Computational Methods in Plasma Physics. Lecture II

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Simple harmonic oscillator

We looked at

$$\frac{d^2z}{dt^2} = -\omega^2 z$$

and wrote it as system of first-order ODEs

$$\frac{dz}{dt} = v; \quad \frac{dv}{dt} = -\omega^2 z$$

Now introduce energy-angle coordinates

$$\omega z = E\sin\theta; \quad v = E\cos\theta$$

then $E^2 = \omega^2 z^2 + v^2 \equiv E_0^2$ is a constant as we showed before. Using these expressions we get the very simple ODE $\dot{\theta} = \omega$. This shows that in phase-space $(v, \omega z)$ the motion is with uniform angular speed along a circle.

Simple harmonic oscillator: Phase-errors

The mid-point scheme had

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (v^n)^2 + \omega^2 (z^n)^2 = E_0^2$$

which means that the mid-point scheme gets the energy coordinate *exactly* correct. However, we have

$$\tan \theta^{n+1} = \frac{\omega z^{n+1}}{v^{n+1}}.$$

Using the expressions for the scheme and Taylor expanding in Δt we get

$$\tan \theta^{n+1} = \tan \theta^n + \frac{\omega E_0^2}{(v^n)^2} \Delta t + \frac{\omega^3 z^n E_0^2}{(v^n)^3} \Delta t^2 + O(\Delta t^3)$$

The first three terms match the Taylor expansion of the exact solution $\tan(\theta^n + \omega \Delta t)$ and the last term is the *phase-error*.

Single particle motion in an electromagnetic field

- In PIC method the Vlasov-Maxwell equation is solved in the *Lagrangian frame*: 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

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

- 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. In general, this would make the scheme nonlinear!

- 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 foo: find $\mathbf{A}$ if $\mathbf{A} = \mathbf{R} + \mathbf{A} \times \mathbf{B}$.
The Boris algorithm updates this equation in three steps:

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

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

$$\mathbf{t} = \frac{q\mathbf{B}}{m}\frac{\Delta t}{2}$$
$$\mathbf{s} = \frac{2\mathbf{t}}{1 + |\mathbf{t}|^2}$$

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

See Birdsall and Langdon text book Section 4-3 and 4-4 and figure 4-4a. Easily extended to relativistic case.

Note 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?

See paper by Qin at. al. Phys. Plasmas, **20**, 084503 (2013) in which it is shown that the Boris algorithm *conserves phase-space volume*. However, they also show that the Boris algorithm is *not* symplectic.

- 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.
- 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.
- 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.

Solving Maxwell equations

Besides pushing particles in electromagnetic fields, we need to compute these fields self-consistently from currents and charges by solving Maxwell equations. First consider Maxwell equations in vacuum:

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$
$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = 0$$

For these we have the conservation laws

$$\frac{d}{dt} \int_\Omega \mathbf{E} \times \mathbf{B} \, d^3\mathbf{x} = 0$$
$$\frac{d}{dt} \int_\Omega \left(\frac{\epsilon_0}{2} |\mathbf{E}|^2 + \frac{1}{2\mu_0} |\mathbf{B}|^2 \right) d^3\mathbf{x} = 0.$$

Note these are *global* conservation laws and one can instead also write *local* conservation laws that include momentum and energy flux terms. How to solve these equations efficiently and maintain (some) conservation and geometric properties?

Solving Maxwell equations

- Maxwell equations have a very special geometric structure. The electric field $\mathbf{E}$ is a *vector* while the magnetic field $\mathbf{B}$ is a *bivector* (this is disguised in the usual formulations of Maxwell equations).
- (In spacetime formulations the complete electromagnetic field is represented as a single bivector in 4D space-time).
- The fact that we are dealing with two objects of *different* geometric types indicates that the discrete Maxwell equations should also inherit this somehow.
- 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

