Numerical Plasma Basics

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1 Movement of charged particles in electromagnetic field

1.1 Boris push

1.1.1 Equations of motion

The charged particle moves in an electromagnetic field under the Lorentz force

$$\frac{d}{dt}\gamma\mathbf{v} = \frac{q}{m}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right). \tag{1}$$

In total we have to integrate the following set of equations:

$$\begin{cases} \frac{d\mathbf{x}}{dt} &= \mathbf{v} \\ \mathbf{u} &= \frac{\mathbf{v}}{\sqrt{1-v^2/c^2}} \\ \frac{d\mathbf{u}}{dt} &= \frac{q}{m}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right) \end{cases} \tag{2}$$

We wish to integrate this motion accurately and use the Boris scheme to do it.
Firstly let us rewrite the equation in simpler form

$$\begin{cases} \frac{d\mathbf{x}}{dt} &= \frac{\mathbf{u}}{\sqrt{1+u^2/c^2}} \\ \frac{d\mathbf{u}}{dt} &= \frac{q}{m}\left(\mathbf{E} + \frac{\mathbf{u}}{\sqrt{1+u^2/c^2}}\times\mathbf{B}\right) \end{cases} \tag{3}$$

This is done from inverting the relation between **u** to **v** in 2. This is shown explicitly as follows

Transforming v to u

Transforming from velocity to momentum (for unit mass) is as follows

$$
\begin{aligned}
\mathbf{u} &= \frac{\mathbf{v}}{\sqrt{1-\frac{v^2}{c^2}}} \\
u^2 &= \frac{v^2}{1-\frac{v^2}{c^2}} \\
u^2\left(1-\frac{v^2}{c^2}\right) &= v^2 \\
u^2 &= v^2\left(1+\frac{u^2}{c^2}\right) \\
v^2 &= \frac{u^2}{1+\frac{u^2}{c^2}} \\
\mathbf{v} &= \frac{\mathbf{u}}{\sqrt{1+\frac{u^2}{c^2}}}
\end{aligned}
\tag{4}
$$

And so we find that

$$
\mathbf{v}_{i+\frac{1}{2}} = \frac{\mathbf{v}_{i+1}+\mathbf{v}_i}{2} = \frac{\mathbf{u}_{i+1}}{2\sqrt{1+u_{i+1}^2/c^2}} + \frac{\mathbf{u}_i}{2\sqrt{1+u_i^2/c^2}}. \tag{5}
$$

No electric field motion

In the case there is no electric field we get an equation of the form $\frac{d\mathbf{u}}{dt} = \mathbf{u} \times \mathbf{Q}$ where $\mathbf{Q}$ is some vector with a direction which is independent of $\mathbf{u}$ (Only the magnitude is dependent). It is important to notice that

$$
\frac{d}{dt}u^2 = \frac{d}{dt}\|\mathbf{u}\|^2 = \frac{d}{dt}(\mathbf{u}\cdot\mathbf{u}) = 2\mathbf{u}\cdot\frac{d\mathbf{u}}{dt} = 2\mathbf{u}\cdot(\mathbf{u}\times\mathbf{Q}) = 0.
$$

This means the magnitude of $\mathbf{u}$ is unchanged by the dynamics and the motion is a pure rotation and so in a pure rotation $\gamma = \sqrt{1+\frac{u^2}{c^2}} = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$ is constant.

1.1.2 Discretization

We discretize the position $\mathbf{x}$ in time on half integer indexes and the velocity on integer. The equations change into:

$$
\begin{cases}
\dfrac{\mathbf{x}_{i+\frac{1}{2}}-\mathbf{x}_{i-\frac{1}{2}}}{\Delta t} = \dfrac{\mathbf{u}_i}{\sqrt{1+u_i^2/c^2}} \\
\dfrac{\mathbf{u}_{i+1}-\mathbf{u}_i}{\Delta t} = \dfrac{q}{m}\left(\mathbf{E}_{i+\frac{1}{2}} + \dfrac{\mathbf{u}_{i+\frac{1}{2}}}{\gamma_{i+\frac{1}{2}}}\times\mathbf{B}_{i+\frac{1}{2}}\right)
\end{cases}
\tag{6}
$$

Transforming away the electric field

The Boris scheme transforms the momentum variable, $\mathbf{u}$, such that the resulting equations has no electric field. The transformed variable equation is purely oscillatory and can be shown to bound the error[2].

