Introduction to Computational Physics

Maxwell & More - 1

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The General Problem Statement I

Vast majority of plasma physics in contained in the Vlasov-Maxwell-Boltzmann equations that describe self-consistent evolution of distribution function $f(\mathbf{x}, \mathbf{v}, t) \in \mathbb{R}^{3\times3\times1}$ and electromagnetic fields:

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f_s) + \nabla_{\mathbf{v}} \cdot (\mathbf{F}_s f_s) = \left(\frac{\partial f_s}{\partial t}\right)_c$$

where $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. The EM fields are determined from Maxwell equations

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

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$$

$$\nabla \times \mathbf{B} - \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J} = \mu_0 \sum_s q_s \int_{-\infty}^{\infty} \mathbf{v} f_s \, d\mathbf{v}^3$$

The General Problem Statement II

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field. This means the polarization, magnetization together with the electric conductivity.

$$\begin{aligned} \mathbf{D} &= \varepsilon_0 \varepsilon_r \mathbf{E} \\ \mathbf{B} &= \mu_0 \mu_r \mathbf{H}. \end{aligned}$$

Remarks

- *highly nonlinear: fields tell particles how to move*
- *particle motion generates fields*
- *acceleration of particles generate radiation*
- *theoretical and computational plasma physics consists of making approximations and solving these equations in specific situations.*
- *for the rest of the discussion we assume*
  - *no material dispersion* ($v \neq v(f)$)
  - $\varepsilon_r = 1, \mu_r = 1$

Why is solving Vlasov-Maxwell equations directly so hard?

Despite being the fundamental equation in plasma physics the Vlasov-Maxwell equations remain highly challenging to solve.

- collisions can further complicate things due to long-range forces in a plasma; dominated by small-angle collisions
- high dimensionality and multiple species with large mass ratios: 6D phase-space, $m_e/m_p = 1/1836$ and possibly dozens of species.
- enormous scales in the system: light speed and electron plasma oscillations; cyclotron motion of electrons and ions; fluid-like evolution on intermediate scales; resistive slow evolution of near-equilibrium states; transport scale evolution in tokamak discharges. 14 orders of magnitude of physics in these equations!

Many approximations developed over the decades

Modern computational plasma physics consists of making justified approximations to the Vlasov-Maxwell system and then coming up with efficient schemes to solve them.

- Major recent theoretical development in plasma physics is the discovery of gyrokinetic equations, an asymptotic approximation for plasmas in strong magnetic fields. Reduces dimensionality to 5D (from 6D) and eliminates cyclotron frequency and gyroradius from the system. Very active area of research.
- Many fluid approximations have been developed to treat plasma via low-order moments: extended MHD models; multi-moment models; various reduced MHD equations
- Numerical methods for these equations have undergone renaissance in recent years: emphasis on *memetic* schemes that preserve conservation laws and some geometric features of the continuous equations. Based on Lagrangian and Hamiltonian formulation of basic equations. Very active area of research.

With advent of large scale computing much research is now focused on schemes that scale well on thousands (millions) of CPU/GPU cores.

Goal of this course is to look at some key schemes and study their properties

Computational plasma physics is vast: we can only cover a (very) small fraction of interesting methods. In this class we will focus on

- Solving the Vlasov-Maxwell equations using particles, the "Particle-in-cell" method; methods to solve Maxwell equations. This is probably the most widely used method that yields reasonable results for many kinetic problems
- Shock-capturing methods for plasma fluid equations. These are particularly relevant to astrophysical problems in which flows can be supersonic or super-Alfvenic. A brief look at fluid solvers for use in fusion machines (tokamaks, stellarators) in which dynamics is much slower.
- Directly discretizing the Vlasov-Maxwell equations as a PDE in 5D/6D. This is an emerging area of active research and may open up study of turbulence in fusion machines and also exploring fundamental plasma physics in phase-space.

