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LASER WAKEFIELD ACCELERATION
Studies using Particle in Cell Method

Master Thesis

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Introduction

Add stuff here Tajima and Dawson 1979.

Chapter 1

Classical Electrodynamics

In order to study complex phenomena such as laser wakefield acceleration, we need to have a solid understanding of the basic physical phenomena that govern the dynamics of charged particles in interaction with electromagnetic fields. In this thesis we will restrict ourselves to classical electrodynamics, ignoring QED effects that are important for very high laser intensities $I \gtrsim 5 \times 10^{22}\,\mathrm{W\,cm^{-2}}$. We will mainly follow the ideas presented in Jackson (1999) and Eisenberg and Greiner (1978, Chapter 2).

We thus begin with Maxwell's equations in free space

$$\boldsymbol{\nabla} \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{1.1a}$$

$$\boldsymbol{\nabla} \cdot \mathbf{B} = 0 \tag{1.1b}$$

$$\boldsymbol{\nabla} \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1.1c}$$

$$\boldsymbol{\nabla} \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}\,, \tag{1.1d}$$

which relate the electromagnetic field to sources. An additional equation must be satisfied in order to ensure charge conservation

$$\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r}, t) + \frac{\partial \rho(\mathbf{r}, t)}{\partial t} = 0\,. \tag{1.2}$$

As we can see above, equations (1.1b) and (1.1c) do not involve sources and thus they state the dynamical properties of the fields. Since equations (1.1a) and (1.1d) describe how the sources influence the fields, we need an additional equation to describe how the fields affect the sources

$$\mathbf{F} = \int \mathrm{d}\mathbf{r}'\, \rho(\mathbf{r}', t)\mathbf{E}(\mathbf{r}', t) + \frac{1}{c}\int \mathrm{d}\mathbf{r}'\, \mathbf{j}(\mathbf{r}', t) \times \mathbf{B}(\mathbf{r}', t)\,.$$

Maxwell's equations (1.1) relate six field quantities ($\mathbf{E}$ and $\mathbf{B}$) to four source quantities (ρ and $\mathbf{j}$). This implies that there are some restrictions on the six quantities. This suggests that we can find a less redundant way to express the fields, and indeed the four quantities given by the vector potential $\mathbf{A}$ and scalar potential ρ provide this representation. Equation (1.1b) implies the existence of a vector potential

$$\mathbf{B}(\mathbf{r}, t) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r}, t)\,. \tag{1.3}$$

Substituting (1.3) in (1.1c) we obtain

$$\boldsymbol{\nabla} \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}\right) = 0 \tag{1.4}$$

and thus the quantity in the parenthesis can always be expressed as the gradient of a scalar field, namely the scalar potential

$$\boldsymbol{\nabla}\phi(\mathbf{r},t) = -\mathbf{E}(\mathbf{r},t) - \frac{\partial \mathbf{A}}{\partial t}\,.$$

With these considerations equation (1.1a) becomes

$$\boldsymbol{\nabla}\cdot\left(\boldsymbol{\nabla}\phi + \frac{\partial \mathbf{A}}{\partial t}\right) = -\frac{\rho}{\varepsilon_0}$$

or

$$\nabla^2\phi + \frac{\partial}{\partial t}\boldsymbol{\nabla}\cdot\mathbf{A} = -\frac{\rho}{\varepsilon_0} \tag{1.5}$$

and equation (1.1d)

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{A}) = \mu_0\mathbf{j} - \frac{1}{c^2}\frac{\partial}{\partial t}\left(\boldsymbol{\nabla}\phi + \frac{\partial \mathbf{A}}{\partial t}\right)\,. \tag{1.6}$$

Using the following vector identity

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{A}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{A}) - \nabla^2\mathbf{A}\,, \tag{1.7}$$

equation (1.6) becomes

$$\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{A}) - \nabla^2\mathbf{A} = \mu_0\mathbf{j} - \frac{1}{c^2}\left(\boldsymbol{\nabla}\frac{\partial\phi}{\partial t} + \frac{\partial^2\mathbf{A}}{\partial t^2}\right)$$

or

$$\nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} = -\mu_0\mathbf{j} + \boldsymbol{\nabla}\left(\boldsymbol{\nabla}\cdot\mathbf{A} + \frac{1}{c^2}\frac{\partial\phi}{\partial t}\right)\,. \tag{1.8}$$

Equations (1.5) and (1.8) were obtained by substituting the potentials obtained from the source-less equations, (1.1b) and (1.1c), into the ones with sources, (1.1a) and (1.1d). They are thus fully equivalent with Maxwell's equations (1.1) and, as we can observe, relate the four quantities given by the potentials to the four quantities for the sources. They also preserve the invariance under Lorentz transformations, with the scalar potential ϕ as the time-like component.

Equations (1.5) and (1.8) can be simplified by decoupling the potentials. This is possible due to the fact that potentials are not unique. To illustrate this point consider

$$\mathbf{A}'(\mathbf{r},t) = \mathbf{A}(\mathbf{r},t) + \boldsymbol{\nabla}\Lambda(\mathbf{r},t)\,.$$

This vector potential gives rise to a magnetic field

$$\boldsymbol{\nabla}\times\mathbf{A}' = \boldsymbol{\nabla}\times\mathbf{A} + \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\Lambda) = \boldsymbol{\nabla}\times\mathbf{A} = \mathbf{B}$$

equal with the original one since $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\varphi) = 0$.

Similarly, for a scalar potential

$$\phi'(\mathbf{r},t) = \phi(\mathbf{r},t) - \frac{\partial\Lambda(\mathbf{r},t)}{\partial t}$$

and the corresponding electric field will be

$$-\boldsymbol{\nabla}\phi' - \frac{\partial\mathbf{A}'}{\partial t} = -\boldsymbol{\nabla}\phi + \boldsymbol{\nabla}\frac{\partial\Lambda}{\partial t} - \frac{\partial\mathbf{A}}{\partial t} - \frac{\partial}{\partial t}\boldsymbol{\nabla}\Lambda = -\boldsymbol{\nabla}\phi - \frac{\partial\mathbf{A}}{\partial t} = \mathbf{E}\,,$$

since the spatial and temporal derivatives commute. These kinds of transformations are called gauge transformations.

1.1 Gauge transformations

The freedom of choosing the gauge leads to the following condition satisfied by the scalar and vector potentials

$$\boldsymbol{\nabla}\cdot\mathbf{A}+\frac{1}{c^2}\frac{\partial\phi}{\partial t}=0\,,$$

called the Lorenz condition.

Indeed, if we consider a set of potentials $\mathbf{A}$ and ϕ that don't satisfy the condition

$$\boldsymbol{\nabla}\cdot\mathbf{A}+\frac{1}{c^2}\frac{\partial\phi}{\partial t}\neq 0=f(\mathbf{r},t)\,,$$

then we can always carry out a gauge transformation to a new set of potentials $\mathbf{A}'$ and ϕ' that satisfy the Lorenz condition, such that

$$\begin{aligned}\boldsymbol{\nabla}\cdot\mathbf{A}+\frac{1}{c^2}\frac{\partial\phi}{\partial t}&=\boldsymbol{\nabla}\cdot(\mathbf{A}'-\boldsymbol{\nabla}\Lambda)+\frac{1}{c^2}\frac{\partial}{\partial t}\left(\phi'+\frac{\partial\Lambda}{\partial t}\right)\\&=\boldsymbol{\nabla}\cdot\mathbf{A}'-\nabla^2\Lambda+\frac{1}{c^2}\frac{\partial\phi'}{\partial t}+\frac{1}{c^2}\frac{\partial^2\Lambda}{\partial t^2}=f(\mathbf{r},t)\end{aligned}$$

or

$$\boldsymbol{\nabla}\cdot\mathbf{A}+\frac{1}{c^2}\frac{\partial\phi}{\partial t}=\Box\,\Lambda\equiv\frac{1}{c^2}\frac{\partial^2\Lambda}{\partial t^2}-\nabla^2\Lambda=f(\mathbf{r},t)\,,$$

where the d'Alambertian operator is defined as

$$\Box\equiv\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\nabla^2$$

when choosing the Minkowski metric $(+,-,-,-)$ and

$$\boldsymbol{\nabla}\cdot\mathbf{A}'+\frac{1}{c^2}\frac{\partial\phi'}{\partial t}=0\,,$$

since they satisfy the Lorenz condition. The transformation we need is thus defined by the solution of $\Box\,\Lambda=f$.

Imposing the Lorenz condition on equations (1.5) and (1.4) decouples the potentials

$$\begin{aligned}\nabla^2\phi-\frac{\partial}{\partial t}\frac{1}{c^2}\frac{\partial\phi}{\partial t}&=-\frac{\rho}{\varepsilon_0}\\\nabla^2\mathbf{A}-\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2}&=-\mu_0\mathbf{j}\end{aligned}$$

yielding the simplified form of Maxwell's equations

$$\begin{aligned}\Box\,\phi&=\frac{\rho}{\varepsilon_0}\\\Box\,\mathbf{A}&=\mu_0\mathbf{j}\,.\end{aligned}$$

This form of Maxwell's equations preserves Lorentz invariance, as the Lorenz gauge condition can be expressed in a covariant way as the contraction of the four-vector $A\equiv(\frac{\phi}{c},\mathbf{A})$ with the four-gradient $(\frac{1}{c}\frac{\partial}{\partial t},-\boldsymbol{\nabla})$.

Since the Lorenz condition doesn't fix the gauge, but only restricts us to transformations with $\Box\,\Lambda=0$, we can impose further conditions in order to fix the gauge, but in general those will not be covariant. One such condition is given by the Coulomb gauge

$$\boldsymbol{\nabla}\cdot\mathbf{A}=0. \tag{1.9}$$

In this gauge equation (1.5) becomes a Poisson equation for the scalar potential

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0} \tag{1.10}$$

with the solution given by the instantaneous Coulomb potential of the charge density in the domain $\rho(\mathbf{r}, t)$

$$\phi(\mathbf{r}, t) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' \ , \tag{1.11}$$

explaining the name of the condition (1.9).

An apparent violation of special relativity shows up in the above result which states that the scalar potential (at time t) is given by the instantaneous Coulomb interactions between charges (also at time t). The contradiction is only apparent and stems from the act that the Coulomb gauge is not Lorentz invariant.

In order to resolve the contradiction we first note that we can only observe the electric field

$$\mathbf{E}(\mathbf{r}, t) = -\boldsymbol{\nabla}\phi(\mathbf{r}, t) - \frac{\partial \mathbf{A}(\mathbf{r}, t)}{\partial t} \, .$$

Thus, the instantaneous propagation is removed by the time derivative of the vector potential.

