Computational Methods in Plasma Physics. Lecture III

Ammar H. Hakim[1]

[1]Princeton Plasma Physics Laboratory, Princeton, NJ

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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

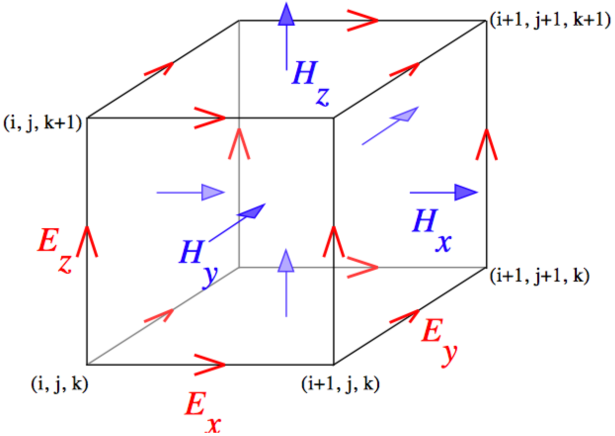

Figure: Standard Yee-cell. Electric field components (vectors) are located on edges while magnetic field components (bivectors) are located on faces.

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).

Maxwell equations are hyperbolic: large class of such equations

A vast class of partial differential equations are *hyperbolic*.

- Consider

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0$$

  where $\mathbf{Q}$ is a vector of *conserved* quantities and $\mathbf{F} = \mathbf{F}(\mathbf{Q})$ is the vector of *fluxes*.

- Compute the *flux-jacobian*

$$\mathbf{A} = \frac{\partial \mathbf{F}}{\partial \mathbf{Q}}.$$

- Now compute the eigenvalues and eigenvectors of $\mathbf{A}$. If these eigenvalues are *real* and eigenvectors are *complete* then this system is called *hyperbolic*.

Example 1: Maxwell equations

Consider the 1D source-free Maxwell equations

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

The flux-jacobian is

$$\mathbf{A} = \begin{bmatrix} 0 & c^2 \\ 1 & 0 \end{bmatrix}.$$

A simple calculation shows that the eigenvalues are $-c, c$ and eigenvectors

$$\mathbf{r}^1 = \begin{bmatrix} 1 \\ -1/c \end{bmatrix} \qquad \mathbf{r}^2 = \begin{bmatrix} 1 \\ 1/c \end{bmatrix}.$$

Example 2: Euler equations

Consider the ideal fluid equations (Euler equations)

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho u \\ E\end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix}\rho u \\ \rho u^2 + p \\ (E+p)u\end{bmatrix} = 0$$

Where, $E = \rho u^2/2 + p/(\gamma - 1)$ is the fluid energy. This is also hyperbolic, with eigenvalues $u \pm c_s$ where $c_s = \sqrt{\gamma p/\rho}$ is the sound speed.

Note that the Euler equations are a *nonlinear* hyperbolic system. Other examples: *ideal MHD* equations, relativistic fluid equations, Einstein field equation for gravitation, ...

Hyperbolic problems need special methods to solve

Major feature of hyperbolic equations are the existence of shocks and other nonlinear features (rarefactions, compression waves, contact discontinuities).

To handle these properly one needs to account for the structure of the equation as revealed by the eigenvalues and eigenvectors.

- These *shock capturing* methods were originally developed in aerospace engineering literature to solve problems of transonic and supersonic flight and reentry vehicles.
- They are built around the concept of a *Reimann solver* that approximate the nonlinear structure at each cell interface.
- In fusion physics, these are not yet widely used. However, they are ubiquitous in astrophysical plasma physics.

Typically, the general belief is that the the evolution of the plasma in a fusion machine is too slow to justify shock capturing methods.

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

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

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.