We define the following

$$\mathbf{u}^- = \mathbf{u}_i + \frac{q}{2m}\mathbf{E}\Delta t, \tag{7}$$

$$\mathbf{u}^+ = \mathbf{u}_{i+1} - \frac{q}{2m}\mathbf{E}\Delta t. \tag{8}$$

The equation of motion 6 transforms as follows

$$\frac{\mathbf{u}^+ - \mathbf{u}^-}{\Delta t} = \frac{q}{2m\gamma_{i+\frac{1}{2}}}\left(\mathbf{u}^+ + \mathbf{u}^-\right) \times \mathbf{B}_{i+\frac{1}{2}}.$$

The equation is a dynamical equation of a pure rotation motion and so γ is constant and can take $\gamma_{i+\frac{1}{2}} = \sqrt{1 + \left(\mathbf{u}^-\right)^2 / c^2}$.

Let us write the solution of $\mathbf{u}^+$ explicitly

$$\mathbf{u}^+ - \mathbf{u}^- = \left(\mathbf{u}^+ + \mathbf{u}^-\right) \times \mathbf{A}$$

$$\mathbf{u}^+ - \mathbf{u}^- = \tilde{A}\left(\mathbf{u}^+ + \mathbf{u}^-\right)$$

$$\mathbf{u}^+ = \left(I - \tilde{A}\right)^{-1}\left(I + \tilde{A}\right)\mathbf{u}^-$$

Using the fact

$$\left(I - \tilde{A}\right)^{-1}\left(I + \tilde{A}\right) = I + \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\left(\tilde{A} + \tilde{A}^2\right),$$

We find

$$\begin{aligned}
\mathbf{u}^+ &= \left[I + \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\left(\tilde{A} + \tilde{A}^2\right)\right]\mathbf{u}^- = \\
&= \mathbf{u}^- + \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\tilde{A}\mathbf{u}^- + \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\tilde{A}^2\mathbf{u}^- = \\
&= \mathbf{u}^- + \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\mathbf{u}^- \times \mathbf{A} + \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\left(\mathbf{u}^- \times \mathbf{A}\right) \times \mathbf{A} = \\
&= \mathbf{u}^- + \mathbf{u}^- \times \mathbf{A}' + \left(\mathbf{u}^- \times \mathbf{A}\right) \times \mathbf{A}',
\end{aligned} \tag{9}$$

where

$$\mathbf{A} = \frac{q\Delta t}{2m\sqrt{1 + \left(\mathbf{u}^-\right)^2}}\mathbf{B}_i, \tag{10}$$

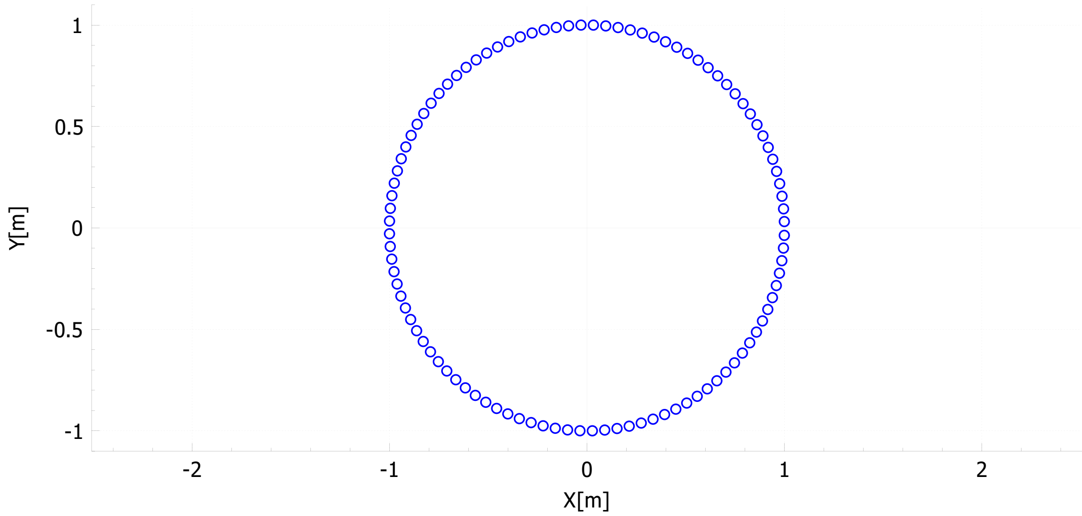
$$\mathbf{A}' = \frac{2}{1 + A_1^2 + A_2^2 + A_3^2}\mathbf{A}. \tag{11}$$

