Solving Maxwell Equations and Intro to Hyperbolic PDEs

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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:

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

For these we have the conservation laws

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

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 E is a *vector* while the magnetic field 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

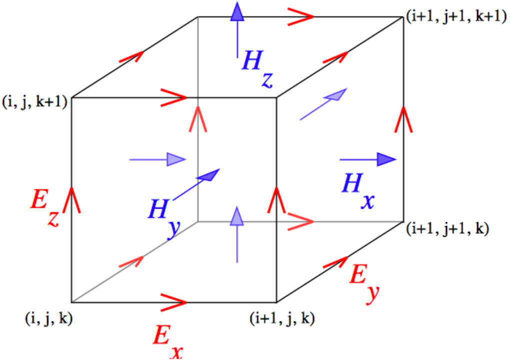


Figure: Standard Yee-cell. Electric field components (vectors) are located on edges while magnetic field components (bivectors) are located on faces.

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:

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

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:

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

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

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

where ϱ_c is the charge density and J is the current density. On the Yell-cell this becomes

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

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).

Methods for solution of hyperbolic/mixed PDEs

Hyperbolic (or mixed) PDEs appear everywhere in physics and engineering: Euler equations, Navier-Stokes equations, MHD equations, Einstein's equation of general relativity, shallow-water equations, ...

- Describe phenomena that travel with *finite-speed*: clearly all fundamental physics must obey causality, hence hyperbolic systems are fundamental (though approximations of hyperbolic equations may violate finite-speed constraint).
- Display very rich structure shocks and other discontinuities, instabilities, turbulence ... and in most problems, a mix of all!
- Specialized methods are needed to solve such systems: naive algorithms can **cause disaster**!

My goal is to develop *conceptual* understanding about such equations and numerical methods to solve them. Literature is too vast to cover in few lectures!

Dissipation, dispersion and robustness

Typically, numerical methods trade between accuracy and robustness. Very accurate schemes are not too robust and highly robust schemes are typically not very accurate. Must find a balance.

- To capture shocks and sharp gradient features some localized diffusion (dissipation) is needed via *limiters* or some other means. Some dissipation may also be needed for stability.
- Dissipation typical leads to a loss of other properties: in particular, for Maxwell equations it can cause EM energy to *decay*. For Euler equations high-k modes may get over-damped due to limiters: not good for turbulence problems.
- An ideal situation is to apply dissipation only where it is needed and use low-dissipation schemes elsewhere. However, this is easier said than done. How to determine where to apply dissipation is very tricky, specially in nonlinear complex flows. Ease to confuse physical features for numerical artifacts (and vice-versa!)

Hyperbolic PDEs describe phenomena that travel at finite speed

An intuitive "definition" that we will initially work with before stating the mathematically rigorous definition:

Definition (Hyperbolic PDEs "Intuitive Definition")

A hyperbolic PDE is one in which all phenomena travel at a finite speed.

Some prototypical examples we will look at more closely:

- Advection equation: simplest trivial *linear* hyperbolic equation. Trivial but very important!
- Maxwell equation of electromagnetism: linear hyperbolic system
- Euler equations: probably historically the most important *nonlinear hyperbolic system*. Basis of vast literature on numerical methods and basis for more complex equations: ideal MHD, (general) relativistic hydro/MHD, Navier-Stokes solvers, etc. Need to understand even if you want to follow literature and apply methods to your own problem.

Hyperbolic PDEs: rigorous definition, no reliance on linearization

Consider a system of conservation laws written as

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

where Q is a vector of conserved quantities and F(Q) is a vector of fluxes. This system is called *hyperbolic* if the flux Jacobian

$$\mathrm{A} \equiv \frac{\partial \mathrm{F}}{\partial \mathrm{Q}}$$

has *real eigenvalues* and a *complete set of linearly independent* eigenvectors. In multiple dimensions if F_i are fluxes in direction i then we need to show that arbitrary linear combinations $\sum_i n_i \partial \mathrm{F}_i / \partial \mathrm{Q}$ have real eigenvalues and linearly independent set of eigenvectors.

