \mathbf{u2}' + \tilde{\mathbf{E}}_{\parallel}\frac{\Delta t}{2} + \frac{\gamma_a}{\Omega}\tilde{\mathbf{E}}_{\perp}\tan\left(\frac{\Omega\Delta t}{2\gamma_a}\right) \qquad (22.)$$

Note that the half acceleration perpendicular to **B**, eqns (20,22), is treated differently than in the classic Boris algorithm, eqns (5,9). Here the **E** field must be decomposed into components parallel and perpendicular to the magnetic field.

For the position one uses the same leap-frog as classic Boris:

$$x(t+\Delta t) = x(0) + v\left(t+\frac{\Delta t}{2}\right)\Delta t \qquad (23.)$$

By making use of the identities:

$$\sin(2\theta) = \frac{2\tan(\theta)}{1+\tan^2(\theta)} \text{ and } \cos(2\theta) = \frac{1-\tan^2(\theta)}{1+\tan^2(\theta)} \quad (24.)$$

One can rewrite the analytic rotation eqn (21) as follows:

$$\mathbf{u2}' = \mathbf{u1}'\left[1-\tan^2\left(\frac{\Omega\Delta t}{2\gamma_a}\right)\right] + \frac{\mathbf{u1}' \times \boldsymbol{\Omega}}{\Omega} 2\tan\left(\frac{\Omega\Delta t}{2\gamma_a}\right)$$

$$+2\tan^2\left(\frac{\Omega\Delta t}{2\gamma_a}\right)\frac{(\mathbf{u1}' \cdot \boldsymbol{\Omega})\boldsymbol{\Omega}}{\Omega^2} / \left[1+\tan^2\left(\frac{\Omega\Delta t}{2\gamma_a}\right)\right] (25.)$$

With the substitution

$$\tan\left(\frac{\Omega\Delta t}{2\gamma_a}\right) \to \frac{\Omega\Delta t}{2\gamma_a} \quad (26.)$$

we recover the Boris algorithm, except for $\gamma_a \to \gamma_B$.

One can also see that the Boris rotation is second order in Δt, and it is straightforward to convert an existing Boris program to the analytic scheme, except for the calculation of γ_a.

γ_B is only first order in Δt, since it neglects magnetic forces.

To find an approximation to γ_a, differentiate eqn (2) to obtain:

$$\frac{d\gamma}{dt} = \frac{1}{2\gamma c^2}\frac{d}{dt}(\mathbf{u}\cdot\mathbf{u}) = \frac{q}{\gamma m c^2}\mathbf{E}\cdot\mathbf{u} \qquad (27.)$$

Making use of $\frac{d\tau}{dt} = \frac{1}{\gamma}$, write this in terms of proper time τ:

$$\frac{d\gamma}{d\tau} = \frac{\gamma d\gamma}{dt} = \frac{1}{c^2}\tilde{\mathbf{E}}\cdot\mathbf{u} \qquad (28.)$$

Substituting the analytic momenta (eqns 14-15), gives the result:

$$\frac{d\gamma}{d\tau} = \frac{\widetilde{E}_\parallel}{c^2}\left\{u_\parallel(0) + \widetilde{E}_\parallel t\right\} + \frac{\widetilde{E}_\perp}{c^2}\left\{u_L(0)\cos\left(\frac{\Omega t}{\gamma_a}\right) + \frac{1}{\Omega}\left[\gamma_a\widetilde{E}_\perp - u_D(0)\right]\sin\left(\frac{\Omega t}{\gamma_a}\right)\right\} \quad (29.)$$

where $u_L = \mathbf{u}\cdot\widehat{E}_\perp$, $u_D = \mathbf{u}\cdot\widehat{E}_\perp\times\widehat{\Omega}$, $\widehat{E}_\perp = \frac{\mathbf{E}_\perp}{E_\perp}$ and $\widehat{\Omega} = \frac{\mathbf{\Omega}}{\Omega}$.