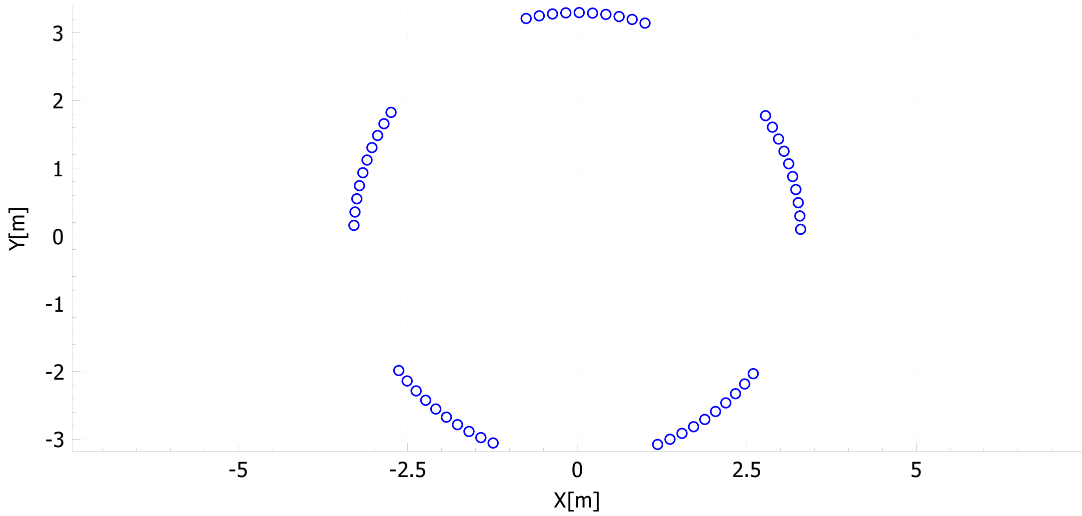
1.2 Uniform magnetic field

Cyclotron rotation period:

$$T = \frac{2\pi m}{eB} \tag{12}$$

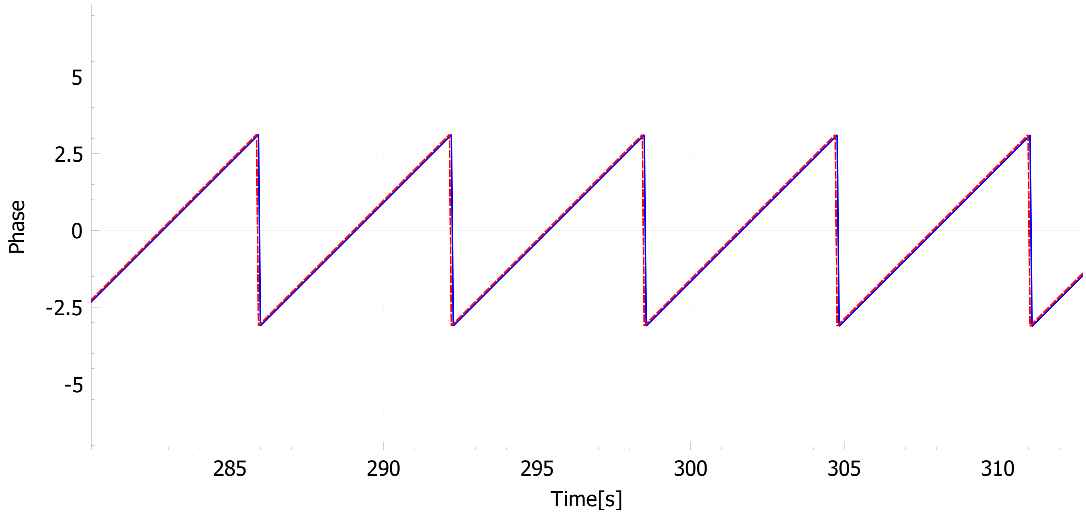
For time steps smaller than T we get a closed circle as expected. For larger than T we get non-closed time steps since each steps propagates more than 1 cycle.



