

Solving Poisson equation with FFT:

$$F_k[f'(x)] = \int_{-L/2}^{L/2} f'(x) \exp(-2\pi i k x) dx$$

$$= [f(x) \exp(-2\pi i k x)]_{-L/2}^{L/2} - \int_{-L/2}^{L/2} f(x) [-2\pi i k \exp(-2\pi i k x)] dx$$

$$= 2\pi i k F_k(f(x))$$

k is quantized, i.e. multiples of 1/L.

Hyperbolic equations

Hyperbolic: $\frac{\partial^2 \phi}{\partial t^2} - c^2 \frac{\partial^2 \phi}{\partial x^2} = 0$ wave equation (Tsunami, sound, electromagnetic waves)

Basic solution methods

Simplest example:

$$\frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} = 0$$

May be viewed as 1D advection.

$$\frac{d}{dt} \phi(t, x = ct + x_{t=0}) = 0$$

A figure: Line of Characteristics.

Now discretize and use j to index x and n to index time.

We could do:

$$\frac{\partial \phi_j^n}{\partial t} \approx \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t}$$

$$\frac{\partial \phi_j^n}{\partial x} \approx \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x}$$

or

$$\frac{\partial \phi_j^n}{\partial x} \approx \frac{\phi_{j+1}^n - \phi_j^n}{\Delta x}$$

or

$$\frac{\partial \phi_j^n}{\partial x} \approx \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x}$$

The last one is second order.

Let's see how do they work.

Finite volume, view the domain as grid cells with $F_{in,out} = c\phi$

Numerically, one could calculate the eigenvalues of the spatial operator.

There is a physical interpretation (for the first two at least).

Domain of dependence (works for upwind, downwind but not in general).

This gives the Courant-Fredrichs-Lewy condition (CFL number) necessary condition for stability.

$$\mu = \frac{c\Delta t}{\Delta x}$$

The eigenvalue analysis tells us about the stability, but there is more to it.

Why upwind is so diffusive?

Modified equations:

$$\phi_{j-1}^n = \phi_j^n - \Delta x \frac{\partial \phi}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 \phi}{\partial x^2} + O(\Delta x^3)$$

$$\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = \frac{\partial \phi}{\partial x} - \frac{\Delta x}{2} \frac{\partial^2 \phi}{\partial x^2} + O(\Delta x^2)$$

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \frac{\partial \phi}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 \phi}{\partial t^2} + O(\Delta t^2)$$

Since

$$\frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} = 0$$

we also have

$$\begin{aligned} \frac{\partial^2 \phi}{\partial t^2} + c \frac{\partial^2 \phi}{\partial x \partial t} &= 0 \\ c \frac{\partial^2 \phi}{\partial t \partial x} + c^2 \frac{\partial^2 \phi}{\partial x^2} &= 0 \end{aligned}$$

Thus

$$\frac{\partial^2 \phi}{\partial t^2} - c^2 \frac{\partial^2 \phi}{\partial x^2} = 0$$

We have

$$\begin{aligned} &\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} \\ &= \frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} - c \frac{\Delta x}{2} \frac{\partial^2 \phi}{\partial x^2} + \frac{\Delta t}{2} \frac{\partial^2 \phi}{\partial t^2} + O(\Delta x^2) + O(\Delta t^2) \\ &= \frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} - c \frac{\Delta x}{2} \left(1 - \frac{c\Delta t}{\Delta x}\right) \frac{\partial^2 \phi}{\partial x^2} + O(\Delta x^2) + O(\Delta t^2) \end{aligned}$$

We see that the upwind scheme approximates a 1D advection-diffusion equation to a higher order. This numerical diffusion is why the method is so diffusive. One could extend the analysis to a higher order and show there is a dispersion error.

Lax-Wendroff method: why don't we subtract that diffusion term?

$$\begin{aligned} & \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} \\ &= \frac{\partial \phi}{\partial x} + c \frac{\partial \phi}{\partial t} - c \frac{\Delta x}{2} \left(1 - \frac{c \Delta t}{\Delta x} \right) \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} + O(\Delta x^2) + O(\Delta t^2) \\ & \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} - \frac{c^2 \Delta t}{2\Delta x} \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} \\ &= \frac{\partial \phi}{\partial x} + c \frac{\partial \phi}{\partial t} + O(\Delta x^2) + O(\Delta t^2) \end{aligned}$$

This could also be seen as centered difference with added numerical diffusion.

With the diffusion term improved, dispersion error becomes apparent:

Dispersion error could be serious. Imagine this is the concentration of a chemical (say O3) that is being transported. You will end up with negative O3. How will that react with other species!

Discrete dispersion relation (Extended Von Neumann analysis)

Because the equation is linear, we can consider a single wavenumber k and frequency ω at a time:

$$\phi_j^n = \exp[i(kj\Delta x - \omega n\Delta t)]$$

The upwind method then gives:

$$\begin{aligned} & \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0 \\ & (e^{-i\omega\Delta t} - 1)\phi_j^n + \mu(1 - e^{-ik\Delta x})\phi_j^n = 0 \\ & \omega = \omega_r + i\omega_i \\ & e^{\omega_i\Delta t} (\cos \omega_r \Delta t - i \sin \omega_r \Delta t) - 1 = \mu(\cos k\Delta x - i \sin k\Delta x - 1) \\ & \begin{cases} A \cos \omega_r \Delta t - 1 = \mu(\cos k\Delta x - 1) \\ A \sin \omega_r \Delta t = \mu \sin k\Delta x \end{cases} \end{aligned}$$

where A is $e^{\omega_i\Delta t}$ the amplification factor.

Eliminate ω_r , we have

$$A^2 = 1 - 2\mu(1 - \mu)(1 - \cos k\Delta x)$$

and we see when $cfl < 1$, it's stable: $A^2 < 1$.

Eliminate A , we have:

$$\omega_r = \frac{1}{\Delta t} \arctan\left(\frac{\mu \sin k\Delta x}{1 + \mu(\cos k\Delta x - 1)}\right)$$

And we can plot the numerical phase speeds as a function of $k\Delta x$.

Do the same for Lax-Wendroff (don't show the formula, but show the plot)

$$\omega_r = \frac{1}{\Delta t} \arctan\left(\frac{\mu \sin k\Delta x}{1 + \mu^2(\cos k\Delta x - 1)}\right)$$

Numerical diffusion, discrete dispersion curve

Flux limiter (just the idea).

Upwind scheme doesn't produce new extremes but is very diffusive. Lax-wendroff is not that diffusive (higher order) but produces new extrema. The idea of a flux limiter is to combine the two. (A bit like shape preserving interpolations).

$$\begin{aligned} & \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} \\ &= -c \frac{\Delta x}{2} \left(1 - \frac{c\Delta t}{\Delta x}\right) \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} \end{aligned}$$

The idea is to somehow limit the antidiffusion so as not to produce new extrema. Best discussed in the context of a finite volume view.