Conservation properties of Vlasov-Maxwell equations

It is important to design methods that preserve at least some properties of continuous Vlasov-Maxwell system. Define the moment operator for any function $\varphi(\mathbf{v})$ as

$$\langle \varphi(\mathbf{v}) \rangle_s \equiv \int_{-\infty}^{\infty} \varphi(\mathbf{v}) f_s(t, \mathbf{x}, \mathbf{v}) \, d^3\mathbf{v}.$$

The Vlasov-Maxwell system conserves particles:

$$\frac{d}{dt} \int_\Omega \sum_s \langle 1 \rangle_s \, d^3\mathbf{x} = 0.$$

The Vlasov-Maxwell system conserves total (particles plus field) momentum.

$$\frac{d}{dt} \int_\Omega \left(\sum_s \langle m_s \mathbf{v} \rangle_s + \varepsilon_0 \mathbf{E} \times \mathbf{B} \right) \, d^3\mathbf{x} = 0.$$

The Vlasov-Maxwell system conserves total (particles plus field) energy.

$$\frac{d}{dt} \int_\Omega \left(\sum_s \langle \frac{1}{2} m_s |\mathbf{v}|^2 \rangle_s + \frac{\varepsilon_0}{2} |\mathbf{E}|^2 + \frac{1}{2\mu_0} |\mathbf{B}|^2 \right) \, d^3\mathbf{x} = 0.$$

Conservation properties of Vlasov-Maxwell equations

Besides the fundamental conservation laws, in the *absence of collisions* we can also show that

$$\frac{d}{dt}\int_K \frac{1}{2} f_s^2 \, d\mathbf{z} = 0,$$

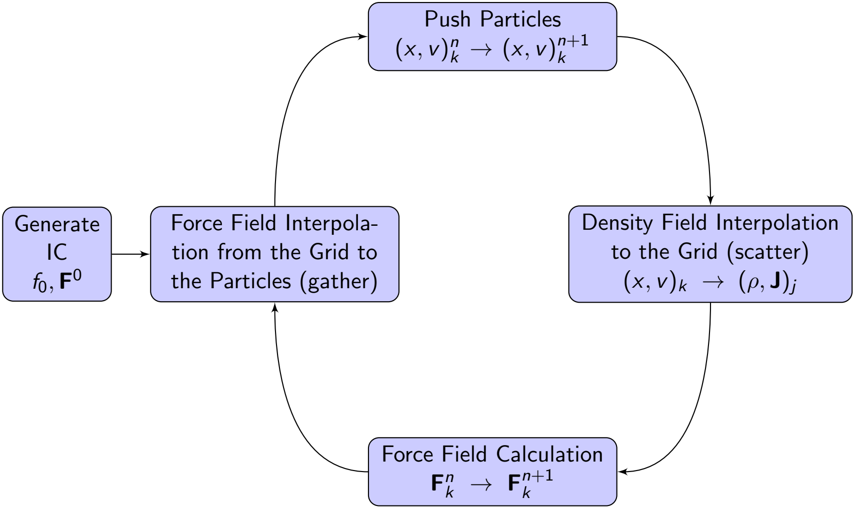
where the integration is taken over the complete phase-space. Also, the entropy is a *non-decreasing* function of time

$$\frac{d}{dt}\int_K -f_s \ln(f_s) \, d\mathbf{z} \geq 0.$$

For collision-less system the entropy remains *constant*.

- It is not always possible to ensure all these properties are preserved numerically. For example: usually one can either ensure momentum *or* energy conservation but not both; it is very hard to ensure $f(t, \mathbf{x}, \mathbf{v}) > 0$.
- Much of modern computational plasma physics research is aimed towards constructing schemes that preserve these properties.

Coupling Particle Dynamics with Fields I



Single particle motion in an electromagnetic field

- In the *Particle-in-cell* (PIC) method the Vlasov-Maxwell equation is solved in the *Lagrangian frame* in which the phase-space is represented by *finite-sized* "macro-particles".
- In the Lagrangian frame the distribution function remains constants along *characteristics* in phase-space.
- These characteristics satisfy the ODE of particles moving under Lorentz force law

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$
$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}(\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t))$$

- We will first focus on solving the equations-of-motion for the macro-particles

Single particle motion in an electromagnetic field

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$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}(\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t))$$

- In the absence of an electric field, the kinetic energy must be conserved

$$\frac{1}{2}|\mathbf{v}|^2 = \text{constant}.$$

This is independent of the spatial or time dependence of the magnetic field. Geometrically this means that in the absence of an electric field the velocity vector rotates and its tip always lies on a sphere.