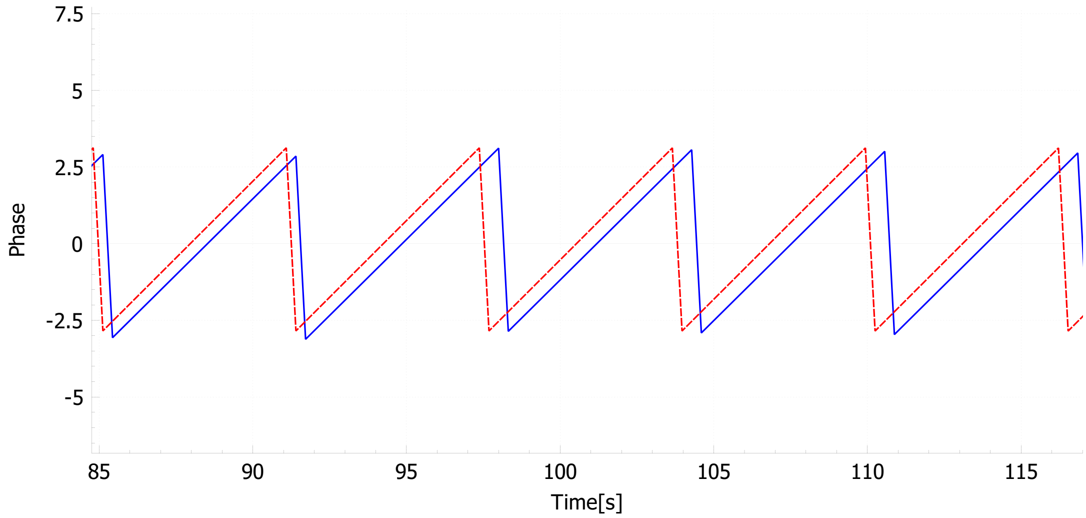


The phase error is approximated by taking $B = (0, 0, 1)$, $r = (1, 0, 0)$ and $v = (0, 1, 0)$ for $\frac{q}{m} = -1$ should have a motion around the unit circle. We normalize and take the arctan to find the phase. We plot it against the theoretical phase $\frac{t}{T}$.

