Hyperbolic PDEs and Finite-Volume Methods II

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Hyperbolic PDEs: rigorous definition, no reliance on linearization

Consider a system of conservation laws written as

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

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

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

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

The Riemann Problem for hyperbolic PDEs

The Riemann problem is a class of *initial value* problems for a hyperbolic PDE

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

on $x \in [-\infty, \infty]$ with initial conditions

$$\mathbf{Q}(x, 0) = \mathbf{Q}_R \quad x > 0$$
$$\mathbf{Q}(x, 0) = \mathbf{Q}_L \quad x < 0$$

where $\mathbf{Q}_{L,R}$ are *constant* initial states.

- Fundamental mathematical problem in theory of hyperbolic PDEs: brings out the key structure of the nonlinear solutions of the system.
- For some important systems like (relativisitic) Euler equations, ideal MHD the Riemann problem can be solved *exactly* (modulo some nonlinear root-finding).
- Good test for shock-capturing schemes as it tests ability to capture discontinuities and complex non-linear phenomena.

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

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

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

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

Definition (Weak-solution)

A function $\mathbf{Q}(x,t)$ 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?

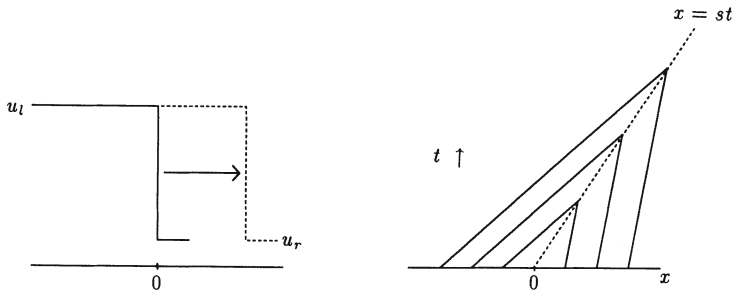
In physical problems there is always some non-ideal effects (viscosity, Landau damping etc) that does not allow a genuine discontinuity to form. However, this "viscous shock layer" can be extremely thin compared to system size. Also, we know entropy must increase in the physical universe.

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 of Burgers' equation: shock

When characteristics *converge* a shock will form



Shock-speed is given by the Rankine-Hugoniot jump condition

Consider a discontinuity in the solution wirh left/right states $\mathbf{Q}_L$ and $\mathbf{Q}_R$. Then the speed at which this discontinuity moves, s, is called the *shock-speed* and is determined by the Rankine-Hugoniot jump condition

$$s(\mathbf{Q}_R - \mathbf{Q}_L) = \mathbf{F}_R - \mathbf{F}_L$$

For Burgers's equation we simply have

$$s = \frac{1}{2}(u_L + u_R).$$

For linear systems of hyperbolic equations as $\mathbf{F} = \mathbf{A}\mathbf{Q}$ we have

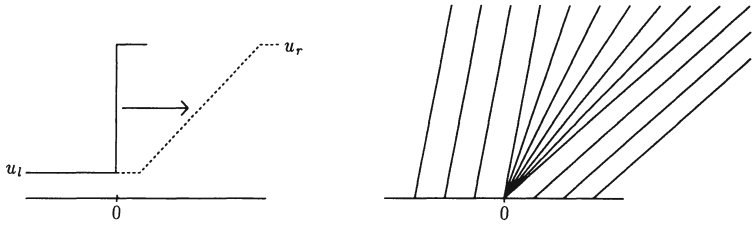
$$s(\mathbf{Q}_R - \mathbf{Q}_L) = \mathbf{A}(\mathbf{Q}_R - \mathbf{Q}_L)$$

which means the eigenvalues of $\mathbf{A}$ are the shock-speeds.

For general nonlinear hyperbolic systems only very specific jumps in which the jump in flux and jump in conserved variables are *linearly dependent* can be shocks.

Weak-solutions of Burgers' equation: rarefaction

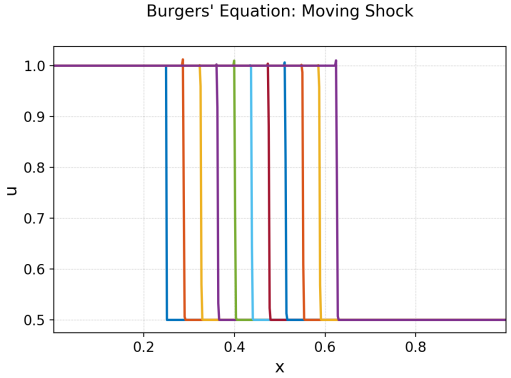
When characteristics *diverge* inifinite solutions to the weak-form! An entropy respecting solution is a *rarefaction*

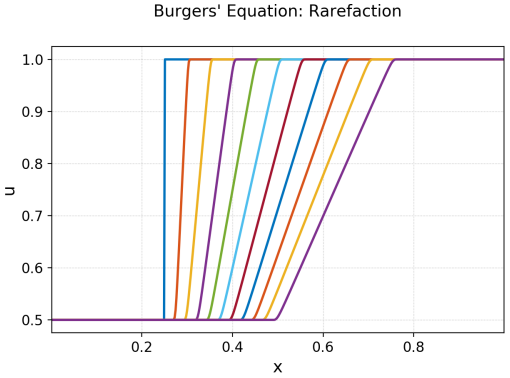


One possible defintion of entropy respecting shocks for Burgers' equation: *only* allow a discontinuity if $u_L > u_R$. So in the above case me must not allow a shock to form.