In the Coulomb gauge, the vector potential is given by

$$\Box\, \mathbf{A} = \mu_0 \mathbf{j} - \frac{1}{c^2} \boldsymbol{\nabla} \frac{\partial \phi}{\partial t} \, . \tag{1.12}$$

Considering the continuity equation (1.2) and the form of the scalar potential in equation (1.11), the second term in equation (1.12) becomes

$$\boldsymbol{\nabla} \frac{\partial \phi}{\partial t} = \boldsymbol{\nabla} \frac{1}{4\pi\varepsilon_0} \int \frac{\frac{\partial \rho}{\partial t}}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' = -\frac{1}{4\pi\varepsilon_0} \boldsymbol{\nabla} \int \frac{\boldsymbol{\nabla}' \cdot \mathbf{j}(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' \ , \tag{1.13}$$

where $\boldsymbol{\nabla}'$ denotes the derivatives with respect to $\mathbf{r}'$. Using the Helmholtz decomposition we can write any sufficiently well behaved vector (the current density in this particular case) as the sum of a divergence-free (transversal) component and a curl-free (longitudinal) one:

$$\mathbf{j} = \mathbf{j}^t + \mathbf{j}^l \, ,$$

where

$$\begin{aligned} \boldsymbol{\nabla} \cdot \mathbf{j}^t &= 0 \\ \boldsymbol{\nabla} \times \mathbf{j}^l &= 0 \, . \end{aligned}$$

Using the vector identity (1.7) and

$$\nabla^2 \frac{1}{|\mathbf{r} - \mathbf{r}'|} = -4\pi\delta(\mathbf{r} - \mathbf{r}')$$

we can write the current density as follows

$$\begin{aligned} \nabla^2 \left(\mathbf{j}^t + \mathbf{j}^l\right) &= \boldsymbol{\nabla}\left(\boldsymbol{\nabla} \cdot \mathbf{j}^l\right) - \boldsymbol{\nabla} \times \left(\boldsymbol{\nabla} \times \mathbf{j}^t\right) \\ \int \frac{\nabla^2 \mathbf{j}}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r} &= \int \frac{\boldsymbol{\nabla}\left(\boldsymbol{\nabla} \cdot \mathbf{j}^l\right)}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' - \int \frac{\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{j}^t)}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' \\ -4\pi \mathbf{j} &= \boldsymbol{\nabla} \int \frac{\boldsymbol{\nabla} \cdot \mathbf{j}^l}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' - \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \int \frac{\mathbf{j}^{\mathbf{t}}}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}\mathbf{r}' \end{aligned}$$

and thus we obtain the two components as

$$\mathbf{j}^t = \frac{1}{4\pi}\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\int\frac{\mathbf{j}(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}'$$
$$\mathbf{j}^l = -\frac{1}{4\pi}\boldsymbol{\nabla}\int\frac{\boldsymbol{\nabla}'\cdot\mathbf{j}(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}'\ .$$

Comparing with equation (1.13) we see that

$$\frac{1}{c^2}\boldsymbol{\nabla}\frac{\partial\phi}{\partial t} = \frac{\varepsilon_0}{c^2}\mathbf{j}^l = \mu_0\mathbf{j}^l$$

and thus the source term in equation (1.12) can be expressed as function of the transverse current:

$$\Box\,\mathbf{A} = \mu_0(\mathbf{j}-\mathbf{j}^l) = \mu_0\mathbf{j}^t$$

and this also why the Coulomb gauge is also called the transverse gauge. This gauge is useful when no sources are present. In this case $\phi = 0$, $\mathbf{A}$ satisfies the homogeneous wave equation and the fields can be expressed only as function of the vector potential

$$\mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t}$$
$$\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}\,.$$

1.2 The Poynting theorem

In order to complete the description of the interaction between fields and sources, we will now focus on how the fields affect the particles. We begin by considering the force acting on a charge q

$$\mathbf{F} = q\mathbf{E} + q\mathbf{v}\times\mathbf{B}\,.$$

The corresponding infinitezimal variation of the force is given by

$$\delta\mathbf{F} = \rho\mathbf{E}\,\delta V + \mathbf{j}\times\mathbf{B}\,\delta V = (\rho\mathbf{E}+\mathbf{j}\times\mathbf{B})\,\delta V \equiv f\,\delta V\,,$$

where $f = \rho\mathbf{E}+\mathbf{j}\times\mathbf{B}$ is the Lorentz force density. We can now consider a uniform charge distribution characterized by ρ. For an infinitezimal volume δV of this charge distribution, the rate of change of the work, or the power given by the fields is given by

$$\mathbf{v}\cdot\mathbf{F} = \rho\mathbf{v}\mathbf{E} + \frac{\mathbf{j}}{q}\cdot(\mathbf{j}\times\mathbf{B}) = \rho\mathbf{v}\mathbf{E}\,.$$

As we can see above, the magnetic force doesn't contribute to the work done by the fields. Thus, the power transferred from the fields to the charges in a finite domain $\mathscr{D}$ is

$$\int_{\mathscr{D}}\mathbf{j}\cdot\mathbf{E}\,\mathrm{d}\mathbf{r}\ .$$

For the energy to conserve, this power must be balanced by a corresponding rate of decrease of energy in the electromagnetic field. Using the Ampère law (1.1d)

$$\int_{\mathscr{D}}\mathbf{j}\cdot\mathbf{E}\,\mathrm{d}\mathbf{r} = \int_{\mathscr{D}}\mathbf{E}\cdot\frac{1}{\mu_0}\left(\boldsymbol{\nabla}\times\mathbf{B}-\frac{1}{c^2}\frac{\partial\mathbf{E}}{\partial t}\right)\mathrm{d}\mathbf{r} = \frac{1}{\mu_0}\int_{\mathscr{D}}\left[\mathbf{E}\cdot(\boldsymbol{\nabla}\times\mathbf{B})-\frac{1}{c^2}\mathbf{E}\cdot\frac{\partial\mathbf{E}}{\partial t}\right]\mathrm{d}\mathbf{r}$$

Using the following vector identity

$$\boldsymbol{\nabla}\cdot(\mathbf{E}\times\mathbf{B}) = \mathbf{B}\cdot(\boldsymbol{\nabla}\times E) - \mathbf{E}\cdot(\boldsymbol{\nabla}\times\mathbf{B})$$

we can express $\mathbf{E}\cdot(\boldsymbol{\nabla}\times\mathbf{B})$ as

$$\mathbf{E}\cdot(\boldsymbol{\nabla}\times\mathbf{B}) = \mathbf{B}\cdot(\boldsymbol{\nabla}\times E) - \boldsymbol{\nabla}\cdot(\mathbf{E}\times\mathbf{B}) = -\mathbf{B}\cdot\frac{\partial\mathbf{B}}{\partial t} - \boldsymbol{\nabla}\cdot(\mathbf{E}\times\mathbf{B})\,,$$

where we used equation (1.1c) for the first term.

Using this result, the power transferred by the fields is given by

$$\int_{\mathscr{D}}\mathbf{j}\cdot\mathbf{E}\,\mathrm{d}\mathbf{r} = -\int_{\mathscr{D}}\left[\frac{1}{\mu_0}\boldsymbol{\nabla}\cdot(\mathbf{E}\times\mathbf{B}) + \frac{1}{\mu_0}\mathbf{B}\cdot\frac{\partial\mathbf{B}}{\partial t} + \frac{1}{\mu_0 c^2}\mathbf{E}\cdot\frac{\partial\mathbf{E}}{\partial t}\right]\mathrm{d}\mathbf{r}$$

Considering that

$$\mathbf{E}\cdot\frac{\partial\mathbf{E}}{\partial t} = \frac{1}{2}\frac{\partial}{\partial t}\mathbf{E}^2\,,$$

we obtain

$$\int_{\mathscr{D}}\mathbf{j}\cdot\mathbf{E}\,\mathrm{d}\mathbf{r} = -\int_{\mathscr{D}}\left[\frac{1}{2}\frac{\partial}{\partial t}\left(\varepsilon_0\mathbf{E}^2 + \frac{1}{\mu_0}\mathbf{B}^2\right) + \frac{1}{\mu_0}\boldsymbol{\nabla}\cdot(\mathbf{E}\times\mathbf{B})\right]\mathrm{d}\mathbf{r}\ .$$

The total energy density of the electromagnetic field can be denoted with

$$w_{em} = \frac{1}{2}\left(\varepsilon_0\mathbf{E}^2 + \frac{1}{\mu_0}\mathbf{B}^2\right)$$

and thus we obtain

$$-\int_{\mathscr{D}}\mathbf{j}\cdot\mathbf{E}\,\mathrm{d}\mathbf{r} = \int_{\mathscr{D}}\left[\frac{\partial w_{em}}{\partial t} + \frac{1}{\mu_0}\boldsymbol{\nabla}\cdot(\mathbf{E}\times\mathbf{B})\right]\mathrm{d}\mathbf{r}\ .$$

Since the domain $\mathscr{D}$ is arbitrary, we can write the above as a differential continuity equation

$$\frac{\partial w_{em}}{\partial t} = -\boldsymbol{\nabla}\cdot\mathbf{S} - \mathbf{j}\cdot\mathbf{E}\,, \tag{1.14}$$

where

$$\mathbf{S} = \frac{1}{\mu_0}\mathbf{E}\times\mathbf{B}$$

is the Poynting vector representing the energy flow.

If we consider the domain $\mathscr{D}$ such that no particles will leave it

$$W_{em} = \int_{\mathscr{D}} w_{em}\,\mathrm{d}\mathbf{r}$$

is the energy of the electromagnetic field and W_{mech} is the energy of the particles

$$W_{mech} = \int_{\mathscr{D}} w_{mech}\,\mathrm{d}\mathbf{r} = \int_{\mathscr{D}}\mathbf{j}\cdot\mathbf{E}\,\mathrm{d}\mathbf{r}\ .$$

By using Gauss' theorem, the energy flux corresponding to the Poynting vector becomes

$$\int_{\mathscr{D}}\boldsymbol{\nabla}\cdot\mathbf{S} = \oint_{\Sigma}\mathbf{n}\cdot\mathbf{S}\,\mathrm{d}a\ ,$$

where Σ is the surface enclosing the domain $\mathscr{D}$.

With the above considerations Poynting's theorem gives the conservation of energy for the whole system

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(W_{em} + W_{mech}\right) = -\oint_{\Sigma} \mathbf{n}\cdot\mathbf{S}\,\mathrm{d}a\ , \tag{1.15}$$

stating that the rate of change of the energy of the system composed of the charged particles and corresponding fields is given by minus the flux of the Poynting vector through the surface bounding the domain.

Equation (1.14) is the local form for the Poynting theorem.

If we consider the extension of the domain to infinity $\mathscr{D} \to \mathbb{R}^3$, $\Sigma \to \Sigma_\infty$, then there is no energy flow through the boundary since electromagnetic waves propagate at a constant finite speed c. Then

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(W_{em} + W_{mech}\right) = 0$$

and the entire energy of the electromagnetic field can be converted into the mechanical energy of the particles interacting with the field.

If we consider $\mathscr{D}$ such that it doesn't enclose any sources, than

$$\frac{\mathrm{d}}{\mathrm{d}t}W_{em} = -\oint_{\Sigma} \mathbf{n}\cdot\mathbf{S}\,\mathrm{d}a\ ,$$

which shows that the energy of the electromagnetic field in the domain $\mathscr{D}$ can change through the variation of the flux of the Poynting vector on the boundary of the domain, Σ. Thus we can indeed say that the flux of the Poynting vector is the energy flux.

1.3 Electromagnetic waves

In the of sources, Maxwell's equations become

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{B} &= 0 \qquad & \boldsymbol{\nabla}\times\mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} &= 0 \\ \boldsymbol{\nabla}\cdot\mathbf{D} &= 0 \qquad & \boldsymbol{\nabla}\times\mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} &= 0\,, \end{aligned}$$

where $\mathbf{D} = \varepsilon\mathbf{E}$ and $\mathbf{B} = \mu\mathbf{H}$. In our case, $\varepsilon = \varepsilon_0$ and $\mu = \mu_0$.

If we assume that the time dependence for the solutions is given by $\mathrm{e}^{-\mathrm{i}\omega t}$, then the above equations become

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{B} &= 0 \qquad & \boldsymbol{\nabla}\times\mathbf{E}\,\mathrm{e}^{-\mathrm{i}\omega t} - \mathrm{i}\omega\mathbf{B}\,\mathrm{e}^{-\mathrm{i}\omega t} &= 0 \\ \boldsymbol{\nabla}\cdot\mathbf{D} &= 0 \qquad & \boldsymbol{\nabla}\times\mathbf{H}\,\mathrm{e}^{-\mathrm{i}\omega t} + \mathrm{i}\omega\mathbf{D} &= 0\,. \end{aligned}$$

More complex time dependencies can be treated with a Fourier decomposition since if we have a solution, any linear combinations with that solution are also solutions.