Then use the approximation that $t = \gamma_a\tau$. This equation is true for $t = 0$ and $t = \Delta t$ and is a very good approximation between:

$$\frac{d\gamma}{d\tau} = \frac{\widetilde{E}_\parallel}{c^2}\left\{u_\parallel(0) + \gamma_a\widetilde{E}_\parallel\tau\right\} + \frac{\widetilde{E}_\perp}{c^2}\left\{u_L(0)\cos(\Omega\tau) + \frac{1}{\Omega}\left[\gamma_a\widetilde{E}_\perp - u_D(0)\right]\sin(\Omega\tau)\right\} \quad (30.)$$

The value of γ_a comes from:

$$\gamma_a = \frac{1}{\Delta\tau}\int_0^{\Delta\tau}\gamma(\tau')d\tau' = \frac{\Delta t}{\Delta\tau} \qquad (31.)$$

The integral is done by integrating eqn (29) twice. In this expression Δt is known and $\gamma_a, \Delta\tau$ are unknown. One needs to iterate to find the roots of the equation:

$$\frac{1}{\Delta\tau}\int_0^{\Delta\tau}\gamma(\tau')d\tau' - \frac{\Delta t}{\Delta\tau} = 0 \qquad (32.)$$

One can use an initial guess of $\gamma_a = \gamma(0)$ and $\Delta\tau = \Delta t/\gamma(0)$.

The approximation is accurate to 5-7 digits, so iterating to higher precision is not needed. Usually 1 iteration is enough.

For a 2-1/2D code, the Analytic Boris pusher is about 3x slower per time step than the classic Boris Pusher. The analytic push needs 6 divides, 3 square roots, and 1 tangent. The Boris push needs 4 divides and 2 square roots.

Timings on a single Intel processor

Classic Boris Pusher	35 nsec/particle/step
Analytic Boris Pusher	100 nsec/particle/step

When would one want to use it?
• if larger time steps can be used, e.g. with strong fields
• if high accuracy is required
• debugging other codes

The Analytic pusher is time-reversible to the accuracy of γ_a.
The Boris pusher is time-reversible, even when γ_B is not correct.

Such semi-analytic methods are possible when some slowly-varying term is set to a constant, and the remainder is solved analytically.

Further details in:
V. K. Decyk, W. B. Mori, and F. Li, Computer Physics Comm. 282, 108559 (2023)

An exact analytic pusher developed by Fei Li et al. solves the equations of motion written in terms of proper time:

$$\frac{d\mathbf{u}}{d\tau} = \frac{q}{m}\left[\gamma\mathbf{E} + \mathbf{u}\times\frac{\mathbf{B}}{c}\right] \text{ and } \frac{d\mathbf{x}}{d\tau} = \mathbf{u} \qquad (33.)$$

where the electric and magnetic fields **E** and **B** are constant during a time step, but γ is allowed to vary.

In terms of orthogonal components, the equations of motion are:

$$\frac{du_{\|}}{d\tau} = \gamma\widetilde{E}_{\|} \text{ and } \frac{du_L}{d\tau} = \gamma\widetilde{E}_{\perp} - u_D\Omega \text{ and } \frac{du_D}{d\tau} = u_L\Omega \qquad (34.)$$

We also need an equation for γ:

$$g = \frac{d\gamma}{d\tau} = \frac{1}{c^2}\widetilde{\mathbf{E}}\cdot\mathbf{u} = \frac{1}{c^2}\left[\widetilde{E}_{\|}u_{\|} + \widetilde{E}_{\perp}u_L\right] \qquad (35.)$$

Taking successive derivations g results in:

$$\frac{dg}{d\tau} = \frac{1}{c^2}\left[\gamma\widetilde{E}^2 - \widetilde{E}_{\perp}\Omega u_D\right]$$

$$\frac{d^2g}{d\tau^2} = \frac{1}{c^2}\left[\widetilde{E}^2 g - \widetilde{E}_{\perp}\Omega^2 u_L\right] = \left[\frac{\widetilde{E}^2}{c^2} - \Omega^2\right]g + \frac{\widetilde{E}_{\|}\Omega^2}{c^2}u_{\|} \qquad (36.)$$

$$\frac{d^4g}{d\tau^4} + \left[\Omega^2 - \frac{\widetilde{E}^2}{c^2}\right]\frac{d^2g}{d\tau^2} - \left[\frac{\widetilde{E}_{\|}^{\,2}\Omega^2}{c^2}\right]g = 0 \qquad (37.)$$

If $g \propto e^{i\omega\tau}$ in eqn (37), one obtains the eigenfunction equation:

$$\omega^4 - \omega^2\left[\Omega^2 - \widetilde{E}^2 / c^2\right] - \Omega^2\widetilde{E}_{\|}^{\,2} / c^2 = 0 \qquad (38.)$$

F. Li, V. K. Decyk, K. G. Miller, A. Tableman, F. S. Tsung, M.Vranic, R. A. Fonseca, and W. B. Mori, .J. Computational Physics 438, 110367 (2021).