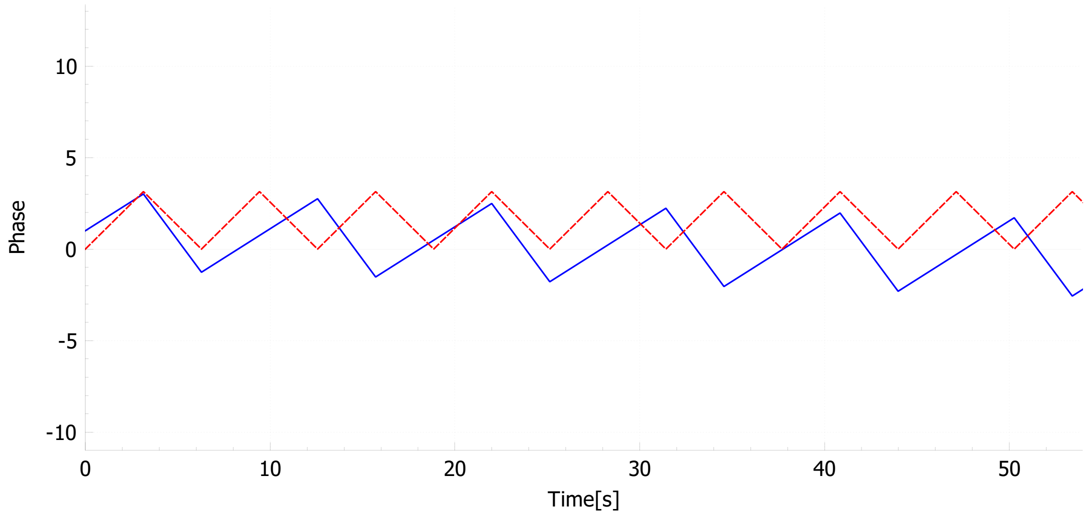
For $\Delta t = \frac{T}{100}$



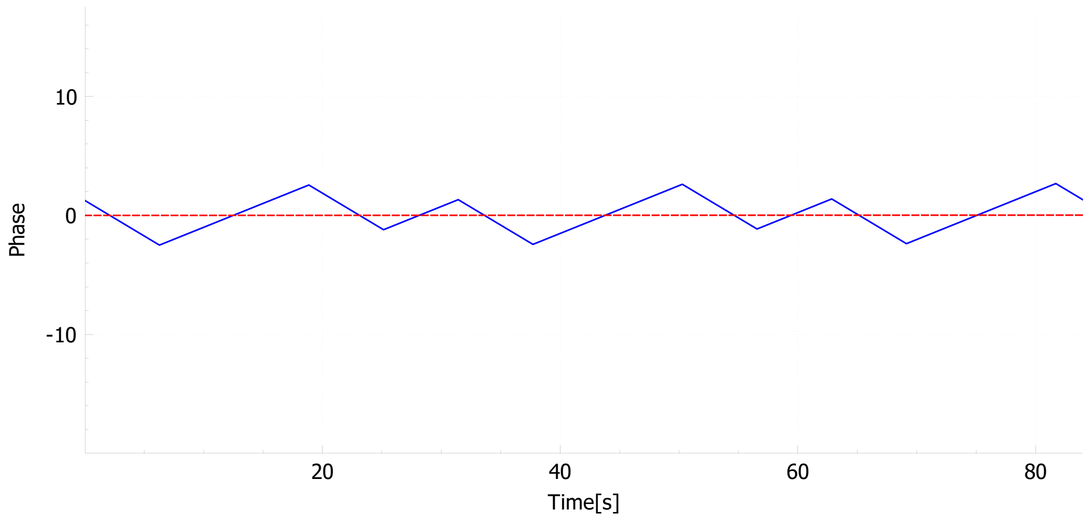
For $\Delta t = \frac{T}{50}$



For $\Delta t = \frac{T}{5}$



For $\Delta t = \frac{T}{5}$



In here the theoretical phase is 0 since each step should match the starting point due to periodicity. What we see here is purely integration errors.

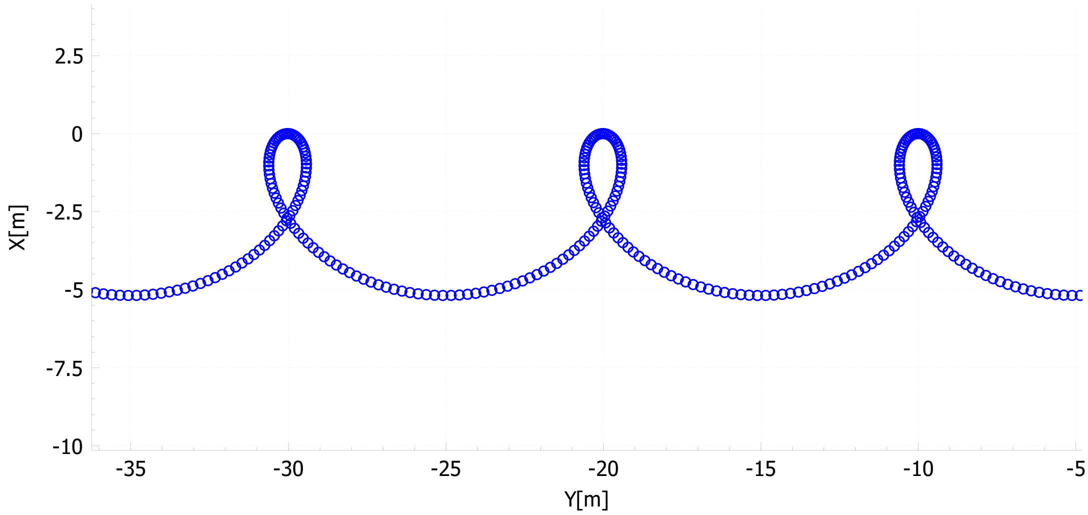
1.3 Drift velocity

Adding a constant electric field in the x direction results with a drift in the y direction. The drift velocity is given by