If we consider only the curl equations

$$\begin{aligned} \boldsymbol{\nabla}\times\mathbf{E} - \mathrm{i}\omega\mathbf{B} &= 0 \\ \boldsymbol{\nabla}\times\mathbf{B} + \mathrm{i}\omega\mu\epsilon\mathbf{E} &= 0 \end{aligned}$$

and take the curl

$$\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{E} - \mathrm{i}\omega\boldsymbol{\nabla}\times\mathbf{B} = \boldsymbol{\nabla}\underbrace{\left(\boldsymbol{\nabla}\cdot\mathbf{E}\right)}_{0} - \nabla^2\mathbf{E} + (\mathrm{i}\omega)^2\mu\varepsilon\mathbf{E} = 0$$

we obtain the Helmholtz wave equations

$$\left(\nabla^2 + \omega^2 \mu\varepsilon\right) \mathbf{E} = 0$$
$$\left(\nabla^2 + \omega^2 \mu\varepsilon\right) \mathbf{B} = 0$$

or in a more compact notation

$$\left(\nabla^2 + \omega^2 \mu\varepsilon\right) \begin{pmatrix} \mathbf{E} \\ \mathbf{B} \end{pmatrix} = 0 \, .$$

Taking the plane wave

$$\mathrm{e}^{\mathrm{i}kx - \mathrm{i}\omega t}$$

as a solution for the Helmholtz wave equation (1.3), we can study what properties arise for wave number k and the frequency ω. Thus we can see that

$$-k^2 + \omega^2 \mu\varepsilon = 0$$

or

$$k = \omega\sqrt{\mu\varepsilon} \, .$$

The phase velocity of a wave v_ϕ is defined as

$$v_\phi = \frac{\omega}{k} \, .$$

In this case, the phase velocity of a plane wave satisfying the Helmholtz equation is

$$v_\phi = \frac{1}{\sqrt{\mu\varepsilon}} = \frac{c}{n} \, ,$$

where n is the refraction index of the media in which the wave propagates and is given by

$$n = \sqrt{\frac{\mu}{\mu_0}\frac{\varepsilon}{\varepsilon_0}} \, .$$

A general solution for the wave equation can be constructed by using the superposition principle

$$u(x,t) = a\,\mathrm{e}^{\mathrm{i}kx - \mathrm{i}\omega t} + b\,\mathrm{e}^{-\mathrm{i}kx - \mathrm{i}\omega t} \, .$$

This general solution can be seen as a superposition of incoming and outgoing plane waves.

Let us now consider an electromagnetic plane wave, that is a plane wave that satisfies both the Helmholtz wave equation (1.3) and Maxwell's equations (1.1)

$$\mathbf{E}(\mathbf{x}, t) = \boldsymbol{\mathcal{E}}\,\mathrm{e}^{\mathrm{i}k\mathbf{n}\cdot\mathbf{x} - \mathrm{i}\omega t}$$
$$\mathbf{B}(\mathbf{x}, t) = \boldsymbol{\mathcal{B}}\,\mathrm{e}^{\mathrm{i}k\mathbf{n}\cdot\mathbf{x} - \mathrm{i}\omega t} \, .$$

First, let us consider the Laplacian in the Helmholtz equation

$$\frac{\partial^2}{\partial x_i^2}\mathcal{E}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j - \mathrm{i}\omega t} = \frac{\partial}{\partial x_i}\mathrm{i}kn_j\delta_{ij}\mathcal{E}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j - \mathrm{i}\omega t} = -k^2 n_i n_i \mathcal{E}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j - \mathrm{i}\omega t} \, .$$

With this consideration, Helmholtz equation yields

$$-k^2 n_i n_i \mathcal{E}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j - \mathrm{i}\omega t} + \mu\varepsilon\omega^2\mathcal{E}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j - \mathrm{i}\omega t} = 0$$

or

$$k^2\mathbf{n}\cdot\mathbf{n} = \mu\varepsilon\omega^2\,.$$

Considering that $k = \sqrt{\mu\varepsilon}\omega$, we obtain that the norm of $\mathbf{n}$ must be 1

$$\mathbf{n}\cdot\mathbf{n} = 1\,.$$

Now we continue with Maxwell's equations. We begin with the divergence equations

$$\boldsymbol{\nabla}\cdot\mathbf{B} = 0 \implies \partial_i\mathcal{B}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j-\mathrm{i}\omega t} = 0\,,$$

where we have used the notation

$$\partial_i \equiv \frac{\partial}{\partial x_i}\,.$$

Thus $\mathrm{i}kn_i\mathcal{B}_i = 0$ and the magnetic field $\mathbf{B}$ and $\mathbf{n}$ are perpendicular since

$$\mathbf{n}\cdot\boldsymbol{\mathcal{B}} = 0\,.$$

Similarly, for the electric field

$$\boldsymbol{\nabla}\cdot\mathbf{D} = 0 \implies \partial_i\varepsilon\mathcal{E}_i\,\mathrm{e}^{\mathrm{i}kn_jx_j-\mathrm{i}\omega t} = 0$$

and

$$\mathrm{i}kn_i\mathcal{E}_i = 0 \implies \mathbf{n}\cdot\boldsymbol{\mathcal{E}} = 0\,.$$

Thus, since the electric and magnetic fields are perpendicular to the propagation direction given by the $\mathbf{n}$ versor, the electromagnetic plane wave is a transverse wave.

If we now consider the curl equation

$$\boldsymbol{\nabla}\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}\,,$$

we obtain

$$\begin{aligned}
\varepsilon_{ijk}\partial_jE_k &= -(-\mathrm{i}\omega)\mathcal{B}_i\,\mathrm{e}^{\mathrm{i}kn_ix_i-\mathrm{i}\omega t}\\
\varepsilon_{ijk}\partial_j\mathcal{E}_k\,\mathrm{e}^{\mathrm{i}kn_ix_i-\mathrm{i}\omega t} &= \mathrm{i}\omega\mathcal{B}_i\,\mathrm{e}^{\mathrm{i}kn_ix_i-\mathrm{i}\omega t}\\
\varepsilon_{ijk}\mathcal{E}_k\mathrm{i}kn_j &= \mathrm{i}\omega\mathcal{B}_i\,.
\end{aligned}$$

Thus $\mathbf{n}\times\boldsymbol{\mathcal{E}}\sqrt{\mu\varepsilon} = \boldsymbol{\mathcal{B}}$ or

$$\mathbf{n}\times\boldsymbol{\mathcal{E}}\frac{n}{c} = \boldsymbol{\mathcal{B}}\,.$$

In vacuum ($n = 1$), we observe that the electric and magnetic field differ in magnitude by a factor of c

$$|\boldsymbol{\mathcal{E}}| = |c\boldsymbol{\mathcal{B}}|\,.$$

If we consider a coordinate system spanned by the versors $(\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \mathbf{n})$, then the electric and magnetic field magnitudes can be written as

$$\boldsymbol{\mathcal{E}} = \boldsymbol{\epsilon}_1E_0 \qquad \boldsymbol{\mathcal{B}} = \boldsymbol{\epsilon}_2\sqrt{\mu\varepsilon}E_0\,.$$

A plane wave with its electric field always in a direction $\boldsymbol{\epsilon}_1$ is called *linearly polarized* with the polarization vector $\boldsymbol{\epsilon}_1$.

According to the Poynting theorem, the plane wave transports energy. The Poynting vector in this case is given by

$$\mathbf{S} = \mathbf{E}\times\mathbf{H} = \mathbf{e}_i\varepsilon_{ijk}\boldsymbol{\epsilon}_{1j}E_0\boldsymbol{\epsilon}_{2k}\frac{1}{\mu}\sqrt{\mu\varepsilon} = \sqrt{\frac{\varepsilon}{\mu}}E_0^2\mathbf{n}$$

1.4 Electron in a Plane Wave

In this section we will consider the classical dynamics of an electron in a laser pulse following the discussion in Karsch (2018). The starting point is the equation of motion for the electron

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -e\left[\mathbf{E}(\mathbf{r},t) + \mathbf{v}\times\mathbf{B}(\mathbf{r},t)\right] . \qquad (1.18)$$

1.4.1 Non-relativistic treatment

1.4.2 Relativistic treatment

1.5 The Ponderomotive Force

1.5.1 Non-relativistic treatment

1.5.2 Relativistic treatment

Chapter 2

Particle in Cell Method

As we outlined in Chapter 1, the interaction of some charged particles with an electromagnetic field can be viewed as the action of the sources on the fields and the action of the fields on the sources.

In the same manner, simulating the interaction self-consistently requires a *field solver* that computes the structure of the fields considering the sources and a *particle pusher* that solves the (relativistic) equations of motion for the particles. In the particle in cell method, a finite-difference time-domain (FDTD) method is used for solving Maxwell's equations and a modified leapfrog method is used for the particle pusher as presented in Arber *et al.* 2015.

2.1 Numerical Methods Introduction

The numerical methods mentioned above are based on the idea of discretizing the derivative operator. There are multiple ways of discretizing this operator, but all of them can be derived from the Taylor series expansion.

$$f(x_0 + h) = f(x_0) + \frac{f'(x_0)}{1!}h + \frac{f''(x_0)}{2!}h^2 + \cdots + \frac{f^{(n)}(x_0)}{n!}h^n + \dots$$

The main discretizations options are the forward, backward and central differences. For the forward discretization we consider

$$f(x_0 + h) = f(x_0) + \frac{f'(x_0)}{1!}h + \frac{f''(x_0)}{2!}h^2 + \cdots$$

and we rearrange the terms in the following way

$$\frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0) + \frac{f''(x_0)}{2}h + \cdots$$

and thus, when $h \to 0$, the derivative in first order is given by

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} + \mathcal{O}(h)\,.$$

The local truncation error is given by the error of the approximation in one time step. The forward and backward discretizations are both of order one. The central discretization is second order accurate and can be derived as follows.

We first begin with the forward and backward discretizations for half of a timestep:

$$f(x_0 + \frac{h}{2}) = f(x_0) + f'(x_0)\frac{h}{2} + \frac{f''(x_0)}{2}\frac{h^2}{4} + \frac{f^{(3)}(x_0)}{3!}\frac{h^3}{8} + \cdots$$
$$f(x_0 - \frac{h}{2}) = f(x_0) - f'(x_0)\frac{h}{2} + \frac{f''(x_0)}{2}\frac{h^2}{4} - \frac{f^{(3)}(x_0)}{3!}\frac{h^3}{8} + \cdots .$$

Then we take the difference and obtain

$$f(x_0 + \frac{h}{2}) - f(x_0 - \frac{h}{2}) = f'(x_0)h + 2\frac{f^{(3)}(x_0)}{3!}\frac{h^3}{8} + \cdots$$

and we can see that indeed the central difference is second order accurate

$$f'(x_0) = \frac{f(x_0 + \frac{h}{2}) - f(x_0 - \frac{h}{2})}{h} + \mathcal{O}\big(h^2\big) .$$

As an application of the methods discussed above, we will now derive the so called leapfrog method for solving second order differential equations following Hockney and Eastwood (1988, Chapter 4). More concretely, we will take a look at solving the equations of motion for a particle. As a first step, the equations of motion can be written as a system of first order differential equations

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$$
$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{F} ,$$

where $\mathbf{F}$ is the total force on the particle. Replacing the derivatives with their finite difference approximations, we obtain

$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\Delta t} = \mathbf{v}_{n+1/2} \tag{2.1a}$$
$$m\frac{\mathbf{v}_{n+1/2} - \mathbf{v}_{n-1/2}}{\Delta t} = \mathbf{F}(\mathbf{x}_n) . \tag{2.1b}$$

Replacing the velocity, we obtain

$$\frac{\mathbf{x}_{n+1} - 2\mathbf{x}_n + \mathbf{x}_{n-1}}{\Delta t^2} = \frac{\mathbf{F}(\mathbf{x}_n)}{m} .$$

2.1.1 Accuracy

The accuracy of an integration method is given by difference between the true solution and the approximate solution at a given timestep, that is the local error. There are two types of local errors: truncation errors and roundoff errors. Truncation errors are given by the approximations employed in the numerical method. On the other hand, roundoff errors are consequence of implementing the numerical method on a computer with finite precision. In general, for low order methods, the truncation errors are significantly bigger than roundoff errors, and thus we can consider that the accuracy is given only by truncation error.