Weak-solutions: shock and rarefaction

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

The Euler equations for invicid fluids are important in themselves, and form the basis of many other more complex equation systems (Navier-Stokes, multi-fluid plasma equations, MHD, ...)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{Continuity}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\mathbf{I}) = 0 \qquad \text{Momentum}$$

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

where

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

is the total energy of the system. If we solve the system in this *conservative* form, then density, momentum and energy are conserved automatically, even locally.

Euler equations: hyperbolicity

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

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 $p\to 0$ all eigenvalues become u and for cold-fluid ($p=0$) the system does not possess complete set of eigenvectors. (Cold fluid model is important in plasmas and 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 *balance laws* (not conservation laws) for transport of KE and IE

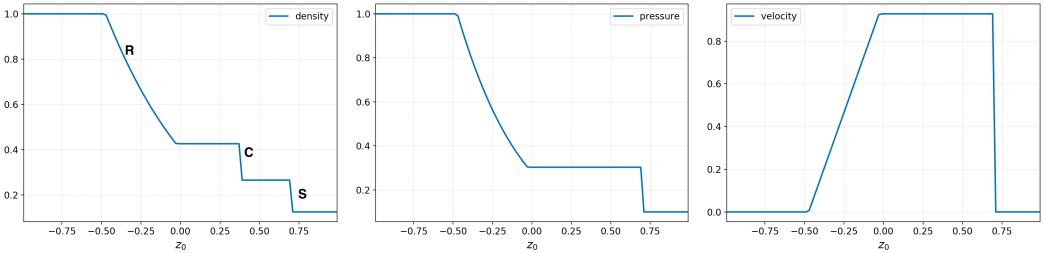
$$\frac{\partial}{\partial t}(\text{KE}) + \nabla \cdot (\text{KE}\,\mathbf{u}) = -\mathbf{u} \cdot \nabla p$$
$$\frac{\partial}{\partial t}(\text{IE}) + \nabla \cdot (\text{IE}\,\gamma\mathbf{u}) = \mathbf{u} \cdot \nabla p$$

It is important to ensure that in the *numerics* exchange of kinetic and internal energy is only via the RHS terms (pressure work).

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.



Beyond hyperbolic PDEs: Source terms, non-ideal effects

In most physics applications one must add source terms and non-ideal effects to the underlying hyperbolic PDE, converting it into a PDE of *mixed* type. Typically we will have systems of the form

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial x} + \ldots = \mathbf{S}$$

where $\mathbf{G}(\mathbf{Q}, \partial\mathbf{Q}/\partial x)$ are *viscous*/non-ideal fluxes that depend on *gradients* of $\mathbf{Q}$ (viscous stress-tensor in Navier-Stokes equations, heat-conducion etc) and $\mathbf{S}(\mathbf{Q}, x, t)$ are *source* terms.

The presence of non-ideal and source terms can *significantly* change the physics and required numerics.

Example: Ideal multifluid equations (five-moment)

Multi-fluid plasma equations are an important example. Ignoring non-ideal terms:

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) = 0$$

$$\frac{\partial}{\partial t}(\rho_s \mathbf{u}_s) + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + p_s \mathbf{I}) = \frac{q_s \rho_s}{m_s}(\mathbf{E} + \mathbf{u}_s \times \mathbf{B})$$

$$\frac{\partial \mathcal{E}_s}{\partial t} + \nabla \cdot [(\mathcal{E}_s + p_s)\mathbf{u}_s] = \frac{q_s \rho_s}{m_s}\mathbf{u}_s \cdot \mathbf{E}$$

for each plasma species s (electrons, ions, ...). These are coupled to Maxwell equations

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

$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \sum_s \frac{q_s \rho_s}{m_s}\mathbf{u}_s$$

Multifluid equations (five-moment): conservation properties

Note that in multifluid system total momentum (fluid+field) and total energy (fluid+field) is conserved. Hence, conservation properties are *indirect*: ensuring conservation of total momentum and total energy (specially locally) is non-trivial.

$$\frac{\partial}{\partial t}\left(\sum_s \rho_s \mathbf{u}_s + \epsilon_0 \mathbf{E}\times\mathbf{B}\right) + \nabla\cdot\left[\sum_s(\rho_s\mathbf{u}_s\mathbf{u}_s + p_s\mathbf{I}) + \left(\frac{\epsilon_0}{2}|\mathbf{E}|^2 + \frac{1}{2\mu_0}|\mathbf{B}|^2\right)\mathbf{I} - \left(\epsilon_0\mathbf{E}\mathbf{E} + \frac{1}{\mu_0}\mathbf{B}\mathbf{B}\right)\right] = 0$$