Single particle motion in an electromagnetic field

- A mid-point scheme for this equation system would look like

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^{n}}{\Delta t} = \frac{\mathbf{v}^{n+1} + \mathbf{v}^{n}}{2}$$

$$\frac{\mathbf{v}^{n+1} - \mathbf{v}^{n}}{\Delta t} = \frac{q}{m}\left(\overline{\mathbf{E}}(\mathbf{x}, t) + \frac{\mathbf{v}^{n+1} + \mathbf{v}^{n}}{2} \times \overline{\mathbf{B}}(\mathbf{x}, t)\right)$$

  The overbars indicate some averaged electric and magnetic fields evaluated from the new and old positions.

- Instead, we will use a *staggered* scheme in which the position and velocity are staggered by half a time-step.

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^{n}}{\Delta t} = \mathbf{v}^{n+1/2}$$

$$\frac{\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}^{n}, t^{n}) + \frac{\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}^{n}, t^{n})\right)$$

The Boris algorithm for the staggered scheme

The velocity update formula is

$$\frac{\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}^n, t^n) + \frac{\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}^n, t^n)\right)$$

This appears like an implicit method: most obvious is to construct a linear 3×3 system of equations and invert them to determine $\mathbf{v}^{n+1}$. Puzzle to test your vector-identity knowledge: find $\mathbf{A}$ if $\mathbf{A} = \mathbf{R} + \mathbf{A} \times \mathbf{B}$.

The Boris algorithm updates this equation in three steps:

$$\begin{aligned}
\mathbf{v}^{-} &= \mathbf{v}^{n-1/2} + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2} \\
\frac{\mathbf{v}^{+} - \mathbf{v}^{-}}{\Delta t} &= \frac{q}{2m}(\mathbf{v}^{+} + \mathbf{v}^{-}) \times \mathbf{B}^n \\
\mathbf{v}^{n+1/2} &= \mathbf{v}^{+} + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2}
\end{aligned}$$

Exercise: convince yourself that this is indeed equivalent to the staggered expression above. So we have two electric field updates with half time-steps and a rotation due to the magnetic field. Once the updated velocity is computed, we can trivially compute the updated positions.

The Boris algorithm for the staggered scheme

How to do the rotation? The Boris algorithm does this in several steps:

- Compute the $\mathbf{t}$ and $\mathbf{s}$ vectors as follows

$$\mathbf{t} = \tan\left(\frac{qB}{m}\frac{\Delta t}{2}\right)\frac{\mathbf{B}}{B} \approx \frac{q\mathbf{B}}{m}\frac{\Delta t}{2}$$
$$\mathbf{s} = \frac{2\mathbf{t}}{1+|\mathbf{t}|^2}$$

- Compute $\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$ and finally $\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$.

Note that using the approximate form in computing $\mathbf{t}$ will lead to *an error in the gyroangle*.

Exercise: show that in the absence of an electric field the Boris algorithm conserves kinetic energy.

Why is the Boris algorithm so good? Can one do better? I

- The relativistic Boris algorithm does not properly compute the $\mathbf{E} \times \mathbf{B}$ velocity. This can be corrected. For example Vay, Phys. Plasmas, **15**, 056701 (2008). The Vay algorithm however, breaks the phase-space volume preserving property of the Boris algorithm.
- See paper by Qin at. al. Phys. Plasmas, **20**, 084503 (2013) in which it is shown that the Boris algorithm *conserves phase-space volume*.
- Toggweiler, M., AA, Arbenz, P., & Yang, J. (2014). A novel adaptive time stepping variant of the Boris-Buneman integrator for the simulation of particle accelerators with space charge. JCP, **273**, 255-267.
- Higuera and Cary, Phys. Plasmas, **24**, 052104 (2017) showed how to compute the correct $\mathbf{E} \times \mathbf{B}$ drift velocity and restore volume preserving property. Seems this is probably the current-best algorithm for updating Lorentz equations.