In order to better illustrate the concept of truncation errors, we will exemplify its computation for the leapfrog method. Let us consider the local truncation error at the timestep n, δ^n and $\mathbf{X}$ the true solution

$$\frac{\mathbf{X}_{n+1} - 2\mathbf{X}_n + \mathbf{X}_{n-1}}{\Delta t^2} = \frac{\mathbf{F}(\mathbf{X}_n)}{m} + \delta^n .$$

If we expand $\mathbf{X}_{n+1}$ and $\mathbf{X}_{n-1}$ in Taylor series around $\mathbf{X}_n$

$$\begin{aligned}\mathbf{X}_{n+1} &= \mathbf{X}_n + \frac{\mathrm{d}\mathbf{X}_n}{\mathrm{d}t}\Delta t + \frac{1}{2}\frac{\mathrm{d}^2\mathbf{X}_n}{\mathrm{d}t^2} - \cdots \\ \mathbf{X}_{n-1} &= \mathbf{X}_n - \frac{\mathrm{d}\mathbf{X}_n}{\mathrm{d}t}\Delta t + \frac{1}{2}\frac{\mathrm{d}^2\mathbf{X}_n}{\mathrm{d}t^2} - \cdots \,,\end{aligned}$$

we obtain

$$\frac{\mathrm{d}^2\mathbf{X}_n}{\mathrm{d}t^2} + \frac{\Delta t^2}{12}\frac{\mathrm{d}^4\mathbf{X}}{\mathrm{d}t^4} + \mathcal{O}\big(\Delta t^5\big) = \frac{\mathbf{F}(\mathbf{X}_n)}{m} + \delta^n \,,$$

and thus

$$\delta^n \sim \mathcal{O}\big(\Delta t^2\big)$$

which shows that the leapfrog algorithm is of order 2.

2.1.2 Stability

A numerical method is considered asymptotically stable if the solution obtained for a linear problem is asymptotically bounded. As in the previous case we will show an example for the leapfrog method, following the ideas exposed in Butcher 2016 and in Leimkuhler and Reich (2004, Section 2.6).

A linear problem can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{z} = A\mathbf{z} \,,$$

where we used the following notation to denote the dynamical state of the system

$$\mathbf{z} = \begin{pmatrix}\mathbf{q} \\ \mathbf{p}\end{pmatrix} .$$

The solution can be written as

$$\mathbf{z}(t) = R(t)\mathbf{z}_0 \,,$$

where $R(t)$ is a matrix which can give the solution at any time by evolving the initial conditions.

The discrete version of the problem is given by

$$\mathbf{z}_{n+1} = \hat{R}(\Delta t)\mathbf{z}_n \,, \tag{2.2}$$

where $\hat{R}(\Delta t)$ is called the propagation matrix. With this considerations, asymptotic stability can be expressed as a function of the eigenvalues of $\hat{R}(\Delta t)$, since the solution is obtained with powers of $\hat{R}$ from the initial conditions

$$\mathbf{z}_n = [\hat{R}]^n\mathbf{z}_0 \,.$$

More concretely, a method is asymptotically stable if the eigenvalues of $\hat{R}$ are inside the unit disk in the complex plane and simple (not repeated) if on the unit circle (Leimkuhler and Reich 2004, p. 28).

One of the most studied linear problems is the harmonic oscillator and we can use it as our model linear problem

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + \frac{\omega^2\mathbf{q}^2}{2} \,.$$

The equations of motion are given by the corresponding Hamilton equations

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} = \frac{p_i}{m}$$
$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} = -\omega^2 q_i\,.$$

Taking $m = 1$ and writing the above equations in matrix form yields

$$\dot{\mathbf{z}} = \begin{pmatrix} p \\ -\omega^2 q \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}$$

and thus we obtain

$$\dot{\mathbf{z}} = A\mathbf{z},$$

with

$$A = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}\,.$$

The solution is given by

$$\mathbf{z}(t) = R(t)\mathbf{z}_0,$$

with

$$R(t) = \begin{pmatrix} \cos(\omega t) & \frac{1}{\omega}\sin(\omega t) \\ -\omega\sin(\omega t) & \cos(\omega t) \end{pmatrix}\,.$$

In order to analyze the stability of the leapfrog algorithm, it is convenient to express the equations in a different form, also called the Störmer–Verlet method

$$\mathbf{q}_{n+1} = \mathbf{q}_n + \Delta t \mathbf{v}_{n+1/2}$$
$$M\mathbf{v}_{n+1/2} = M\mathbf{v}_n - \frac{\Delta t}{2}\boldsymbol{\nabla} V(\mathbf{q}_n)$$
$$M\mathbf{v}_{n+1} = M\mathbf{v}_{n+1/2} - \frac{\Delta t}{2}\boldsymbol{\nabla} V(\mathbf{q}_{n+1})\,.$$

In our particular case, the gradient of the potential is given by $\omega^2 q$ and the above reduces to

$$\mathbf{q}_{n+1} = \mathbf{q}_n + \Delta t(\mathbf{v}_n - \frac{\Delta t}{2}\omega^2\mathbf{q}^n) = \mathbf{q}_n\left(1 - \frac{\Delta t^2\omega^2}{2}\right) + \mathbf{v}_n\Delta t$$
$$\mathbf{p}_{n+1} = \mathbf{p}_n - \frac{\Delta t^2}{2}\omega^2\mathbf{q}_n - \frac{\Delta t^2}{2}\omega^2\mathbf{q}_{n+1} = \mathbf{p}_n - \frac{\Delta t^2}{2}\omega^2\mathbf{q}_n - \frac{\Delta t}{2}\omega^2\left(\mathbf{q}_n + \mathbf{v}_n - \frac{\Delta t}{2}\omega^2\mathbf{q}_n\right)\,,$$

or

$$\begin{pmatrix} \mathbf{q}_{n+1} \\ \mathbf{p}_{n+1} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\Delta t^2\omega^2}{2} & \Delta t \\ -\Delta t\omega^2\left(1 - \frac{\Delta t^2\omega^2}{4}\right) & 1 - \frac{\Delta t^2\omega^2}{2} \end{pmatrix} \begin{pmatrix} \mathbf{q}_n \\ \mathbf{p}_n \end{pmatrix}\,.$$

Comparing with equation (2.2) we obtain

$$\hat{R}(\Delta t) = \begin{pmatrix} 1 - \frac{\Delta t^2\omega^2}{2} & \Delta t \\ -\Delta t\omega^2\left(1 - \frac{\Delta t^2\omega^2}{4}\right) & 1 - \frac{\Delta t^2\omega^2}{2} \end{pmatrix}\,.$$

The eigenvalues of $\hat{R}$ are given by the solution of $\det\left(\hat{R} - \lambda I\right) = 0$, or more explicitly

$$\begin{vmatrix} 1 - \frac{\Delta t^2\omega^2}{2} & \Delta t \\ -\Delta t\omega^2\left(1 - \frac{\Delta t^2\omega^2}{4}\right) & 1 - \frac{\Delta t^2\omega^2}{2} \end{vmatrix} = 0\,.$$

This reduces to

$$\left(1-\frac{\Delta t^2\omega^2}{2}-\lambda\right)^2+\frac{\Delta t^2\omega^2}{2}\left(2-\frac{\Delta t^2\omega^2}{2}\right)=0\,.$$

Using the notation $\frac{\Delta t^2 w^2}{2}\equiv\mu^2$, we obtain

$$\left(1-\mu^2-\lambda\right)^2+\mu^2\left(2-\mu^2\right)=0\,,$$

which can be further expanded to

$$\lambda^2+\left(1-\mu^2\right)^2-2\left(1-\mu^2\right)\lambda+\mu^2\left(2-\mu^2\right)=0\,,$$

yielding the solutions

$$\begin{aligned}\lambda_{1,2}&=\frac{1}{2}\left\{2(1-\mu^2)\pm\sqrt{4(1-\mu^2)^2-4\left[(1-\mu^2)^2+\mu^2(2-\mu^2)\right]}\right\}\\&=1-\mu^2\pm\sqrt{\mu^2(\mu^2-2)}\,.\end{aligned}$$

We notice that for $\mu^2<2$ the solutions are complex and

$$\begin{aligned}|\lambda_{1,2}|^2&=(1-\mu^2)+\mu^2(\mu^2-2)\\&=1+\mu^4-2\mu^2+\mu^4-2\mu^2\\&=1+\mu^4-4\mu^2\,.\end{aligned}$$

The method will be stable for $|\lambda|^2<1$, or

$$\mu^2(\mu^2-4)<0\implies\mu<2,\text{for }\mu\neq0\,.$$

For $\mu^2>2$ the eigenvalues are real and with modulus greater than 1. Thus the stability condition for the Störmer–Verlet method is given by $\mu<2$, or

$$\Delta t^2\omega^2<4\,,$$

indicating a sampling of at least π points per period, or a step size $\Delta t<2/\omega$.

In the context of ordinary differential equations, a stability region of the method is usually defined via a stability function $R(z)$ in the complex plane (Butcher 2016, p. 81). Such approach cannot be used in this case since the stability function is defined for a singe ordinary differential equation, but in the case of Hamiltonian dynamics we always have $2n$ ordinary differential equations, with $n>1$.

2.2 The particle pusher

Having (briefly) developed some general aspects of the theory of numerical methods for solving differential equations, we now continue with the more concrete case of numerically solving the equations of motion for a charged particle. In the non-relativistic case, the (continuous) equations of motion have the following form

$$\begin{aligned}\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}&=\mathbf{v}\\\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}&=\frac{q}{m}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)\,.\end{aligned}$$

Since the above equations are symmetric with respect to time reversal, it is desired that we obtain a discretization which is also time-reversible. Buneman (1967) explained that we can use centered differences for this task and in the particular case of the Lorentz force we can average the velocity in order to represent the $\mathbf{v} \times \mathbf{B}$ product symmetrically. Thus we obtain

$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\Delta t} = \mathbf{v}_{n+1} \tag{2.3a}$$

$$\frac{\mathbf{v}_{n+1/2} - \mathbf{v}_{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}_n) + \frac{\mathbf{v}_{n+1/2} + \mathbf{v}_{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}_n)\right) . \tag{2.3b}$$

As explained in Birdsall and Langdon (2005, Chapter 4–3), there are several methods for solving the above equations, implying a partial (Buneman 1967) or complete (Boris 1970) separation of the electric and magnetic force contributions. In the following we will detail the second method, which is also called the Boris push.

Let us introduce the following notation

$$\mathbf{v}^- = \mathbf{v}_{n-1/2} - \frac{q\mathbf{E}}{m}\frac{\Delta t}{2}$$
$$\mathbf{v}^+ = \mathbf{v}_{n+1/2} + \frac{q\mathbf{E}}{m}\frac{\Delta t}{2} ,$$

such that

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{\mathbf{v}_{n+1/2} - \mathbf{v}_{n-1/2}}{\Delta t} + \frac{q\mathbf{E}}{m} .$$

Substituting in equation (2.3b) we obtain

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{q}{2m}(\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B} , \tag{2.4}$$

which can be seen as a rotation. Indeed, if we take the scalar product with $(\mathbf{v}^+ + \mathbf{v}^-)$, we get

$$(\mathbf{v}^+ + \mathbf{v}^-) \cdot \frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{q}{2m}\underbrace{(\mathbf{v}^+ + \mathbf{v}^-) \cdot (\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}}_{0}$$

or

$$|\mathbf{v}^+|^2 - |\mathbf{v}^-|^2 = 0 ,$$

implying that $|\mathbf{v}^+| = |\mathbf{v}^-|$.