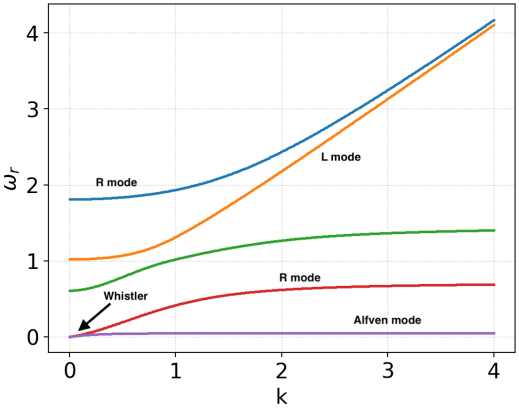
$$\frac{\partial}{\partial t}\left(\sum_s \mathcal{E}_s + \frac{\epsilon_0}{2}|\mathbf{E}|^2 + \frac{1}{2\mu_0}|\mathbf{B}|^2\right) + \nabla\cdot\left[\sum_s(\mathcal{E}_s + p_s)\mathbf{u}_s + \frac{1}{\mu_0}\mathbf{E}\times\mathbf{B}\right] = 0.$$

Multifluid equations (five-moment): eigensystem

The multifluid system is not hyperbolic! However, it has a very complicated eigenstructure (called "dispersion relations" when studying linear plasma problems)

- The presence of the Lorentz force terms add many new time-scales: plasma-frequency, electron/ion cyclotron frequencies ...
- Adding non-ideal terms adds even more scales: diffusion and viscous time-scales.

Understanding the frequencies in the system is critical to determine stable time-steps for explicit schemes. More on this later when we discuss time-stepping.



Essence of the finite-volume method

Consider a PDE of the form (non necessarily hyperbolic)

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

Now make a grid with cells $I_j = [x_{j-1}, x_{j+1/2}]$ and $\Delta x = x_{j+1/2} - x_{j-1/2}$. The finite-volume method *usually* evolves the cell-averages of the solution:

$$\frac{\partial \mathbf{Q}_j}{\partial t} + \frac{\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}}{\Delta x} = 0$$

where

$$\mathbf{Q}_j(t) \equiv \frac{1}{\Delta x} \int_{I_j} \mathbf{Q}(x,t)\, dx$$

are the *cell-averages* and

$$\mathbf{F}_{j\pm1/2} \equiv \mathbf{F}(\mathbf{Q}_{j\pm1/2})$$

are *numerical fluxes* at cell interfaces.

Essence of the finite-volume method

The finite-volume method *usually* evolves the cell-averages of the solution:

$$\frac{\partial \mathbf{Q}_j}{\partial t} + \frac{\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}}{\Delta x} = 0$$

This equation is an *exact* evolution equation for the cell-averages.However, notice that

- We only know cell-averages $\mathbf{Q}_j$ in each cell; we *do not* know the *cell-edge* values $\mathbf{Q}_{j\pm1/2}$ needed to compute the numerical flux $\mathbf{F}_{j\pm1/2}$.
- The finite-volume method consists of determining these *edge values* and *constructing a numerical-flux* so the cell-averages can be updated.
- Time-stepping can be done with a ODE solver (method-of-lines) or using a *single-step* method (fully discrete scheme).

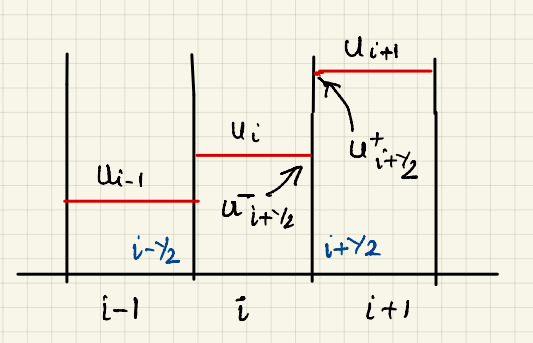
Essence of the finite-volume method

Instead of computing one edge value we will compute *two* values: one the left and one on right of cell. With this, the numerical-flux will then be

$$\mathbf{F}_{j+1/2} = \mathbf{F}_{j+1/2}(\mathbf{Q}^{-}_{j+1/2}, \mathbf{Q}^{+}_{j+1/2})$$

We must impose the consistency condition:

$$\mathbf{F}_{j+1/2}(\mathbf{Q}, \mathbf{Q}) = \mathbf{F}(\mathbf{Q}).$$



Cell-averages v/s cell-center values

- Typically, finite-volume schemes evolve the cell-average values; finite-difference schemes evolve cell-center (or nodal) values.
- For some low-order (first and some second-order) schemes the *forms* of the scheme may look superficially the same. However, this is not true in general and one must *very carefully* distinguish between cell-average and point-wise values. Otherwise incorrect schemes can result that "look okay" but do not achieve full accuracy.
- What we evolve (cell-average, nodal values or in DG moments or interior node values) is called the *solution representation*.

Remember Your Representation

When studying or designing numerical schemes **never** confuse one solution representation for another.