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LASER WAKEFIELD ACCELERATION
Studies using Particle in Cell Method

Master Thesis

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Contents

Introduction

Add stuff here Tajima and Dawson 1979.

Chapter 1

Classical Electrodynamics

Introduction stuff, cite Eisenberg and Greiner (1978) and Jackson (1999).

We will 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, which must satisfy an additional equation 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 (1.1c) and (1.1b) 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 suggets 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 paranthesis 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 (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 (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

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

eq. (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 eq. (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 eq. (1.11), the second term in eq. (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 Helmholz 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

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

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 (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 eq. (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 homogenuous 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 (1.1c) for the first term.

Using this result, the power transferred by the fileds 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 wity

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

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 fileds 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

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 discusion in Karsch (2018). The starting point is the equation of motion for the electron

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -e\left[\mathbf{E}(\mathbf{r},t) + \mathbf{v}\times\mathbf{B}(\mathbf{r},t)\right]\ . \tag{1.16}$$

1.4.1 Non-relativistic treatment

1.4.2 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 rquires 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 rearange 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 centeral diference 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

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

Replacing the velocity, we obtain

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

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 $\mathbf{X}_n$

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

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

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

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 can be 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

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

$$\frac{\mathbf{v}_{n+1/2} - \mathbf{v}_{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}_n) + \frac{\mathbf{v}_{n+1/2} + \mathbf{v}_{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}_n)\right). \tag{2.4}$$

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 (2.4) we obtain

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{q}{2m}(\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}, \tag{2.5}$$

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

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

Rewriting equation (2.5) we obtain

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

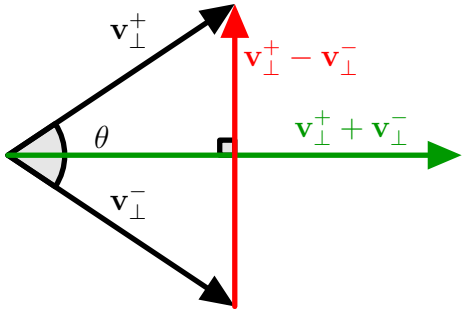

Figure 2.1: Boris rotation angle

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

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

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

$$\tan\frac{\theta}{2} = \frac{qB}{m}\frac{\Delta t}{2}\,. \tag{2.6}$$

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 trinagle 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 (2.6) $\mathbf{t}$ is given by