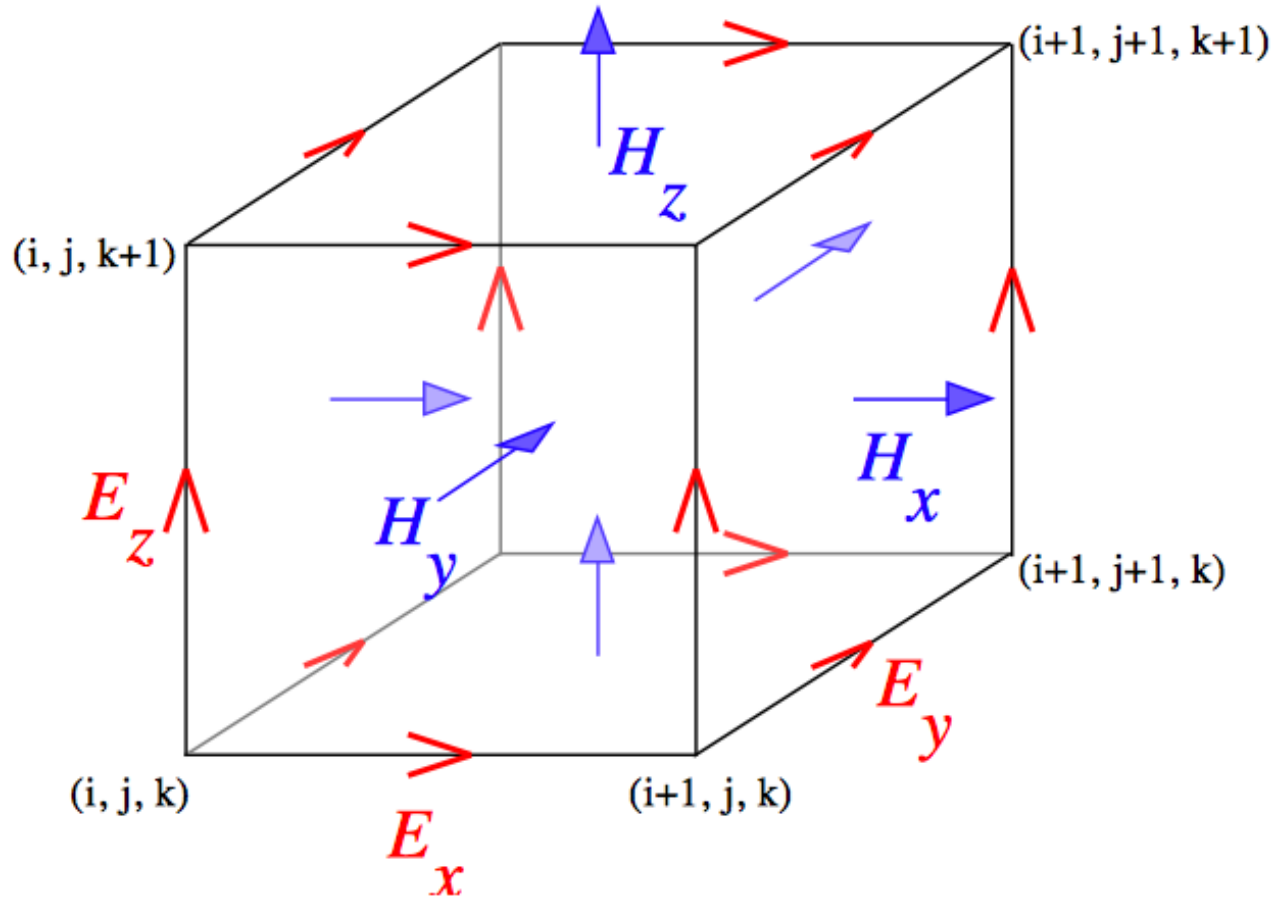

Figure: Standard Yee-cell. Electric field components (vectors) are located on edges while magnetic field components (bivectors) are located on faces.

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:

$$\mathbf{B}^{n+1/2} = \mathbf{B}^{n-1/2} - \Delta t \, \nabla_E \times \mathbf{E}^n$$
$$\mathbf{E}^{n+1} = \mathbf{E}^n + \Delta t / c^2 \, \nabla_F \times \mathbf{B}^{n+1/2}$$

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:

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

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).

Other schemes: Finite-Volume method for Maxwell equations

Consider the 1D source-free Maxwell equations

$$\frac{\partial}{\partial t}\begin{bmatrix} E_y \\ B_z \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} c^2 B_z \\ E_y \end{bmatrix} = 0.$$

Basic idea is to transform the equation into uncoupled advection equations for the *Riemann variables*. This is always possible in 1D for *linear hyperbolic* systems. For the above system, multiply the second equation by c and add and subtract from the first equation to get

$$\frac{\partial}{\partial t}\left(E_y + cB_z\right) + c\frac{\partial}{\partial x}\left(E_y + cB_z\right) = 0$$
$$\frac{\partial}{\partial t}\left(E_y - cB_z\right) - c\frac{\partial}{\partial x}\left(E_y - cB_z\right) = 0.$$

Note that these are two uncoupled passive advection equations for the variables $w^{\pm} = E_y \pm cB_z$ with advection speeds $\pm c$.

Finite-Volume method for Maxwell equations

- Instead of using the Yee-cell one can solve Maxwell equations using finite-volume methods developed in aerospace and fluid mechanics.
- In these schemes one uses the local characterstic direction to "upwind" values at cell faces, adding stability to the scheme when simulating small-scale features.
- Finite-volume schemes are as cheap (or expensive) as Yell-cell based FDTD schemes and are also easy to implement for Maxwell equations. However, they suffer from some disadvantages.
- First, it is very hard to ensure divergence relations are maintained. One needs to correct the divergence errors somehow, by adding some additional equations to the system.
- Energy is not conserved by finite-volume schemes that use upwinding. Special choices of basis-functions can be used to construct energy conserving schemes, but these have other issues (also shared by FDTD schemes).
- However, in some situations, FV based Maxwell solvers are useful and have been successfully applied in many large-scale problems.

Choice of numerical fluxes for Maxwell equations impacts energy conservation

The electromagnetic energy is given by

$$\mathcal{E} = \frac{\epsilon_0}{2} E_y^2 + \frac{1}{2\mu_0} B_z^2$$

Notice that this is the L_2 norm of the electromagnetic field.

- Hence, as we will show tomorrow, if we use upwinding to compute numerical fluxes, the *electromagnetic energy will decay*.
- If we use central fluxes (average left/right values) then the EM energy will remain conserved by the *time-continuous* scheme. However, the Runge-Kutta time-stepping will add small diffusion that will decay the total energy a little.
- However, the energy decay rate will be *independent* of the spatial resolution and will reduce with smaller time-steps.