If we decompose the $\mathbf{v}^-$ into its parallel and perpendicular components with respect to $\mathbf{B}$, we can reduce the rotation of $\mathbf{v}^-$ to the rotation of its perpendicular component $\mathbf{v}^-_\perp$.

The angle of rotation between $\mathbf{v}^-_\perp$ and $\mathbf{v}^-_\perp$, denoted with θ in figure 2.1, can be expressed as

$$\tan\frac{\theta}{2} = \frac{|\mathbf{v}^+_\perp - \mathbf{v}^-_\perp|}{|\mathbf{v}^+_\perp + \mathbf{v}^-_\perp|} .$$

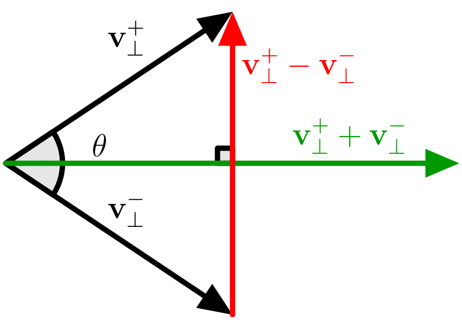

Figure 2.1: Boris rotation angle

Rewriting equation (2.4) we obtain

$$\mathbf{v}^+ - \mathbf{v}^- = \frac{q\Delta t}{2m}(\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}$$

and if we substitute $\mathbf{v}^\pm = \mathbf{v}^\pm_\perp + \mathbf{v}^\pm_\parallel$

$$\mathbf{v}^+_\perp - \mathbf{v}^-_\perp = \frac{q\Delta t}{2m}(\mathbf{v}^+_\perp + \mathbf{v}^-_\perp) \times \mathbf{B} .$$

Furthermore, since all the vectors above have the same direction by construction, we can factor out the versors and obtain

$$\frac{|\mathbf{v}_\perp^+ - \mathbf{v}_\perp^-|}{|\mathbf{v}_\perp^+ + \mathbf{v}_\perp^-|} = \frac{q|\mathbf{B}|}{m}\frac{\Delta t}{2}$$

and thus

$$\tan\frac{\theta}{2} = \frac{qB}{m}\frac{\Delta t}{2}\,. \tag{2.5}$$

Since for the rotation described above only the components perpendicular to the direction of $\mathbf{B}$ matter, we can simplify the notation and use $\mathbf{v}_\pm$ instead of $\mathbf{v}_\perp^\pm$. We will now introduce an additional vector $\mathbf{v}'$ given by the addition between $\mathbf{v}_-$ and another vector, such that $\mathbf{v}'$ is perpendicular to $\mathbf{v}_+ - \mathbf{v}_-$.

It is convenient to write $\mathbf{v}'$ as $\mathbf{v}' = \mathbf{v}_- + \mathbf{v}_- \times \mathbf{t}$. In the right triangle formed by $\mathbf{v}'$ with $\mathbf{v}_-$ and $\mathbf{v}_- \times \mathbf{t}$ as seen in figure 2.2, we have

$$\tan\frac{\theta}{2} = \frac{|\mathbf{v}_- \times \mathbf{t}|}{|\mathbf{v}_-|} = |\mathbf{t}|$$

and thus by using equation (2.5) $\mathbf{t}$ is given by

$$\mathbf{t} = \frac{q\mathbf{B}}{m}\frac{\Delta t}{2}\,.$$

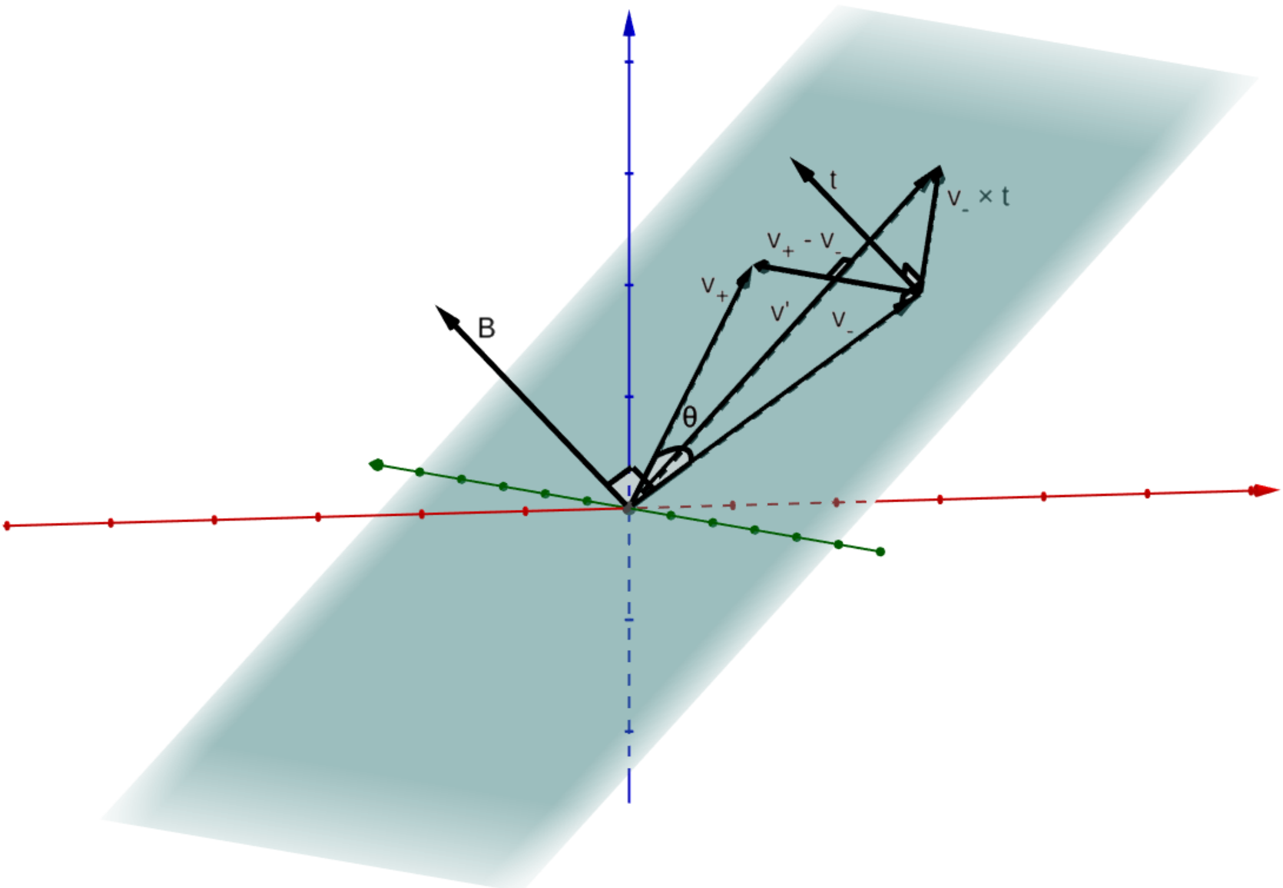

Figure 2.2: Boris rotation construction in 3D

As can be seen in figure 2.2, $\mathbf{v}_+ - \mathbf{v}_- \parallel \mathbf{v}' \times \mathbf{B}$. This encourages the following notation: $\mathbf{v}_+ - \mathbf{v}_- \equiv \mathbf{v}' \times \mathbf{s}$, where $\mathbf{s}$ can be determined by the condition that $|\mathbf{v}_+|^2 = |\mathbf{v}_-|^2$. Thus, expanding $\mathbf{v}' \times \mathbf{s}$ gives

$$\mathbf{v}' \times \mathbf{s} = (\mathbf{v}_- + \mathbf{v}_- \times \mathbf{t}) \times \mathbf{s} = \mathbf{v}_- \times \mathbf{s} + \mathbf{t}\underbrace{(\mathbf{v}_- \cdot \mathbf{s})}_{0} - \mathbf{v}_-(\mathbf{t} \cdot \mathbf{s})$$

and if we consider the definition for $\mathbf{s}$

$$\mathbf{v}_+ = \mathbf{v}_- + \mathbf{v}' \times \mathbf{s} = \mathbf{v}_- + \mathbf{v}_- \times \mathbf{s} - \mathbf{v}_-(\mathbf{t} \cdot \mathbf{s})\,.$$

Taking the scalar product with $\mathbf{v}_-$ gives

$$\mathbf{v}_+ \cdot \mathbf{v}_- = |\mathbf{v}_-|^2 - |\mathbf{v}_-|^2(\mathbf{t} \cdot \mathbf{s})$$

or

$$|\mathbf{v}_-|^2 \cos\theta = |\mathbf{v}_-|^2(1 - \mathbf{t} \cdot \mathbf{s})\,.$$

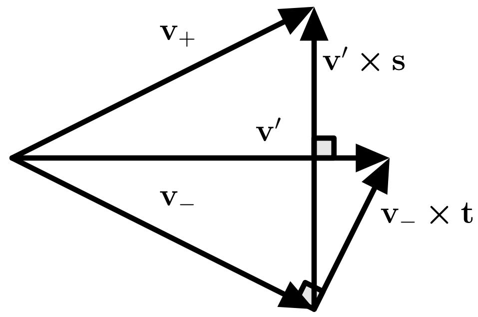

Figure 2.3: The velocities projected in the plane perpendicular to $\mathbf{B}$

Using the trigonometry identity

$$\cos\theta = \frac{1 - \tan^2\frac{\theta}{2}}{1 + \tan^2\frac{\theta}{2}}\,,$$

we obtain

$$\mathbf{t} \cdot \mathbf{s} = 1 - \frac{1 - \tan^2\frac{\theta}{2}}{1 + \tan^2\frac{\theta}{2}}\,,$$

which is equivalent to

$$\mathbf{t} \cdot \mathbf{s} = \frac{2t^2}{1 + t^2}$$

and thus we obtain that

$$\mathbf{s} = \frac{2\mathbf{t}}{1 + t^2}\,.$$

As a summary, the Boris push algorithm solves equation (2.3b) with the following steps:

1. $\mathbf{v}^- = \mathbf{v}_{n-1/2} + \frac{q\mathbf{E}}{m}\frac{\Delta t}{2}$
2. rotate $\mathbf{v}^-$ to obtain $\mathbf{v}^+$ using
   (a) $\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$, where $\mathbf{t} = \frac{q\mathbf{B}}{m}\frac{\Delta t}{2}$
   (b) $\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$, where $\mathbf{s} = \frac{2\mathbf{t}}{1+t^2}$
3. $\mathbf{v}_{n+1/2} = \mathbf{v}^+ + \frac{q\mathbf{E}}{m}\frac{\Delta t}{2}$

2.2.1 Conservation properties

When solving (continuous) differential equations with (discrete) numerical methods, an important aspect is that we want the algorithm to be as close as possible to the original continuous system in terms of symmetries and conserved quantities (Stuart and Humphries 1996).

In what follows we will look at the conservation properties of the Boris push and show why are they important for simulating the dynamics of charged particles following the ideas presented in Qin *et al.* (2013).

Mathematically speaking, a Hamiltonian system is given by the phase space (an even dimensional manifold[1]), a symplectic structure on it and the Hamiltonian function (Arnol'd 1989, p. 160). In order to explain what the symplectic structure is, we will start with a short discussion about 2-forms (Arnol'd 1989, p. 164).