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

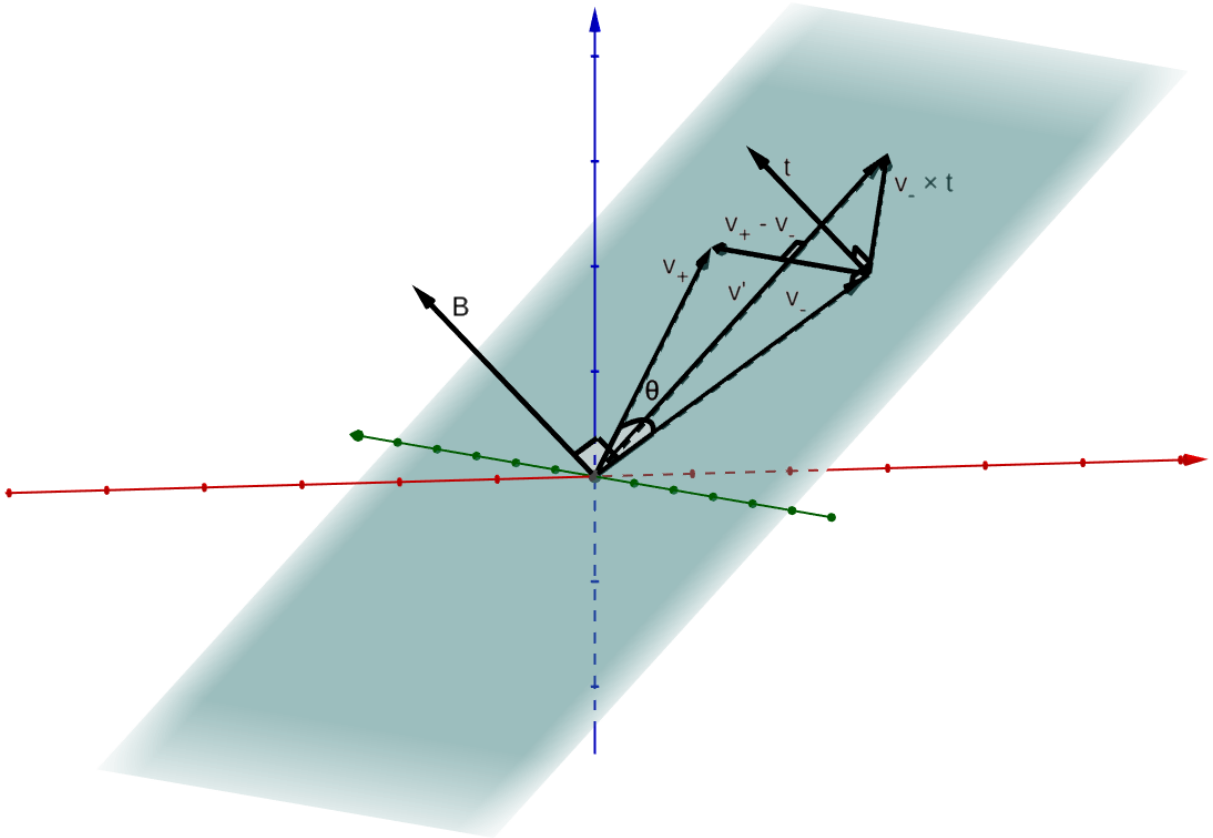

Figure 2.2: Boris rotation construction in 3D

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

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

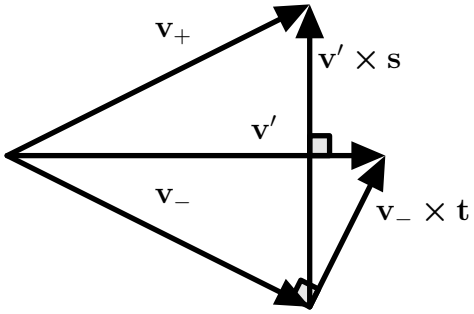

Figure 2.3: The velocities projected in the plane perpendicular to $\mathbf{B}$

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 (2.4) 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.

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.

An 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 beggining 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 evereywhere 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 (2.4) 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 mainfold 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 (2.4) and we obtain

$$\left(I - \hat{\Omega}_n\right) \begin{pmatrix} v^1_{n+1/2} \\ v^2_{n+1/2} \\ v^3_{n+1/2} \end{pmatrix} = \left(I + \hat{\Omega}_n\right) \begin{pmatrix} v^1_{n-1/2} \\ v^2_{n-1/2} \\ v^3_{n-1/2} \end{pmatrix} + \frac{q\Delta t}{m} \begin{pmatrix} E^1_n \\ E^2_n \\ E^3_n \end{pmatrix} , \tag{2.7}$$

where

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

[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 (2.7) 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 (2.3) and (2.4) 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 simplecticty condition can be written as

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

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

Thus, we will have the following set of conditions

$$S_3^T S_1 = S_1^T S_3 \tag{2.8}$$
$$S_1^T S_4 - S_3^T S_2 = I \tag{2.9}$$
$$S_4^T S_1 - S_2^T S_3 = I \tag{2.10}$$
$$S_4^T S_2 = S_2^T S_4 \,. \tag{2.11}$$

If we consider the simplifed case of homogenuous 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

$$S_1 = I \quad S_2 = R\Delta t$$
$$S_3 = 0 \quad S_4 = R \,.$$

If we consider the condition in equation (2.9), 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

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

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.

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

2.4 A survey of available PIC codes

Frequently used simulation programs include

In the above table we used the following abbreviations

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

- 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 golbal 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 ...

Bibliography

Tajima, T. and J. M. Dawson (July 23, 1979). "Laser Electron Accelerator". In: *Physical Review Letters* 43.4, pp. 267–270. DOI: 10.1103/PhysRevLett.43.267.

Eisenberg, Judah M. and Walter Greiner (1978). *Nuclear Theory. 2: Excitation Mechanisms of the Nucleus*. 2., rev. ed., 1. repr. OCLC: 256795525. Amsterdam: North-Holland [u.a.] 421 pp. ISBN: 978-0-7204-0483-8.

Jackson, John David (1999). *Classical Electrodynamics*. 3rd ed. New York: Wiley. 808 pp. ISBN: 978-0-471-30932-1.

Karsch, Stefan (2018). "Applications of High Intensity Laser Pulse". Lecture Notes. Lecture Notes. Ludwig-Maximilians-University Munich. URL: https://www.physik.uni-muenchen.de/lehre/vorlesungen/sose_18/applications_of_high-intensity_laser-pulses/vorlesung/LaserMatter.pdf (visited on 06/09/2019).