This biquadratic equation has two solutions:

$$\omega^2 = \frac{1}{2}\left\{\Omega^2 - \widetilde{E}^2/c^2 \pm \sqrt{\left[\Omega^2 - \widetilde{E}^2/c^2\right]^2 + 4\Omega^2\widetilde{E}_{\parallel}{}^2}\right\} \quad (39.)$$

The positive solution is normally oscillatory:

$$\widetilde{\Omega}^2 = \frac{1}{2}\left\{\Omega^2 - \widetilde{E}^2/c^2 + \sqrt{\left[\Omega^2 - \widetilde{E}^2/c^2\right]^2 + 4\Omega^2\widetilde{E}_{\parallel}{}^2}\right\} \quad (40.)$$

The negative solution is normally exponential:

$$\lambda^2 = \frac{1}{2}\left\{\sqrt{\left[\Omega^2 - \widetilde{E}^2/c^2\right]^2 + 4\Omega^2\widetilde{E}_{\parallel}{}^2} - \left[\Omega^2 - \widetilde{E}^2/c^2\right]\right\} \quad (41.)$$

The cyclotron frequency now depends on the electric field $\tilde{\mathbf{E}}$, and the general solution has the form:

$$g = \frac{d\gamma}{d\tau} = A\cos\left(\widetilde{\Omega}\tau\right) + B\sin\left(\widetilde{\Omega}\tau\right) + C\cosh(\lambda\tau) + D\sinh(\lambda\tau) \quad (42.)$$

$\Delta\tau$ comes from eqn (32), with $\gamma(\tau)$ the integral of eqn (42).

The general solution is complex, partly because varying γ couples $u_{\parallel}$ and u_L. But special cases are interesting.

If $\widetilde{E}_{\perp} = 0$, there are two solutions, $\omega^2 = \Omega^2,\ \omega^2 = -\frac{\widetilde{E}_{\parallel}{}^2}{c^2}$.

In proper time: $u_{\parallel}(\tau) = u_{\parallel}(0)\cosh\left(\frac{\widetilde{E}_{\parallel}\tau}{c}\right) + c\,\gamma(0)\sinh\left(\frac{\widetilde{E}_{\parallel}\tau}{c}\right)$.

In laboratory time: $u_{\parallel}(\tau) = u_{\parallel}(0) + \widetilde{E}_{\parallel}t$.

Linear time maps to hyperbolic proper time!

If $\tilde{E}_{\parallel} = 0$, there are two solutions, $\omega^2 = \Omega^2 - \tilde{E}^2/c^2$, $\omega^2 = 0$.

$$u_{\parallel}(\tau) = u_{\parallel}(0) \tag{43.}$$

$$u_L(\tau) = u_L(0)\cos(\tilde{\Omega}\tau) + \frac{1}{\tilde{\Omega}}\frac{du_L(0)}{d\tau}\sin(\tilde{\Omega}\tau) \tag{44.}$$

$$u_D(\tau) = \frac{\tilde{\Omega}}{\Omega}u_L(0)\sin(\tilde{\Omega}\tau) - \frac{1}{\Omega}\frac{du_L(0)}{d\tau}\cos(\tilde{\Omega}\tau) + \gamma(\tau)v_E \tag{45.}$$

where

$$\gamma(\tau) = \gamma(0) + \frac{\tilde{E}_{\perp}}{\tilde{\Omega}c^2}\left\{u_L(0)\sin(\tilde{\Omega}\tau) - \frac{1}{\tilde{\Omega}}\frac{du_L(0)}{d\tau}\left[\cos(\tilde{\Omega}\tau) - 1\right]\right\} \tag{46.}$$

$$\frac{1}{\Omega}\frac{du_L(0)}{d\tau} = \gamma(0)v_E - u_D(0) \text{ and } \tilde{\Omega} = \sqrt{\Omega^2 - \frac{\tilde{E}_{\perp}^2}{c^2}} \text{ if } \Omega^2 > \frac{\tilde{E}_{\perp}^2}{c^2} \tag{47.}$$

Comparing with the analytic Boris solution, the structure of the solution is the same, but the oscillation frequency Ω is modified and that γ_a has been replaced by either $\gamma(0)$ or $\gamma(\tau)$. Note $\gamma(\tau)v_E$ momentum drift oscillates, but velocity drift does not.

Timings on a single Intel processor

Classic Boris Pusher	35 nsec/particle/step
Analytic Boris Pusher	100 nsec/particle/step
Exact Analytic Pusher	175 nsec/particle/step

For small enough time steps, the Boris and Analytic Pushers should reproduce the exact results.