Why is the Boris algorithm so good? Can one do better? II

Remark

The saga for better particle push algorithms is not over! For example, an active area of research is to discover good algorithms for asymptotic systems, for example, when gyroradius is much smaller than gradient length-scales or gyrofrequency is much higher than other time-scales in the system. Common in most magnetized plasmas.

Recall Maxwell's Equations I

Consider a general first order linear PDE system

$$\frac{\partial \mathbf{u}}{\partial t} = -\mathcal{L}\mathbf{u} = f$$

where u is called a state variable, $\mathcal{L}$ is a linear operator depending on a set of parameters q, and f is a source term.
Examples are,

- $\mathcal{L} = c\frac{\partial}{\partial x}$ yields a wave equation.
- $\mathbf{u} = (H, E)^T$ and

  $$\mathcal{L} = \begin{bmatrix} 0 & \frac{1}{\mu}\frac{\partial}{\partial x} \\ -\frac{1}{\varepsilon}\frac{\partial}{\partial x} & 0 \end{bmatrix}$$

  yields 1D Maxwell's equations in a dielectric, equivalent to the wave equation with speed $c = \sqrt{1/\varepsilon\mu}$.

Recall Maxwell's Equations II

- $\mathbf{u} = (\mathbf{H}, \mathbf{E})^T$ and

$$\mathcal{L} = \begin{bmatrix} 0 & \frac{1}{\mu}\nabla\times \\ -\frac{1}{\varepsilon}\nabla\times & 0 \end{bmatrix}$$

  yields 3D Maxwell curl equations in a non-dispersive dielectric.

E as electric field and **H** as magnetic field vector.
With ρ and **J** we have electric and current charge densities respectively.
The flux densities are denoted by **D** for the electric flux density and and **B** the magnetic flux density. Appropriate initial conditions and boundary conditions are always assumed.

Recall Maxwell's Equations III

$$
\begin{aligned}
&\text{Gauss' law} && \nabla \cdot \mathbf{E}(\mathbf{x}, t) = \frac{1}{\varepsilon_0}\rho(\mathbf{x}, t) && \text{(1a)}\\
&\text{Faraday's law} && \nabla \times \mathbf{E}(\mathbf{x}, t) = -\frac{\partial \mathbf{H}(\vec{x}, t)}{\partial t} && \text{(1b)}\\
&\text{Ampère's law} && \nabla \times \mathbf{H}(\mathbf{x}, t) = \mu_0 \mathbf{J}(\mathbf{x}, t) + \frac{1}{c^2}\frac{\partial \mathbf{E}(\mathbf{x}, t)}{\partial t} && \text{(1c)}\\
&\text{no mag. charges} && \nabla \cdot \mathbf{H}(\mathbf{x}, t) = 0. && \text{(1d)}
\end{aligned}
$$

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field. This means the polarization, magnetization together with the electric conductivity. We are not considering this and furtherrmore assume no material dispersion, i.e.,

Recall Maxwell's Equations IV

the speed of propagation is not frequency dependent. As a consequence the following relations hold:

$$\begin{aligned} \mathbf{D} &= \varepsilon \mathbf{E} \\ \mathbf{B} &= \mu \mathbf{H}. \end{aligned}$$

The time evolution of the fields is thus completely specified by the curl equations

$$\begin{aligned} \varepsilon \frac{\partial \mathbf{E}}{\partial t} &= \nabla \times \mathbf{H} \\ \mu \frac{\partial \mathbf{H}}{\partial t} &= -\nabla \times \mathbf{E}. \end{aligned}$$