Arber, T D et al. (Nov. 1, 2015). "Contemporary Particle-in-Cell Approach to Laser-Plasma Modelling". In: *Plasma Physics and Controlled Fusion* 57.11, p. 113001. ISSN: 0741-3335, 1361-6587. DOI: 10.1088/0741-3335/57/11/113001.

Hockney, Roger W. and James W. Eastwood (1988). *Computer Simulation Using Particles*. Special student ed. Bristol [England]; Philadelphia: A. Hilger. 540 pp. ISBN: 978-0-85274-392-8.

Butcher, J. C. (2016). *Numerical Methods for Ordinary Differential Equations*. Third edition. Chichester, West Sussex, United Kingdom: Wiley. 513 pp. ISBN: 978-1-119-12150-3.

Leimkuhler, B. and Sebastian Reich (2004). *Simulating Hamiltonian Dynamics*. Cambridge Monographs on Applied and Computational Mathematics 14. Cambridge, UK; New York: Cambridge University Press. 379 pp. ISBN: 978-0-521-77290-7.

Buneman, O (June 1967). "Time-Reversible Difference Procedures". In: *Journal of Computational Physics* 1.4, pp. 517–535. ISSN: 00219991. DOI: 10.1016/0021-9991(67)90056-3.

Birdsall, Charles K and A. Bruce Langdon (2005). *Plasma Physics via Computer Simulation*. OCLC: 968173834. Bristol: Institute of Physics Pub. ISBN: 978-1-4822-6306-0. URL: http://public.eblib.com/choice/publicfullrecord.aspx?p=1675636 (visited on 06/21/2019).

Boris, Jay P. (Nov. 2, 1970). "Relativistic Plasma Simulation–Optimization of a Hybrid Code". In: *Fourth Conference on Numerical Simulations of Plasmas*. Naval Research Laboratory, Washington, D.C.: Defense Technical Information Center, pp. 3–67. URL: http://archive.org/details/DTIC_ADA023511 (visited on 08/07/2019).

Qin, Hong et al. (Aug. 1, 2013). "Why Is Boris Algorithm so Good?" In: *Physics of Plasmas* 20.8, p. 084503. ISSN: 1070-664X. DOI: 10.1063/1.4818428.

Arnol'd, V. I. (1989). *Mathematical Methods of Classical Mechanics*. 2nd ed. Graduate Texts in Mathematics. New York: Springer-Verlag. ISBN: 978-0-387-96890-2. URL: https://www.springer.com/gp/book/9780387968902 (visited on 08/11/2019).

Golomb, Solomon W. (Mar. 1, 1985). "Proof without Words: A 2 × 2 Determinant Is the Area of a Parallelogram". In: *Mathematics Magazine* 58.2, p. 107. ISSN: 0025570X. DOI: 10.2307/2689900. JSTOR: 10.2307/2689900?origin=crossref.

Hairer, Ernst, Christian Lubich, and Gerhard Wanner (2006). *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*. 2nd ed. Springer Series in Computational Mathematics 31. OCLC: ocm69223213. Berlin; New York: Springer. 644 pp. ISBN: 978-3-540-30663-4.

Marsden, Jerrold E. and Tudor S. Ratiu (1999). *Introduction to Mechanics and Symmetry: A Basic Exposition of Classical Mechanical Systems*. Red. by Jerrold E. Marsden et al. Vol. 17. Texts in Applied Mathematics. New York, NY: Springer New York. ISBN: 978-1-4419-3143-6 978-0-387-21792-5. DOI: 10.1007/978-0-387-21792-5. URL: http://link.springer.com/10.1007/978-0-387-21792-5 (visited on 08/10/2019).

Hairer, Ernst and Christian Lubich (Dec. 2018). "Energy Behaviour of the Boris Method for Charged-Particle Dynamics". In: *BIT Numerical Mathematics* 58.4, pp. 969–979. ISSN: 0006-3835, 1572-9125. DOI: 10.1007/s10543-018-0713-1.

Higuera, A. V. and J. R. Cary (Apr. 24, 2017). "Structure-Preserving Second-Order Integration of Relativistic Charged Particle Trajectories in Electromagnetic Fields". In: *Physics of Plasmas* 24.5, p. 052104. ISSN: 1070-664X. DOI: 10.1063/1.4979989.