Definition. An exterior form of degree 2 (or a 2-form) is a function of pairs of vectors $\omega^2 : \mathbb{R}^n \times \mathbb{R}^n$, which is bilinear and skew symmetric:

$$\omega^2(\lambda_1 \boldsymbol{\xi}_1 + \lambda_2 \boldsymbol{\xi}_2, \boldsymbol{\xi}_3) = \lambda_1 \omega^2(\boldsymbol{\xi}_1, \boldsymbol{\xi}_3) + \lambda_2 \omega^2(\boldsymbol{\xi}_2, \boldsymbol{\xi}_3)$$
$$\omega^2(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) = -\omega^2(\boldsymbol{\xi}_2, \boldsymbol{\xi}_1)\,,$$

$\forall \lambda_{1,2} \in \mathbb{R}, \boldsymbol{\xi}_{1,2,3} \in \mathbb{R}^n$.

As an example of a 2-form in $n = 2$ dimensions is given by the *oriented area* spanned by 2 vectors in the (oriented) euclidean plane $\mathbb{R}^2$. Let us consider

$$\boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}, \qquad \boldsymbol{\eta} = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix},$$

then the oriented are determined by the two vectors is given by the determinant (Golomb 1985)

$$S(\boldsymbol{\xi}, \boldsymbol{\eta}) = \det \begin{pmatrix} \xi_1 & \eta_1 \\ \xi_2 & \eta_2 \end{pmatrix} = \xi_1 \eta_2 - \xi_2 \eta_1\,.$$

Let us consider an $2d$-dimensional phase space with the coordinates q_i, p_i as presented in Leimkuhler and Reich (2004, p. 183).

Definition 1. A linear map $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called *symplectic* if there exists a 2-form ω such that

$$\omega(A\boldsymbol{\xi}, A\boldsymbol{\eta}) = \omega(\boldsymbol{\xi}, \boldsymbol{\eta})\,,\ \forall \boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^{2d}\,.$$

We can also express the above in matrix notation

$$A^T J^{-1} A = J^{-1}, \qquad \text{where } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

with I the identity matrix in d dimensions.

A useful example that illustrates the concept is given in the case of $d = 1$, where symplecticity implies area conservation under the given linear transformation. In the more general $d > 1$ case, it would imply the conservation of the sum of the respective projected areas.

As we have seen from the beginning of this chapter, differentiable functions are often approximated using linear maps. This provides the motivation for extending the above definition to the non-linear case.

Definition 2. A differentiable map $g : U \to \mathbb{R}^{2d}$, with $U \subset \mathbb{R}^{2d}$ an open set, is called *symplectic* if its corresponding Jacobian matrix $g'(\mathbf{p}, \mathbf{q})$ is everywhere symplectic, i.e.

$$\omega(g'(\mathbf{p}, \mathbf{q})\boldsymbol{\xi}, g'(\mathbf{p}, \mathbf{q})\boldsymbol{\eta}) = \omega(\boldsymbol{\xi}, \boldsymbol{\eta})$$

or in matrix notation $g'(\mathbf{p}, \mathbf{q})^T J^{-1} g'(\mathbf{p}, \mathbf{q}) = J^{-1}$.

[1] A manifold is a topological space that is locally Euclidean.

Having defined symplecticity, we will now try to check if the Boris push algorithm is symplectic. For this task we begin with rewriting equation (2.3b) in a more convenient form

$$\mathbf{v}_{n+1/2} - \frac{q\Delta t}{2m}\mathbf{v}_{n+1/2} \times \mathbf{B}_n = \mathbf{v}_{n-1/2} + \frac{q\Delta t}{2m}\mathbf{v}_{n-1/2} \times \mathbf{B}_n + \frac{q\Delta t}{m}\mathbf{E}_n\,,$$

where $\mathbf{B}_n \equiv \mathbf{B}(\mathbf{x}_n)$ and $\mathbf{E}_n \equiv \mathbf{E}(\mathbf{x}_n)$.

In order to manipulate the above more easily, it is useful to introduce some fundamental group theory notions (Hairer, Lubich, and Wanner 2006, p. 118) and the hat map (Marsden and Ratiu 1999, p. 289).

Definition 3. A *Lie group* G is a group that is also a differentiable manifold and for which the product is given by the differentiable mapping $G \times G \to G$.

The tangent space $\mathfrak{g} = T_I G$ at the identity I of a matrix Lie group G is closed under forming commutators of its elements and defines the *Lie algebra* of G.

Definition 4. The *hat map* $\hat{}\colon \mathbb{R}^3 \to \mathfrak{so}(3)$ is a vector space isomorphism that identifies the Lie algebra $\mathfrak{so}(3)$ of $SO(3)$ with $\mathbb{R}^3$. If we consider $\mathbf{v} = (v_1, v_2, v_3) \in \mathbb{R}^3$, then the hat map is given by

$$\hat{\mathbf{v}} = \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix}.$$

We can observe that

$$\hat{\mathbf{v}}\mathbf{w} = \mathbf{v} \times \mathbf{w}$$

characterizes the isomorphism. Comparing

$$\hat{\mathbf{v}}\mathbf{w} = \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix}\begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \begin{pmatrix} -v_3 w_2 + v_2 w_3 \\ v_3 w_1 - v_1 w_3 \\ -v_2 w_1 + v_1 w_2 \end{pmatrix}$$

with

$$(\mathbf{v} \times \mathbf{w}) = \mathbf{e}_i \epsilon_{ijk} v_j w_k = \mathbf{e}_1(v_2 w_3 - v_3 w_2) + \mathbf{e}_2(v_3 w_1 - v_1 w_3) + \mathbf{e}_3(v_1 w_2 - v_2 w_1)$$

we can see that this is indeed true.

Thus, if we consider $\mathbb{R}^3$ together with the cross product, the hat map $\hat{}$ becomes a Lie algebra isomorphism and we can identify $\mathfrak{so}(3)$ with $\mathbb{R}^3$ having the cross product as Lie bracket[2].

We can now resume rewriting equation (2.3b) and we obtain

$$\left(I - \hat{\Omega}_n\right)\begin{pmatrix} v^1_{n+1/2} \\ v^2_{n+1/2} \\ v^3_{n+1/2} \end{pmatrix} = \left(I + \hat{\Omega}_n\right)\begin{pmatrix} v^1_{n-1/2} \\ v^2_{n-1/2} \\ v^3_{n-1/2} \end{pmatrix} + \frac{q\Delta t}{m}\begin{pmatrix} E^1_n \\ E^2_n \\ E^3_n \end{pmatrix}, \tag{2.6}$$

where

$$\hat{\Omega}_n = \frac{q\Delta t}{2m}\begin{pmatrix} 0 & -B^3_n & B^2_n \\ B^3_n & 0 & -B^1_n \\ -B^2_n & B^1_n & 0 \end{pmatrix}.$$

[2] A bilinear, skew symmetric operation $\mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ that satisfies the Jacobi identity.

Multiplying on the left of equation (2.6) with $\left(I-\hat{\Omega}_n\right)$ yields

$$\begin{pmatrix} v^1_{n+1/2} \\ v^2_{n+1/2} \\ v^3_{n+1/2} \end{pmatrix} = \left(I-\hat{\Omega}_n\right)^{-1}\left(I+\hat{\Omega}_n\right)\begin{pmatrix} v^1_{n-1/2} \\ v^2_{n-1/2} \\ v^3_{n-1/2} \end{pmatrix} + \frac{q\Delta t}{m}\left(I-\hat{\Omega}_n\right)^{-1}\begin{pmatrix} E^1_n \\ E^2_n \\ E^3_n \end{pmatrix}.$$

In order to further simplify the notation, we can use the following notation: $\mathbf{x}_n \equiv \mathbf{x}_k$ and $\mathbf{v}_{n-1/2} \equiv \mathbf{v}_k$ and use the Cayley transform for the first term on the right hand side. For a quadratic Lie group[3], the *Cayley transform*

$$\operatorname{cay}\Omega = (I-\Omega)^{-1}(I+\Omega)$$

maps elements of $\mathfrak{g}$ into G (Hairer, Lubich, and Wanner 2006, p. 128).

In our particular case

$$\left(I-\hat{\Omega}_n\right)^{-1}\left(I+\hat{\Omega}_n\right) = \operatorname{cay}\hat{\Omega}_n \equiv R$$

and we obtain

$$\mathbf{v}_{k+1} = R\mathbf{v}_k + \frac{q\Delta t}{m}\left(I-\hat{\Omega}_n\right)^{-1}\mathbf{E}_k\,.$$

Thus equations (2.3a) and (2.3b) form a one step map Ψ_B which maps $\mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k)$ to $\mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$

$$\Psi_B : \begin{cases} \mathbf{x}_{k+1} = \mathbf{x}_k + R\Delta t\mathbf{v}_k + \dfrac{q\Delta t}{m}\left(I-\hat{\Omega}_n\right)^{-1}\mathbf{E}_k \\ \mathbf{v}_{k+1} = R\mathbf{v}_k + \dfrac{q\Delta t^2}{m}\left(I-\hat{\Omega}_n\right)^{-1}\mathbf{E}_k \end{cases}.$$

As Ψ_B is a function $\Psi_B(\mathbf{z}_k)$, we can compute its Jacobian an check the condition for symplecticity

$$\frac{\partial\Psi_B}{\partial\mathbf{z}_k} = \begin{pmatrix} \frac{\partial\mathbf{x}_{k+1}}{\partial\mathbf{x}_k} & \frac{\partial\mathbf{x}_{k+1}}{\partial\mathbf{v}_k} \\ \frac{\partial\mathbf{v}_{k+1}}{\partial\mathbf{x}_k} & \frac{\partial\mathbf{v}_{k+1}}{\partial\mathbf{v}_k} \end{pmatrix} = \begin{pmatrix} I+\Delta t\frac{\partial\mathbf{v}_{k+1}}{\partial\mathbf{x}_k} & R\Delta t \\ \frac{\partial\mathbf{v}_{k+1}}{\partial\mathbf{x}_k} & R \end{pmatrix}.$$

As we mentioned in definition 2, for the map to be symplectic it has to satisfy

$$\left(\frac{\partial\Psi_B}{\partial\mathbf{z}_k}\right)^T J^{-1}\left(\frac{\partial\Psi_B}{\partial\mathbf{z}_k}\right) = J^{-1}\,.$$

Considering

$$\frac{\partial\Psi_B}{\partial\mathbf{z}_k} = \begin{pmatrix} S_1 & S_2 \\ S_3 & S_4 \end{pmatrix},$$

the symplecticity condition can be written as

$$\begin{aligned} \begin{pmatrix} S_1^T & S_3^T \\ S_2^T & S_4^T \end{pmatrix}\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}\begin{pmatrix} S_1 & S_2 \\ S_3 & S_4 \end{pmatrix} &= \begin{pmatrix} S_3^T & -S_1^T \\ S_4^T & -S_2^T \end{pmatrix}\begin{pmatrix} S_1 & S_2 \\ S_3 & S_4 \end{pmatrix} \\ &= \begin{pmatrix} S_3^TS_1 - S_1^TS_3 & S_3^TS_2 - S_1^TS_4 \\ S_4^TS_1 - S_2^TS_3 & S_4^TS_2 - S_2^TS_4 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \end{aligned}$$

[3]Lie groups of the form $G = \{Y \mid Y^TPY = P\}$, where P is a constant matrix.