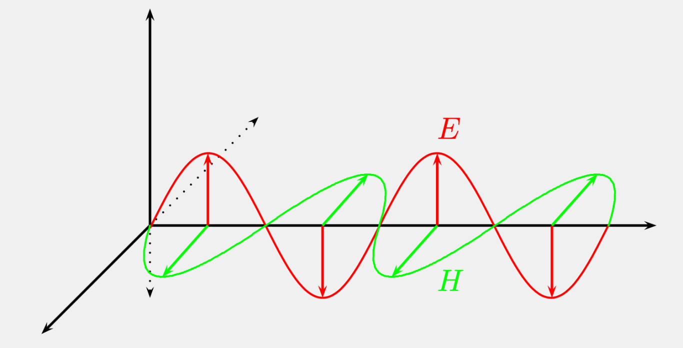
The system above can be combined to a single second order equation for $\mathbf{E}$

$$\varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} = 0.$$

Recall Maxwell's Equations V

This is often referred to as the curl-curl equation or the vector wave equation.

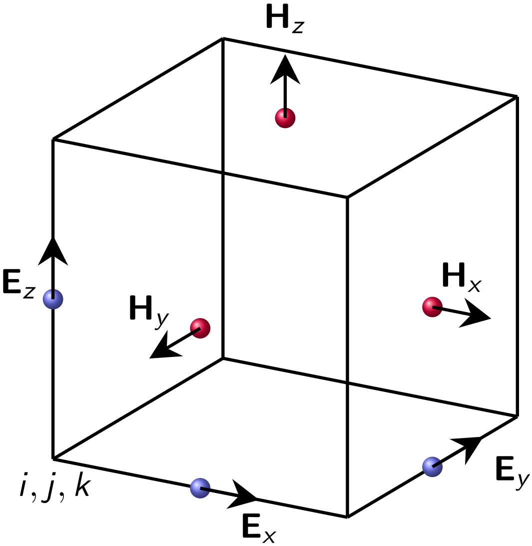
Assuming that the electric field is polarized to oscillate only in the y direction, propagate in the x direction, and there is uniformity in the z direction:



Solving Maxwell equations

- Maxwell equations have a very special geometric structure
- (In spacetime formulations the complete electromagnetic field is represented as a single bivector in 4D space-time).
- In 1966 Kane Yee originated a set of finite-difference equations for the time dependent Maxwell's curl equations
- The Yee algorithm, often called the finite-difference time-domain algorithm is the most successful (and simple) algorithm that accounts of this geometric structure. It is implemented in most PIC codes, though recent research has focused on structure preserving finite-element and other methods.

Solving Maxwell equations: The Yee-cell



Solving Maxwell equations: The Yee-cell

On the Yee-cell the difference approximation to Maxwell equations "falls out", almost like magic. The updates are staggered in time and use two *different* discrete curl operators:

$$
\begin{aligned}
\mathbf{E}^{n+\frac{1}{2}} &= \mathbf{E}^{n-\frac{1}{2}} + \frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{\Delta t}{h}\nabla_F \times \mathbf{B}^n \\
\mathbf{H}^{n+1} &= \mathbf{H}^n + \frac{-1}{\sqrt{\varepsilon_0\mu_0}}\frac{\Delta t}{h}\nabla_E \times \mathbf{E}^n
\end{aligned}
$$

Here the symbols $\nabla_F\times$ and $\nabla_E\times$ are the discrete curl operators:

- The first takes *face-centered* magnetic field and computes it curl. This operator *puts the result on cell edges*.
- The second takes *edge-centered* electric field and computes it curl. This operator *puts the result on cell faces*.
- The structure of Yell-cell also indicates that *currents* must be co-located with the electric field and computed at half time-steps.

This duality neatly reflects the underlying geometry of Maxwell equations. The staggering in time reflects the fact that in 4D the electromagnetic field is a bivector in spacetime.