To compute eigensystem often easier to work in *quasilinear form*

To derive eigensystem it is sometimes easier to work in non-conservative (quasi-linear) form of equations. Start with

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

and introduce an invertible transform $\mathrm{Q} = \varphi(\mathrm{V})$ where V are some other variables (for example: density, velocity and pressure). Then the system converts to

$$\frac{\partial \mathrm{V}}{\partial t} + \underbrace{(\varphi')^{-1}\mathrm{A}\varphi'}_{\mathrm{B}} \frac{\partial \mathrm{V}}{\partial x} = 0.$$

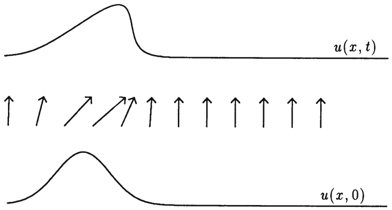
Can easily show eigenvalues of A are same as that of B and right eigenvectors can be computed from $\varphi' \mathrm{r}_p$ and left eigenvectors from $\mathrm{l}_p(\varphi')^{-1}$.

Burgers' equation

Simplest nonlinear scalar equation, has a quadratic nonlinearity:

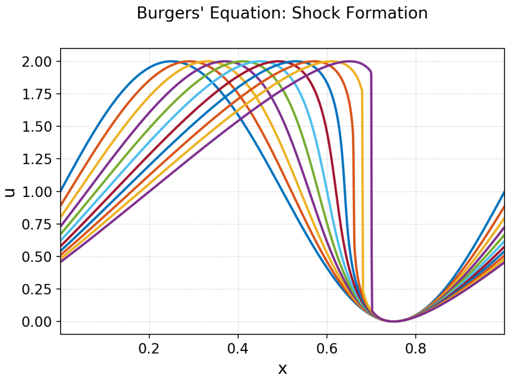
$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right) = 0.$$

Eigenvalue $\lambda = u$. Note that locally, eigenvalue depends on the solution itself: leads to a situation in which after some finite time to the formation of a *shock* as the "characteristics" will intersect.



Burgers' equation: shock formation

Due to varying characteristics speed (eigenvalue) the solution can "pile up" leading to the formation of a shock.



Weak-solutions and entropy conditions

At a shock the solution has a discontinuity. Hence, derivatives are not defined! Differential form of the equations break-down. We must use concept of weak-solutions in this case.

Let $\phi(x,t)$ is a compactly supported (i.e. zero outside some bounded region) smooth function (enough continuous derivatives). Then multiply conservation law

$$\int_0^\infty \int_{-\infty}^\infty \phi(x,t)\left[\frac{\partial \mathsf{Q}}{\partial t} + \frac{\partial \mathsf{F}}{\partial x}\right] dx\, dt = 0$$

by $\phi(x,t)$ and integrating by parts to get the *weak-form*

$$\int_0^\infty \int_{-\infty}^\infty \left[\frac{\partial \phi}{\partial t}\mathsf{Q} + \frac{\partial \phi}{\partial x}\mathsf{F}\right] dx\, dt = -\int_{-\infty}^\infty \phi(x,0)\mathsf{Q}(x,0) dx\, dt.$$

Definition (Weak-solution)

A function $\mathsf{Q}(x,t)$ is said to be a weak-solution if it satisfies the weak-form for all compact, smooth $\phi(x,t)$.

Weak-solutions and entropy conditions

Unfortunately, weak-solutions are not unique! Why does this happen?

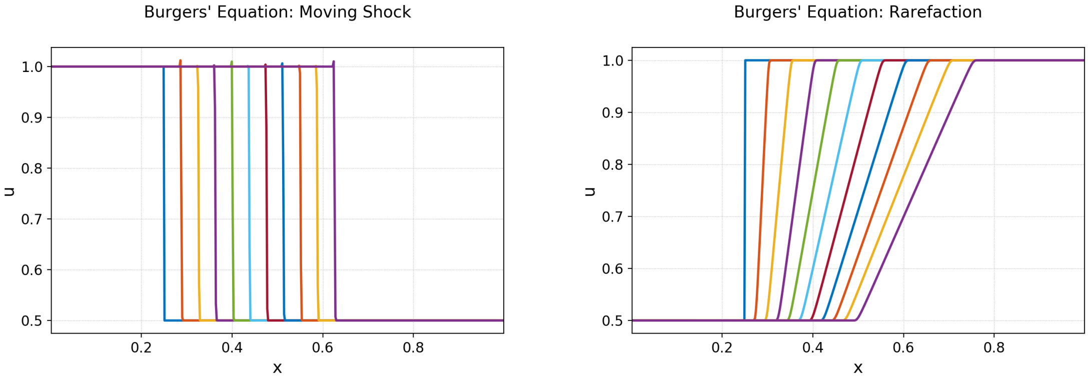
In physical problems there is always some non-ideal effects (viscosity, Landau damping etc) that does not allow a genuine discontinuity to form. However, this "viscous shock layer" can be extremely thin compared to system size. Also, we know entropy must increase in the physical universe.