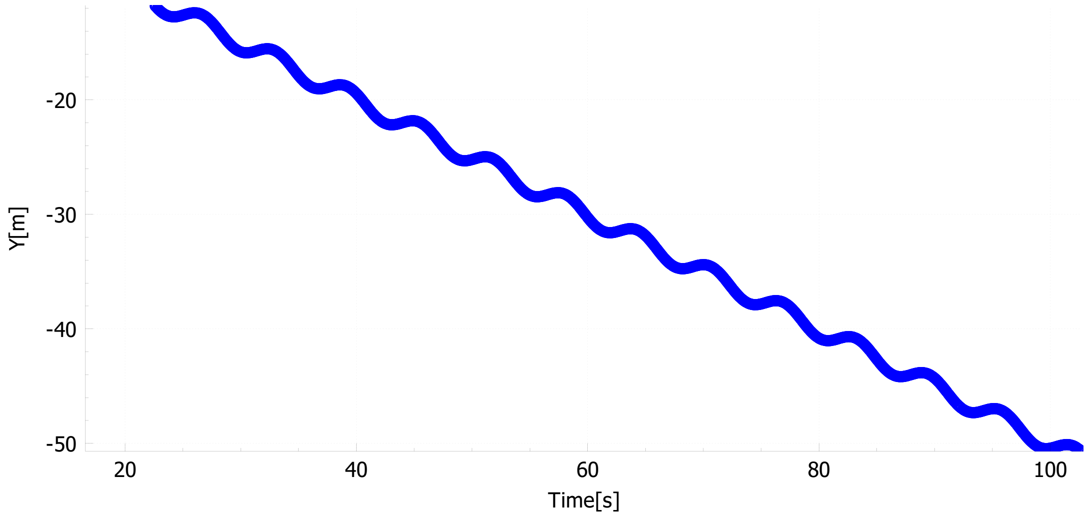
$$\mathbf{v}_d = \frac{\mathbf{E} \times \mathbf{B}}{B^2}.$$

It can be derived be verified by checking when $\mathbf{v}_{\text{total}} = \mathbf{v}_d + \mathbf{v}_r$ that $\frac{d}{dt}\mathbf{v}_{\text{total}}$ is purely oscillatory motion in the case $\gamma \approx 1$. The γ introduces a small deviation which we do not consider since we examine small velocities $v \ll c$.

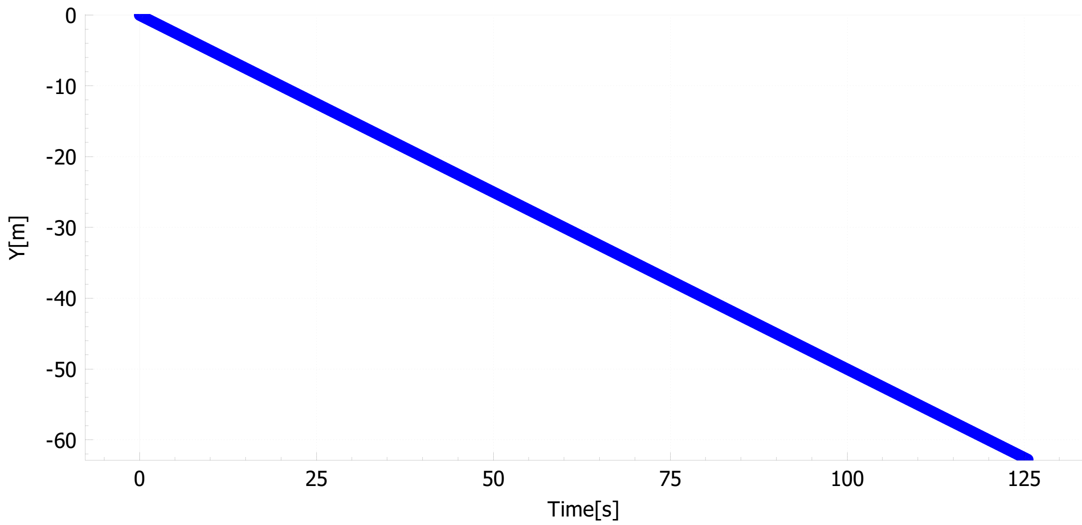
We find



We see here that drift in the y direction which oscillates around a constant velocity as expected.