Divergence relations are exactly maintained

We can show that the discrete Maxwell equations on a Yee-cell maintain the divergence relations exactly:

$$\nabla_F \cdot \mathbf{H}^{n+1/2} = 0$$
$$\nabla_E \cdot \mathbf{E}^n = 0.$$

There is an additional constraint of Maxwell equations in a plasma, that is, the current conservation:

$$\frac{\partial \varrho_c}{\partial t} + \nabla \cdot \mathbf{J} = 0.$$

where ϱ_c is the charge density and $\mathbf{J}$ is the current density. On the Yell-cell this becomes

$$\frac{\varrho_c^{n+1} - \varrho_v^n}{\Delta t} + \nabla_E \cdot \mathbf{J}^{n+1/2} = 0.$$

One must ensure that current from particles is computed carefully to ensure that this expression is satified. See Esirkepov, Comp. Phys. Communications, **135** 144-153 (2001).

Solving Maxwell's Equations in 1D I

- we replace spatial & time derivatives in the two Maxwell's curl equations by central finite difference approximation
- For the time-dependent and source free ($\boldsymbol{J} = 0$) Maxwell's curl equations in vacuum we obtain 6 equations:

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E}, \quad \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon_0} \nabla \times \mathbf{H}$$

$$\begin{aligned}
\frac{\partial \mathbf{E}_x}{\partial t} &= \frac{1}{\varepsilon_0}\left(\frac{\partial \mathbf{H}_z}{\partial y} - \frac{\partial \mathbf{H}_y}{\partial z}\right), & \frac{\partial \mathbf{H}_x}{\partial t} &= \frac{1}{\varepsilon_0}\left(\frac{\partial \mathbf{E}_y}{\partial z} - \frac{\partial \mathbf{E}_z}{\partial y}\right) \\
\frac{\partial \mathbf{E}_y}{\partial t} &= \frac{1}{\varepsilon_0}\left(\frac{\partial \mathbf{H}_x}{\partial z} - \frac{\partial \mathbf{H}_z}{\partial x}\right), & \frac{\partial \mathbf{H}_y}{\partial t} &= \frac{1}{\varepsilon_0}\left(\frac{\partial \mathbf{E}_z}{\partial x} - \frac{\partial \mathbf{E}_x}{\partial z}\right) \\
\frac{\partial \mathbf{E}_z}{\partial t} &= \frac{1}{\varepsilon_0}\left(\frac{\partial \mathbf{H}_y}{\partial x} - \frac{\partial \mathbf{H}_x}{\partial y}\right), & \frac{\partial \mathbf{H}_z}{\partial t} &= \frac{1}{\varepsilon_0}\left(\frac{\partial \mathbf{E}_x}{\partial y} - \frac{\partial \mathbf{E}_y}{\partial x}\right)
\end{aligned}$$

Let's look at 1d, i.e.

Solving Maxwell's Equations in 1D II

- linearly polarized wave along z-axis
- exciting an electric field which has $\mathbf{E}_x$
- propagation along the z-axis
- no variation in the x-y plane: $\partial/\partial_x = \partial/\partial_y = 0$

Now the above 6 equations from 2 Maxwell's curl equations reduce to 2 equations for 1-D FDTD.

$$\frac{\partial \mathbf{E}_x}{\partial t} = \frac{1}{\varepsilon_0}\left(-\frac{\partial \mathbf{H}_y}{\partial z}\right), \qquad \frac{\partial \mathbf{H}_y}{\partial t} = \frac{1}{\varepsilon_0}\left(-\frac{\partial \mathbf{E}_x}{\partial z}\right)$$

Discretize in space and time: $z = k\Delta z$ and $t = n\Delta t$.

Solving Maxwell's Equations in 1D III

$$\frac{\mathbf{E_x}{}_k^{n+\frac{1}{2}} - \mathbf{E_x}{}_k^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\varepsilon_0}\frac{\mathbf{H_y}{}_{k+\frac{1}{2}}^{n} - \mathbf{H_y}{}_{k-\frac{1}{2}}^{n}}{\Delta z}$$
$$\frac{\mathbf{H_y}{}_{k+\frac{1}{2}}^{n+1} - \mathbf{H_y}{}_{k+\frac{1}{2}}^{n}}{\Delta t} = -\frac{1}{\mu_0}\frac{\mathbf{E_x}{}_{k+1}^{n+\frac{1}{2}} - \mathbf{E_x}{}_{k}^{n+\frac{1}{2}}}{\Delta z}$$