This indicates we can recover uniqueness in two ways

- Add a viscous (diffusion) term and take limit of viscosity going to zero. (Generally not convenient for numerical work)
- Impose *entropy condition*: construct an *entropy* function such that it remains conserved for smooth solutions but *increases* across a shock. Entropy is naturally suggested in most physical problems.

Weak-solutions and entropy conditions

When characteristics *diverge* (right plot below) the weak-solution is not unique. A false "shock" solution also is a weak-solution. Imposing *entropy condition* gives a *rarefaction* wave seen in the right plot.



Euler equations of invicid fluids

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

Here $\mathcal{E} = p/(\gamma-1) + \rho u^2/2$ is the total energy. Eigenvalues of this system are $\{u - c_s, u, u, u, u + c_s\}$ where $c_s = \sqrt{\gamma p/rho}$ is the sound speed. See class notes for left/right eigenvectors.

Note: in the limit $p \rightarrow 0$ all eigenvalues become u and for cold-fluid ($p = 0$) the system does not possess complete set of eigenvectors. (Cold fluid model is important to model dust, for example, in astrophysical systems or in say volcanic explosions).

Euler equations: transport of kinetic energy

The energy conservation equation for Euler equation is

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot [(\mathcal{E} + p)\mathbf{u}] = 0$$

where

$$\mathcal{E} = \underbrace{\frac{p}{\gamma - 1}}_{\text{IE}} + \underbrace{\frac{1}{2}\rho u^2}_{\text{KE}}.$$

We can derive instead a *balance law* (not conservation law) for transport of KE

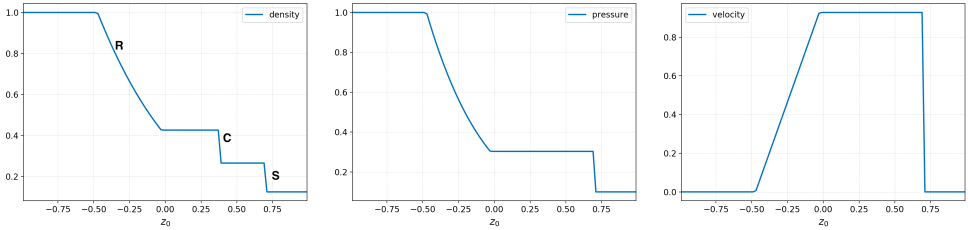
$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2\right) + \nabla \cdot \left(\frac{1}{2}\rho u^2 \mathbf{u}\right) = -\mathbf{u} \cdot \nabla p + \frac{q}{m}\rho \mathbf{u} \cdot \mathbf{E}$$

For turbulence calculations it is important to ensure that in the *numerics* exchange of kinetic and internal energy (and in case of plasma field-particle energy) is only via the RHS terms (pressure work and work done by electric field).

Many shock-capturing and higher-order methods can mess this up for high-k (short wavelength) modes due leading to incorrect energy spectra. (No Free Lunch Principle).

Euler equations: shocks, rarefactions and contacts

In addition to shocks and rarefactions which we saw in Burgers's equation, Euler equations also support *contact discontinuities*, across which density has a jump but not pressure or velocity.



Ideal MHD equations

Ideal MHD equations are very important to both fusion and astrophysical problems. Written in non-conservative form they are

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \mathrm{u} \cdot \nabla \rho + \rho \nabla \cdot \mathrm{u} &= 0 \\
\frac{\partial \mathrm{u}}{\partial t} + \mathrm{u} \cdot \nabla \mathrm{u} + \frac{\nabla p}{\rho} &= \frac{1}{\mu_0 \rho} (\nabla \times \mathrm{B}) \times \mathrm{B} \\
\frac{\partial p}{\partial t} + \mathrm{u} \cdot \nabla p + \gamma p \nabla \cdot \mathrm{u} &= 0 \\
\frac{\partial \mathrm{B}}{\partial t} - \nabla \times (\mathrm{u} \times \mathrm{B}) &= 0
\end{aligned}
$$

with the constraint $\nabla \cdot \mathrm{B} = 0$. The eigensystem is complicated to compute! (Try doing it yourself). Eigenvalues are $u \pm c_f$, $u \pm c_s$, $u \pm c_a$, and u (7 eigenvalues for 8 equations). Here c_f, c_s are the fast/slow magnetosonic speeds and c_a is the Alfven speed. See Ryu and Jones ApJ **442** 228-258, 1995 (linked on website).