Thus, we will have the following set of conditions

$$
\begin{align}
S_3^T S_1 &= S_1^T S_3 \tag{2.7a}\\
S_1^T S_4 - S_3^T S_2 &= I \tag{2.7b}\\
S_4^T S_1 - S_2^T S_3 &= I \tag{2.7c}\\
S_4^T S_2 &= S_2^T S_4 \,. \tag{2.7d}
\end{align}
$$

If we consider the simplified case of homogeneous electric and magnetic fields, then

$$\frac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} = \frac{\partial}{\partial \mathbf{x}_k}(R\mathbf{v}_k) + \frac{q\Delta t}{m}\frac{\partial}{\partial \mathbf{x}_k}\left[\left(I - \hat{\Omega}_k\right)^{-1}\mathbf{E}_k\right] = 0$$

and

$$\begin{aligned} S_1 &= I \quad & S_2 &= R\Delta t\\ S_3 &= 0 \quad & S_4 &= R\,. \end{aligned}$$

If we consider the condition in equation (2.7b), we obtain

$$S_1^T S_4 - S_3^T S_2 = R \neq I$$

and thus the Boris push algorithm is not symplectic. In spite of that, the algorithm presents desirable properties such as near-conservation of energy when the magnetic field is constant or the electric potential is quadratic and for more general cases it has a linear energy error (Hairer and Lubich 2018). This properties encourage a more detailed analysis of the properties of the Boris push method.

One of the properties of a symplectic algorithm is that it conserves the phase space volume. This can be understood as a generalization of the are conservation example in $2d, d = 1$ to higher dimensions. For a map to be volume preserving, the determinant of its Jacobian must be one

$$\det \frac{\partial \Psi_B}{\partial \mathbf{z}_k} = 1\,.$$

In our case this becomes

$$\left|\frac{\partial \Psi_B}{\partial \mathbf{z}_k}\right| = \begin{vmatrix} I + \Delta t \frac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & R\Delta t \\ \frac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & R \end{vmatrix} = \begin{vmatrix} I & 0 \\ \frac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & R \end{vmatrix} = \left|R\right| \,,$$

where we have subtracted the second row multiplied by Δt from the first one. Since $R \in SO(3)$, as a property of the Cayley transform,

$$\left|R\right| = 1$$

and thus the Boris push is volume preserving.

2.2.2 Shape functions

2.2.3 The relativistic case

The Boris push algorithm also has a relativistic variant, which takes into account the γ factor. The relativistic version is also volume preserving (Higuera and Cary 2017).

2.3 The field solver

We now turn our attention to the electromagnetic field equations. In order to compute the time evolution of the fields, we will use the equations containing their time derivatives, namely

$$\frac{\partial \mathbf{B}}{\partial t} = -\boldsymbol{\nabla} \times \mathbf{E} \tag{2.8}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c^2 \boldsymbol{\nabla} \times \mathbf{B} - \frac{1}{\varepsilon_0}\mathbf{j}\,. \tag{2.9}$$

Kane Yee (1966) proposed a method for solving Maxwell's equations in isotropic media involving a leapfrog-like algorithm, but with staggering also in space. In order to illustrate this more easily, we will begin with the one dimensional case

$$\begin{aligned} \frac{\partial B_y}{\partial t} &= -\frac{\partial E_x}{\partial z} \\ \frac{\partial E_x}{\partial t} &= -c^2 \frac{\partial B_y}{\partial z} - \frac{1}{\varepsilon_0} j_x\,, \end{aligned}$$

in which the equations are discretized as follows:

$$\frac{B_y^{n+1/2}(k+\frac{1}{2}) - B_y^{n-1/2}(k+\frac{1}{2})}{\Delta t} = -\frac{E_x^n(k+1) - E_x^n(k)}{\Delta z} \tag{2.10a}$$

$$\frac{E_x^{n+1}(k) - E_x^n(k)}{\Delta t} = -c^2 \frac{B_y^{n+1/2}(k+\frac{1}{2}) - B_y^{n+1/2}(k-\frac{1}{2})}{\Delta z} - \frac{1}{\varepsilon_0} j_x^{n+1/2}(k)\,. \tag{2.10b}$$

Let us now take a closer look at these discretizations by comparing with the typical form of the leapfrog algorithm (2.1a). For the magnetic field in equation (2.10a), the time derivatives of the fields are computed using the $B^{n+1/2} - B^{n-1/2}$ difference with the source term at step n. At the same time, for the electric field, the $E(k+1) - E(k)$ difference is used and the source term is at $k + \frac{1}{2}$. Thus, the values for the electric field are taken at integer k and n, but for the magnetic field, we use the values at half-integer k and n, creating thus a staggering in both space and time. Moving on to equation (2.10b), the time derivative for the electric field uses the $E^{n+1} - E^n$ difference with the source term at $n + \frac{1}{2}$ and similarly the magnetic field has the spatial derivative using the $B(k+\frac{1}{2}) - B(k-\frac{1}{2})$ difference with the source term at k. This swap in the steps used by the derivatives can be explained by the fact that in both equations we are observing the field at the same (space-time) points.

We can now generalize equations (2.10) to the 3-dimensional case. In this case Faraday's law in equation (2.8) becomes

$$\begin{aligned} \frac{\partial B_x}{\partial t} &= -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z} \\ \frac{\partial B_y}{\partial t} &= -\frac{\partial E_x}{\partial z} + \frac{\partial E_z}{\partial x} \\ \frac{\partial B_z}{\partial t} &= -\frac{\partial E_y}{\partial x} + \frac{\partial E_x}{\partial y}\,. \end{aligned}$$

To better emphasize the differences from equation (2.10a), we will focus on the O_y components. Thus the discrete form will be given by

$$\begin{aligned} &\frac{B_y^{n+1/2}(i+\frac{1}{2}, j, k+\frac{1}{2}) - B_y^{n-1/2}(i+\frac{1}{2}, j, k+\frac{1}{2})}{\Delta t} = \\ &- \frac{E_x^n(i+\frac{1}{2}, j, k+1) - E_x^n(i+\frac{1}{2}, j, k)}{\Delta z} + \frac{E_z^n(i+1, j, k+\frac{1}{2}) - E_z^n(i, j, k+\frac{1}{2})}{\Delta x}\,. \end{aligned} \tag{2.11}$$

Since it is quite tedious to write everything explicitely, several shorthand notations have been developed. For example, Lehe (2018 15–26 January[a]) uses

$$F^n_{i,j,k} \equiv F^n(i,j,k)$$

and

$$\partial_t F|^n_{i,j,k} \equiv \frac{F^{n+\frac{1}{2}}_{i,j,k} - F^{n-\frac{1}{2}}_{i,j,k}}{\Delta t} \qquad \partial_x F|^n_{i,j,k} \equiv \frac{F^n_{i+\frac{1}{2},j,k} - F^n_{i-\frac{1}{2},j,k}}{\Delta x}$$
$$\partial_y F|^n_{i,j,k} \equiv \frac{F^n_{i,j+\frac{1}{2},k} - F^n_{i,j-\frac{1}{2},k}}{\Delta y} \qquad \partial_z F|^n_{i,j,k} \equiv \frac{F^n_{i,j,k+\frac{1}{2}} - F^n_{i,j,k-\frac{1}{2}}}{\Delta z}\,.$$

With these notations, equation (2.11) becomes

$$\partial_t B_y|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} = -\partial_z E_x|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} + \partial_x E_z|^n_{i+\frac{1}{2},j,k+\frac{1}{2}}$$

and by applying the same for the rest of the components we obtain

$$\begin{aligned}
\partial_t B_x|^n_{i,j+\frac{1}{2},k+\frac{1}{2}} &= -\partial_y E_z|^n_{i,j+\frac{1}{2},k+\frac{1}{2}} + \partial_z E_y|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} \\
\partial_t B_y|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} &= -\partial_z E_x|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} + \partial_x E_z|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} \\
\partial_t B_z|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} &= -\partial_x E_y|^n_{i+\frac{1}{2},j+\frac{1}{2},k} + \partial_y E_x|^n_{i+\frac{1}{2},j+\frac{1}{2},k}\,.
\end{aligned}$$

In a similar fashion, Ampère's law in equation (2.9) becomes

$$\begin{aligned}
\frac{\partial E_x}{\partial t} &= -c^2\frac{\partial B_y}{\partial z} + c^2\frac{\partial B_z}{\partial y} - \frac{1}{\varepsilon_0}j_x \\
\frac{\partial E_y}{\partial t} &= -c^2\frac{\partial B_z}{\partial x} + c^2\frac{\partial B_x}{\partial z} - \frac{1}{\varepsilon_0}j_y \\
\frac{\partial E_z}{\partial t} &= -c^2\frac{\partial B_x}{\partial y} + c^2\frac{\partial B_y}{\partial x} - \frac{1}{\varepsilon_0}j_z
\end{aligned}$$

and the analogue of equation (2.10b) for the Ox axis will be

$$\begin{aligned}
\frac{E_x^{n+1}(i+\frac{1}{2},j,k) - E_x^n(i+\frac{1}{2},j,k)}{\Delta t} &= -c^2\frac{B_y^{n+1/2}(i+\frac{1}{2},j,k+\frac{1}{2}) - B_y^{n+1/2}(i+\frac{1}{2},j,k-\frac{1}{2})}{\Delta z} \\
&\quad + c^2\frac{B_z^{n+1/2}(i+\frac{1}{2},j+\frac{1}{2},k) - B_z^{n+1/2}(i+\frac{1}{2},j-\frac{1}{2},k)}{\Delta x} - \frac{1}{\varepsilon_0}j_x^{n+1/2}\,.
\end{aligned} \tag{2.12}$$

Using the compact notation above, we obtain

$$\begin{aligned}
\partial_t E_x|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k} &= c^2\partial_y B_z|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k} - c^2\partial_z B_y|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k} - \frac{1}{\varepsilon_0}j_x|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k} \\
\partial_t E_y|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k} &= c^2\partial_z B_x|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k} - c^2\partial_x B_z|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k} - \frac{1}{\varepsilon_0}j_y|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k} \\
\partial_t E_z|^{n+\frac{1}{2}}_{i,j,k+\frac{1}{2}} &= c^2\partial_x B_y|^{n+\frac{1}{2}}_{i,j,k+\frac{1}{2}} - c^2\partial_y B_x|^{n+\frac{1}{2}}_{i,j,k+\frac{1}{2}} - \frac{1}{\varepsilon_0}j_z|^{n+\frac{1}{2}}_{i,j,k+\frac{1}{2}}\,.
\end{aligned}$$

We can observe that we have only used tow of the four Maxwell equations to describe the evolution of the fields, so we should check that the other two equations are satisfied. Let us begin with the divergence of the magnetic field

$$\boldsymbol{\nabla}\cdot\mathbf{B} = 0\,.$$

Assuming that the relation is initially valid and

$$\frac{\partial \mathbf{B}}{\partial t} = -\boldsymbol{\nabla} \times \mathbf{E}$$

is satisfied all the time, then

$$\frac{\partial \boldsymbol{\nabla} \cdot \mathbf{B}}{\partial t} = \boldsymbol{\nabla} \cdot \frac{\partial \mathbf{B}}{\partial t} = \boldsymbol{\nabla} \cdot (-\boldsymbol{\nabla} \times \mathbf{E}) = 0\,.$$

The discretized equations thus satisfy $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$ since the above equation vanishes by the cancelation of identical derivative terms. The discretized version of this condition can be written as

$$\partial_x B_x\big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + \partial_y B_y\big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + \partial_z B_z\big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = 0\,.$$

We will now continue with the divergence of the electric field

$$\boldsymbol{\nabla} \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}\,.$$

Again, we suppose that the relation is satisfied initially and that

$$\frac{\partial \mathbf{E}}{\partial t} = c^2 \boldsymbol{\nabla} \times \mathbf{B} - \frac{1}{\varepsilon_0}\mathbf{j}$$

is vaild all the time. Then

$$\frac{\partial}{\partial t}\left(\boldsymbol{\nabla} \cdot \mathbf{E} - \frac{\rho}{\varepsilon_0}\right) = -\frac{1}{\varepsilon_0}\left[\frac{\partial \rho}{\partial t} - \boldsymbol{\nabla} \cdot \left(\frac{1}{\mu_0}\boldsymbol{\nabla} \times \mathbf{B} - \mathbf{j}\right)\right] = -\frac{1}{\varepsilon_0}\left(\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{j}\right)$$

and we can observe that $\boldsymbol{\nabla} \cdot \mathbf{E} = \rho/\varepsilon_0$ is satisfied *if* the continuity equation is respected for all time steps. In its discrete form, the continuity equation is given by

$$\partial_t \rho\big|^{n+\frac{1}{2}}_{i,j,k} + \partial_x j_x\big|^{n+\frac{1}{2}}_{i,j,k} + \partial_y j_y\big|^{n+\frac{1}{2}}_{i,j,k} + \partial_z j_z\big|^{n+\frac{1}{2}}_{i,j,k} = 0\,.$$

2.3.1 Current deposition

2.3.2 Stability

In order to study the stability of the Yee algorithm, we wll take a claser look at the propagation of an electromagnetic wave in vacuum following Lehe (2018 15–26 January[b]).