Taking the initial velocity to be the drift results with a straight line motion.



Surprisingly the drift seems to be independent of the integration step and only the osculations are affected. This can be explained by that the Boris step implements a transformation removing the electric field from the equation which is similar to what the drift velocity is. The drift velocity is the velocity for which the resulting motion is purely rotational (has no electric field) with respect to it.

2 Electromagnetic Wave in 1d Vacuum

2.1 Theory

The vacuum Maxwell equations read

$$\begin{cases} \boldsymbol{\nabla} \cdot \mathbf{E} = 0, \\ \boldsymbol{\nabla} \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t}, \\ \boldsymbol{\nabla} \cdot \mathbf{B} = 0, \\ \boldsymbol{\nabla} \times \mathbf{B} = \dfrac{1}{c^2}\dfrac{\partial \mathbf{E}}{\partial t}. \end{cases}$$

We consider the 1d propagation of a wave in the z axis direction. Since the wave is perpendicular to the fields they change only in the x–y components. We focus on linearly polarized wave, the electric field oscillates in the x direction and the magnetic field in the y direction. The equations reduce into.

$$\begin{cases} \dfrac{\partial E_x}{\partial x} = 0, \\ \dfrac{\partial E_x}{\partial z} = -\dfrac{\partial B_y}{\partial t}, \\ \dfrac{\partial B_y}{\partial y} = 0, \\ -\dfrac{\partial B_y}{\partial z} = \dfrac{1}{c^2}\dfrac{\partial E_x}{\partial t}. \end{cases}$$

Since we are interested in the z axis propagation we can ignore the first and third equations. The boundary condition are periodic in the z direction with length L. We rescale B into $\tilde{B} = cB$ for simplicity. Simplification yields

$$\begin{cases} \dfrac{\partial \tilde{B}_y}{\partial t} &= -c\dfrac{\partial E_x}{\partial z}, \\ \dfrac{\partial E_x}{\partial t} &= -c\dfrac{\partial \tilde{B}_y}{\partial z}. \end{cases}$$

This 2 variable 2 first order PDEs can be solved easily using the periodic boundary condition to find that

$$\begin{cases} E_x &= A \sin\left(\dfrac{2\pi n}{L}(z \pm ct) + \varphi\right), \\ B_y &= -\dfrac{A}{c} \sin\left(\dfrac{2\pi n}{L}(z \pm ct) + \varphi\right), \end{cases}$$

where n is some integer. Let $k_n = \frac{2\pi n}{L}$ and we focus on negatively signed solutions with unit amplitude and no phase for simplicity, due to linearity and mirror symmetry this do not add more information. Those are the initial conditions used in the simulations.

2.2 Simulation

Let us now discretize the equations finding

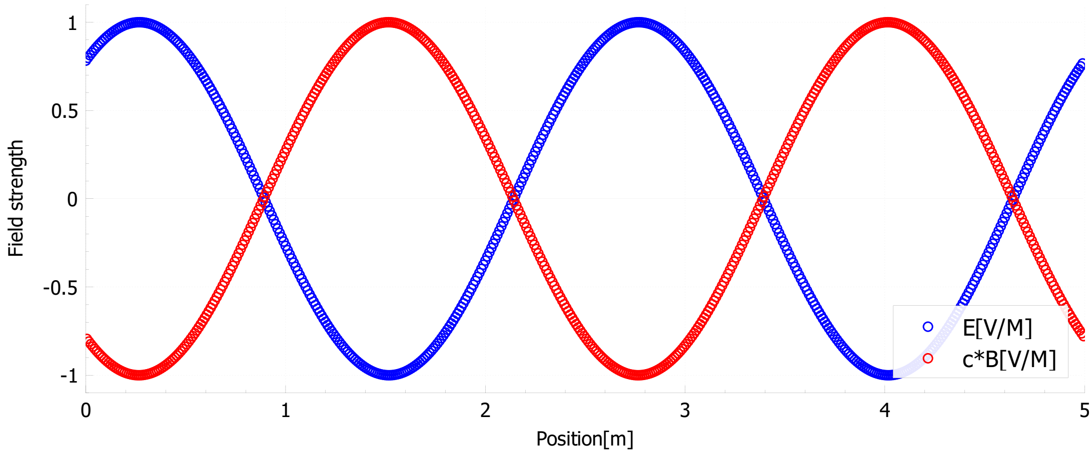
$$\begin{cases} \dfrac{B_{i+\frac{1}{2},j} - B_{i-\frac{1}{2},j}}{\Delta t} &= -c\dfrac{E_{i,j+\frac{1}{2}} - E_{i,j-\frac{1}{2}}}{\Delta z}, \\ \dfrac{E_{i+1,j+\frac{1}{2}} - E_{i,j+\frac{1}{2}}}{\Delta t} &= -c\dfrac{B_{i+\frac{1}{2},j+1} - B_{i+\frac{1}{2},j}}{\Delta z}. \end{cases}$$