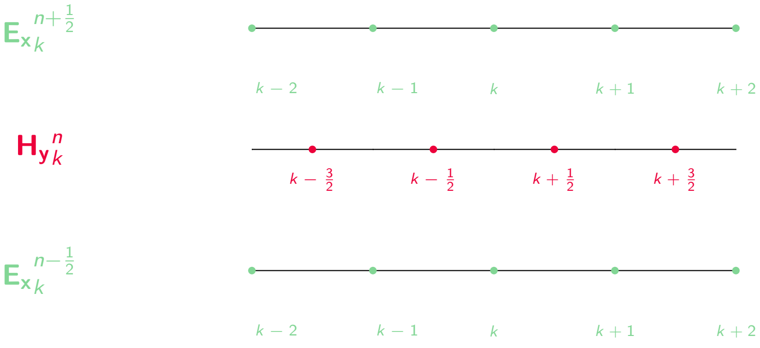
Now we can rearrange these equation to obtain $\mathbf{E_x}{}_k^{n+\frac{1}{2}}$ and $\mathbf{H_y}{}_{k+\frac{1}{2}}^{n+1}$

$$\mathbf{E_x}{}_k^{n+\frac{1}{2}} = \mathbf{E_x}{}_k^{n-\frac{1}{2}} - \frac{\Delta t}{\varepsilon_0 \Delta z}\left(\mathbf{H_y}{}_{k+\frac{1}{2}}^{n} - \mathbf{H_y}{}_{k-\frac{1}{2}}^{n}\right)$$
$$\mathbf{H_y}{}_{k+\frac{1}{2}}^{n+1} = \mathbf{H_y}{}_{k+\frac{1}{2}}^{n} - \frac{\Delta t}{\mu_0 \Delta z}\left(\mathbf{E_x}{}_{k+1}^{n+\frac{1}{2}} - \mathbf{E_x}{}_{k}^{n+\frac{1}{2}}\right)$$

Solving Maxwell's Equations in 1D IV

Graphically:

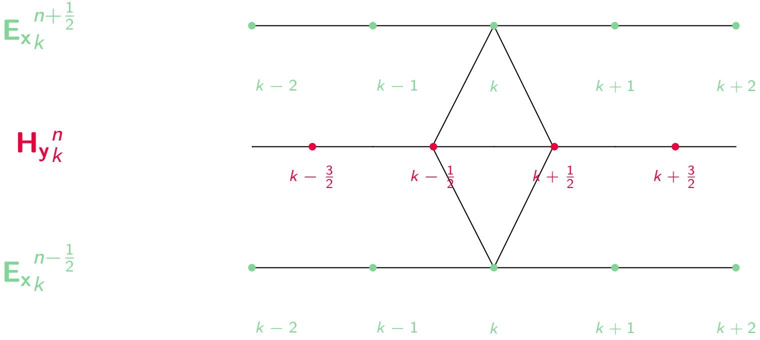
$$\mathbf{E_x}_k^{n+\frac{1}{2}} = \mathbf{E_x}_k^{n-\frac{1}{2}} - \frac{\Delta t}{\varepsilon_0 \Delta z}\left(\mathbf{H_y}_{k+\frac{1}{2}}^{n} - \mathbf{H_y}_{k-\frac{1}{2}}^{n}\right)$$



Solving Maxwell's Equations in 1D V

Graphically:

$$\mathbf{E_x}_k^{n+\frac{1}{2}} = \mathbf{E_x}_k^{n-\frac{1}{2}} - \frac{\Delta t}{\varepsilon_0 \Delta z}\left(\mathbf{H_y}_{k+\frac{1}{2}}^{n} - \mathbf{H_y}_{k-\frac{1}{2}}^{n}\right)$$



Solving Maxwell's Equations in 1D VI

Summarizing:

- we have interleaving of the $\mathbf{E}$ and $\mathbf{H}$ fields in space and time in the FDTD formulation
- to calculate $\mathbf{E_x}_k$ the neighbouring values of $\mathbf{H_x}_{k\pm\frac{1}{2}}$ of the previous time instant are needed
- to calculate $\mathbf{H_x}_{k+\frac{1}{2}}$ the neighbouring values of $\mathbf{E_x}_k$ and $\mathbf{E_x}_{k+1}$ of the previous time instant are needed

Minimizing numerical error

- ε_0 and μ_0 differ by several orders of magnitude, hence the fields will also do so
- the umerical error is minimized by making the following change of variables as

$$\tilde{\mathbf{E}}_\mathbf{x} = \sqrt{\frac{\varepsilon_0}{\mu_0}}\mathbf{E_x}$$

Stability I

How do we determine the time step?

- An EM wave propagating in free space cannot go faster than c, the speed of light.
- To propagate a distance of one cell requires a minimum time of $\Delta t = \Delta x / c$.

With a two- dimensional simulation, we must allow for the propagation in the diagonal direction, which brings the requirement to $\Delta t = \Delta x/(\sqrt{2}\, c)$. The same geometric consideration in a three-dimensional setting requires $\Delta t = \Delta x/(\sqrt{3}\, c)$. This is summarized by the Courant Condition

$$\Delta t = \frac{\Delta x}{\sqrt{d}\, c}$$

with d the spatial dimension.

Absorbing Boundary Condition in One Dimension I

Absorbing boundary conditions are necessary to keep outgoing E and B fields from being reflected back into the problem space.

- in calculating the E field, we need to know the surrounding B values
- at the edge of the computational domain we will not have the value of one side.
- we know however, that the fields at the edge must be propagating outward.

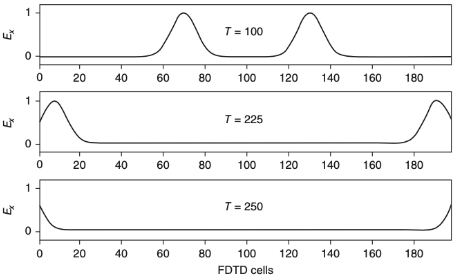
We will use this fact to estimate the value at the end by using the value next to it, this was shown by B. Mur back in 1981.
Suppose we are looking for a boundary condition at the end where $k = 0$.
If a wave is going toward a boundary in free space, it is traveling at c. So, in one time step of the FDTD algorithm, it travels

$$c\Delta t = \frac{\Delta x}{2}.$$

Absorbing Boundary Condition in One Dimension II

Hence, it takes two time steps for the field to cross one cell. A viable approach tells us that an acceptable boundary condition might be

$$\mathbf{E_x}^n(0) = \mathbf{E_x}^{n-2}(1)$$



Appendix: Find $\mathbf{A}$ if $\mathbf{A} = \mathbf{R} + \mathbf{A} \times \mathbf{B}$

Take the cross-product with $\mathbf{B}$:

$$\mathbf{A} \times \mathbf{B} = \mathbf{R} \times \mathbf{B} + (\mathbf{A} \times \mathbf{B}) \times \mathbf{B}$$

Use $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{C} \times \mathbf{B}) \times \mathbf{A} = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$ to write

$$(\mathbf{A} \times \mathbf{B}) \times \mathbf{B} = (\mathbf{B} \cdot \mathbf{A})\mathbf{B} - B^2\mathbf{A}$$

to get

$$\mathbf{A} \times \mathbf{B} = \mathbf{R} \times \mathbf{B} + (\mathbf{B} \cdot \mathbf{A})\mathbf{B} - B^2\mathbf{A}.$$

From the original equation we have $\mathbf{A} \times \mathbf{B} = \mathbf{A} - \mathbf{R}$ and $\mathbf{B} \cdot \mathbf{A} = \mathbf{B} \cdot \mathbf{R}$. Plugging these into the last expression we finally get

$$\mathbf{A} = \frac{\mathbf{R} + \mathbf{R} \times \mathbf{B} + (\mathbf{B} \cdot \mathbf{R})\mathbf{B}}{1 + B^2}.$$

One can use this to find an explicit expression for the velocity update in the Boris scheme.