In order to simplify the calculations, we will begin with the one dimensional case with the electric field on Ox and the magnetic field on Oy. In this case, the propagation of electromagnetic waves is described by equations (2.10), with the current density term dropped. With a more compact notation, this gives

$$\frac{B_{y\,k+1/2}^{\;n+1/2} - B_{y\,k+1/2}^{\;n-1/2}}{\Delta t} = -\frac{E_{x\,k+1}^{\;n} - E_{x\,k}^{\;n}}{\Delta z} \tag{2.13a}$$

$$\frac{E_{x\,k}^{\;n+1} - E_{x\,k}^{\;n}}{\Delta t} = -c^2 \frac{B_{y\,k+1/2}^{\;n+1/2} - B_{y\,k-1/2}^{\;n+1/2}}{\Delta z}\,. \tag{2.13b}$$

In order to better motivate the following derivation, let us consider the continuous (3D) case first. Equations (2.13) are the 1D discretizations of

$$\frac{\partial \mathbf{B}}{\partial t} = -\boldsymbol{\nabla} \times \mathbf{E}$$

$$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \boldsymbol{\nabla} \times \mathbf{B}\,.$$

If we take the time derivative of the second equation, we obtain

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} = \frac{\partial}{\partial t}\boldsymbol{\nabla}\times\mathbf{B} = \boldsymbol{\nabla}\times\left(\frac{\partial \mathbf{B}}{\partial t}\right) = \boldsymbol{\nabla}\times(-\boldsymbol{\nabla}\times\mathbf{E}) = -\boldsymbol{\nabla}\underbrace{(\boldsymbol{\nabla}\cdot\mathbf{E})}_{\text{0 in vacuum}} + \nabla^2\mathbf{E}\,,$$

in which we can recognise the wave equation

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} - \nabla^2\mathbf{E} = \Box\,\mathbf{E} = 0\,.$$

Thus if we divide equation (2.13b) by c^2 and take the time derivative, we should obtain the discretized wave equation. Using centered time differences between equation (2.13b) at time step n and $n-1$, we obtain

$$\frac{1}{c^2}\frac{1}{\Delta t}\left(\frac{E_{x\,k}^{\,n+1} - E_{x\,k}^{\,n}}{\Delta t} - \frac{E_{x\,k}^{\,n} - E_{x\,k}^{\,n-1}}{\Delta t}\right) = \frac{1}{\Delta t}\left(-\frac{B_{y\,k+1/2}^{\,n+1/2} - B_{y\,k-1/2}^{\,n+1/2}}{\Delta z} + \frac{B_{y\,k+1/2}^{\,n-1/2} - B_{y\,k-1/2}^{\,n-1/2}}{\Delta z}\right).$$

The time and space derivatives commute, so we can rearrange the terms in the right hand side to match a centered time derivative and thus obtain

$$\begin{aligned}
\frac{1}{c^2}\frac{E_{x\,k}^{\,n+1} - E_{x\,k}^{\,n}}{\Delta t^2} - \frac{1}{c^2}\frac{E_{x\,k}^{\,n} - E_{x\,k}^{\,n-1}}{\Delta t^2} &= -\frac{B_{y\,k+1/2}^{\,n+1/2} - B_{y\,k-1/2}^{\,n+1/2}}{\Delta z\Delta t} + \frac{B_{y\,k+1/2}^{\,n-1/2} - B_{y\,k-1/2}^{\,n-1/2}}{\Delta z\Delta t} \\
&= -\frac{B_{y\,k+1/2}^{\,n+1/2} - B_{y\,k+1/2}^{\,n-1/2}}{\Delta z\Delta t} + \frac{B_{y\,k-1/2}^{\,n+1/2} - B_{y\,k-1/2}^{\,n-1/2}}{\Delta z\Delta t} \\
&= \frac{E_{x\,k+1}^{\,n} - E_{x\,k}^{\,n}}{\Delta z^2} - \frac{E_{x\,k}^{\,n} - E_{x\,k-1}^{\,n}}{\Delta z}\,,
\end{aligned}$$

where in the last step we used equation (2.13a). We can observe that the terms can be rearranged such that we obtain second order centered time derivatives. Thus we obtain the 1D discrete wave equation

$$\frac{1}{c^2}\frac{E_{x\,k}^{\,n+1} - 2E_{x\,k}^{\,n} + E_{x\,k}^{\,n-1}}{\Delta t^2} = \frac{E_{x\,k+1}^{\,n} - 2E_{x\,k}^{\,n} + E_{x\,k-1}^{\,n}}{\Delta z^2}\,. \tag{2.14}$$

We will now take a closer look at the behaviour of the propagating wave solutions

$$E_{x\,l}^{\,n} = E_0\,\mathrm{e}^{\mathrm{i}kl\Delta z - \mathrm{i}\omega n\Delta t}\,,$$

where we changed to using the l for indexing as not confuse it with the wavenumber k. Using this solution in equation (2.14) gives

$$\begin{aligned}
\frac{E_0\,\mathrm{e}^{\mathrm{i}kl\Delta z}}{c^2}\frac{\mathrm{e}^{-\mathrm{i}\omega(n+1)\Delta t} - 2\,\mathrm{e}^{-\mathrm{i}\omega n\Delta t} + \mathrm{e}^{-\mathrm{i}\omega(n-1)\Delta t}}{\Delta t^2} &= E_0\,\mathrm{e}^{-\mathrm{i}\omega n\Delta t}\frac{\mathrm{e}^{\mathrm{i}k(l+1)\Delta z} - 2\,\mathrm{e}^{\mathrm{i}kl\Delta z} + \mathrm{e}^{\mathrm{i}k(l-1)\Delta z}}{\Delta z^2} \\
\frac{\mathrm{e}^{\mathrm{i}kl\Delta z - \mathrm{i}\omega n\Delta t}}{c^2}\frac{\mathrm{e}^{-\mathrm{i}\omega\Delta t} - 2 + \mathrm{e}^{\mathrm{i}\omega\Delta t}}{\Delta t^2} &= \mathrm{e}^{-\mathrm{i}\omega n\Delta t + \mathrm{i}kl\Delta z}\frac{\mathrm{e}^{\mathrm{i}k\Delta z} - 2 + \mathrm{e}^{-\mathrm{i}k\Delta z}}{\Delta z^2} \\
\frac{1}{c^2}\frac{\mathrm{e}^{-\mathrm{i}\omega\Delta t} - 2 + \mathrm{e}^{\mathrm{i}\omega\Delta t}}{\Delta t^2} &= \frac{\mathrm{e}^{\mathrm{i}k\Delta z} - 2 + \mathrm{e}^{-\mathrm{i}k\Delta z}}{\Delta z^2} \\
\frac{1}{c^2\Delta t^2}\left(\mathrm{e}^{-\mathrm{i}\omega\Delta t/2} - \mathrm{e}^{\mathrm{i}\omega\Delta t/2}\right)^2 &= \frac{1}{\Delta z^2}\left(\mathrm{e}^{-\mathrm{i}k\Delta z/2} - \mathrm{e}^{\mathrm{i}k\Delta z/2}\right)^2.
\end{aligned}$$

Using Euler's formula

$$\mathrm{e}^{\mathrm{i}x} = \cos x + \mathrm{i}\sin x\,,$$

we obtain

$$\frac{1}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z^2}\sin^2\left(\frac{k\Delta z}{2}\right). \tag{2.15}$$

Equation (2.15) is a dispersion relation for the discrete one dimensional wave propagation. In the continuous case the dispersion relation is $\omega^2 = c^2k^2$.

If we take the square root of equation (2.15)

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

we observe that we obtain real solutions for ω, for any k

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

only if $c\Delta t \leq \Delta z$.

Thus the phase velocity of electromagnetic waves $v_\phi = \omega/k$ will be given by

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

This means that in a 1D PIC code that is using the Yee discretizations, electromagnetic waves in vacuum propagate with a velocity depending on k, instead at the (constant) speed of light. This phenomena is called *numerical dispersion*. Since the wavenumber is inverse proportional to the wavelength, electromagnetic waves with shoter wavelengths will propagate slower.

For $c\Delta t \geq \Delta z$, the discrete dispersion relation given by equation (2.15) has no real solutions in the limit $k \to \pi/\Delta z$. The solution is imaginary and the corresponding mode is said to be unstable. As a consequence, PIC codes using FDTD methods like presented here are restricted to $c\Delta t \leq \Delta z$. This is called the *Courant limit*. This coupling between Δz and Δt places an upper bound on how fast can a simulation advance. Moreover, Δz is tightly coupled with the physics of the simulation, since it must be chose such that it can resolve the smallest features of the given problem.

This kind of analysis can be extended in a straightforward way to the 3D case. In this case the discrete version of the solution to the wave equation will be given by

$$E = E_0\,\mathrm{e}^{\mathrm{i}k_x x + \mathrm{i}k_y y + \mathrm{i}k_z z - \mathrm{i}\omega t}.$$

Similarly, the 3D dispersion relation will be given by

$$\frac{1}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right) + \frac{1}{\Delta y^2}\sin^2\left(\frac{k_y\Delta y}{2}\right) + \frac{1}{\Delta z^2}\sin^2\left(\frac{k_z\Delta z}{2}\right)$$

and the 3D Courant condition by

$$c\Delta t \leq \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}.$$

As we can see from the dispersion relation, in the 3D case, the phase velocity will depend on wavelength and propagation direction.

Name	Type	GPU ready	Scalability
EPOCH	EM 3D	No	MPI
Osiris	EM 3D, RZ*, RZ**	No	MPI, OpenMP, SIMD
VSim	EM 3D	No	MPI
PIConGPU	EM 3D	Yes	MPI, CUDA-ALPAKA
FBPIC	EM 3D, RZ***	Yes	MPI, NUMBA
Warp	EM 3D, PS*, RZ*, RZ**	No	MPI, OpenMP
WarpX	EM 3D, PS*, RZ*, RZ**	No	MPI, OpenMP, SIMD
VPIC	EM 3D	No	MPI, pthreads, SIMD
Architect	EM RZ	No	MPI
Wake	QS RZ	No	MPI
QuickPIc	QS RZ	No	MPI
PICLS	EM 3D	No	MPI

Table 2.1: Commonly used simulation programs

2.4 A survey of available PIC codes

Frequently used simulation programs include

In the above table we used the following abbreviations

- EM: Electromagnetic PIC
- QS: Quasi-Static PIC
- 3D: Cartesian coordinates, up to 3D
- RZ: Cylindrical geometry with FDTD method in r and z directions
- RZ*: Cylindrical geometry with Fourier azimuthal decomposition
- RZ**: Cylindrical geometry with FDTD method in r direction and FFT-based pseudo-spectral method in z direction
- RZ***: Cylindrical geometry with Henkel transform in r direction and FFT-based pseudo-spectral method in z direction
- PS: Pseudo-spectral Maxwell solver with global Fourier transform
- PS*: Pseudo-spectral Maxwell solver with domain decomposition and local Fourier transform

2.5 EPOCH

Chapter 3

Results

Add something

Chapter 4

Conclusions

In this thesis we have studied ...

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