Beginning with an initial condition at $i = 1$, notice we need to apply a correction depending on the time step, Δt, since the field are not defined on the same time and space positions.

We propagate the the evolution in time with

$$\begin{cases} B_{i+\frac{1}{2},j} &= B_{i-\frac{1}{2},j} - c\dfrac{\Delta t}{\Delta z}\left(E_{i,j+\frac{1}{2}} - E_{i,j-\frac{1}{2}}\right), \\ E_{i+1,j+\frac{1}{2}} &= E_{i,j+\frac{1}{2}} - c\dfrac{\Delta t}{\Delta z}\left(B_{i+\frac{1}{2},j+1} - B_{i+\frac{1}{2},j}\right). \end{cases}$$

Due to periodic time boundary conditions we simply plug in $j_{\max} + 1 = 1$ and the algorithm is set.



2.3 Dispersion relation

Let us assume the dispersion relation is not accurate in the numerics. This means the solution involves some unknown dispersion of $\omega(k)$. Let us plug in the solution

$$\begin{cases} E_x &= \sin(kz - \omega t), \\ B_y &= -\dfrac{1}{c}\sin(kz - \omega t), \end{cases}$$

into the discretesized equations. Since we assume there is a solution of this form we find an implicit relation of ω and k. Using the trigonometric identity

$$\sin\alpha - \sin\beta = 2\sin\left(\frac{\alpha-\beta}{2}\right)\cos\left(\frac{\alpha+\beta}{2}\right),$$

we find that

$$2\frac{\sin\left(\frac{\omega\Delta t}{2}\right)}{\Delta t}\cos(jk\Delta z - i\omega\Delta t) = 2c\frac{\sin\left(\frac{k\Delta z}{2}\right)}{\Delta z}\cos(k\Delta z - i\omega\Delta t).$$

This is the result from both equations and simplification yields

$$\frac{\Delta z}{\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right) = c\sin\left(\frac{k\Delta z}{2}\right).$$

Solving to find

$$\omega = \frac{2}{\Delta t}\arcsin\left(\frac{c\Delta t}{\Delta z}\sin\frac{k\Delta z}{2}\right).$$

It is clear that as $\Delta t, \Delta z \to 0$ we get $\omega = ck$. As this size get finite size we deviate from this simple dispersion. Considering first order correction the dispersion is

$$\omega = \sqrt{\frac{\Delta z}{\Delta t}c\,|k|}.$$

Taking $\frac{\Delta z}{\Delta t} \approx c$ should lower non-natural dispersion. Taking $\frac{\Delta z}{\Delta t} = c$ seems to eliminate this sort of dispersion problems. If $c > \frac{\Delta z}{\Delta t}$ this dispersion relation has no real solutions and probably our assumption that the oscillatory solution is a vacuum solution is no longer valid. This relates to stability since the wave propagates with velocity c we cannot have the wave move less than 1 cell. In our simulation we take $\Delta t = \frac{\Delta z}{2c}$, this guarantees that the dispersion has a real solution.

References

[1] C.K. Birdsall. *Plasma Physics via Computer Simulation.* CRC Press, oct 2004.

[2] Hong Qin, Shuangxi Zhang, Jianyuan Xiao, Jian Liu, Yajuan Sun, and William M. Tang. Why is Boris algorithm so good? *Physics of Plasmas*, 20(8):084503, aug 2013.

[3] Seiji Zenitani and Takayuki Umeda. On the Boris solver in particle-in-cell simulation. *Physics of Plasmas*, 25(11):112110, nov 2018.