Lecture 17

Partial differential equations.

- Flux-conservative equations, FTCS scheme.
- Von Neumann stability analysis.
- Lax scheme.
- Other kinds of errors.

This is a vast subject. Dealing with PDEs is what several physicists do for a living (including your instructor…). We can only attempt to give a brief introduction, outlining some of the basic ideas.

Mathematical literature classifies PDEs into three broad groups: hyperbolic, parabolic and elliptic.

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

Wave equation (hyperbolic)

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial u}{\partial x} \right)$$

Diffusion equation (parabolic)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y)$$

Poisson equation (elliptic)

Numerically, it is more important to notice that the first two equations define initial value problems, whereas the latter constitutes a boundary value problem.

We already saw in the context of ODEs the implications of these statements: in initial value problems one “marches along” in time whereas in boundary value problems we cannot “integrate from the boundary” and in general one ends up with much more costly methods.

Finite difference methods consist, as we saw in the case of ODEs, in discretizing the derivatives and therefore turning the system into a set of algebraic equations (linear or non-linear) that one handles with the techniques we discussed before in the course. The only novelty is that one has to discretize in more than one dimension and pay attention to the boundary conditions.

We will now discuss in some detail some special types of PDEs and how one solves them.

Flux conservative initial value problems:

A large class of IVP equations in one spatial dimension can be cast in "flux conservative form",

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{\partial \mathbf{F}(\mathbf{u})}{\partial x}$$

For example, the wave equation, $\dfrac{\partial^2 u}{\partial t^2} = v^2 \dfrac{\partial^2 u}{\partial x^2}$

$$\frac{\partial r}{\partial t} = v\frac{\partial s}{\partial x} \qquad \frac{\partial s}{\partial t} = v\frac{\partial r}{\partial x}$$

with

$$r \equiv v\frac{\partial u}{\partial x} \qquad s \equiv \frac{\partial u}{\partial t}$$

(analogous to Maxwell's equations)

For simplicity, let us consider the case of one “advective equation” (advective refers to the fact that the variable “u” moves along like a fluid with velocity v),

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x}$$ Has as solution, $$u = f(x - vt)$$

The first thing that comes to mind when discretizing this equation is the FTCS scheme (forward time centered in space),

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right)$$

This scheme is explicit (one obtains an equation determining u at the step n+1 in time as a function of u at various points in space at time step n.

Because we have taken an Euler type step in time, we can suspect that this discretization might have a problem.

Von Neumann stability analysis:

We assume that the coefficients of the equations are slowly varying in space and time. Then the solution can be expanded in eigen-modes,

$$u_j^n = \xi^n e^{ikj\Delta x}$$

Where k is a real spatial wavenumber and ξ is a complex number that depends on k. Since the eigenmode's amplitude is given by a power of ξ, the scheme in question will be stable if | ξ |<1. Otherwise it will blow up as we step forward in time.

Let us substitute in the equation for the FTCS scheme,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) \qquad \frac{\xi^{n+1} - \xi^n}{\Delta t} = -v\frac{\left(\xi^n e^{ik\Delta x} - \xi^n e^{-ik\Delta x}\right)}{2\Delta x}$$

Or, $$\xi(k) = 1 - i\frac{v\Delta t}{\Delta x}\sin k\Delta x$$

Which implies | ξ |>1. FTCS is "unconditionally unstable".

Lax method:

Starting from the FTCS scheme, $$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right)$$

Replace $$u_j^n \rightarrow \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right)$$ (spatial average)

Which yields,

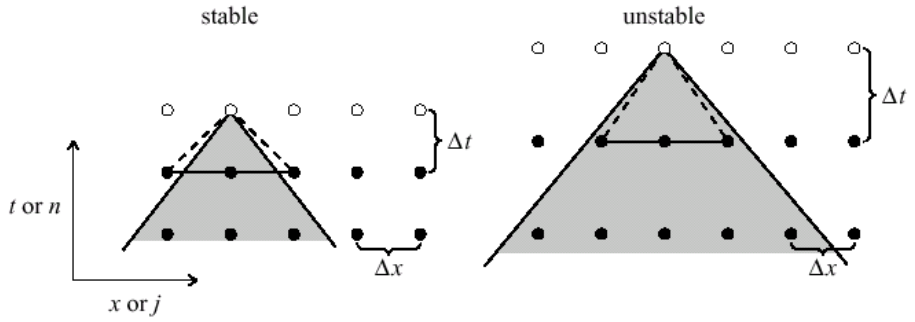
$$u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{v\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right)$$

If we now do a von Neumann stability analysis, one gets,

$$\xi = \cos k\Delta x - i\frac{v\Delta t}{\Delta x}\sin k\Delta x$$ So stability is achieved if, $$\frac{|v|\Delta t}{\Delta x} \leq 1$$

This condition is called “Courant condition” (Courant-Friedrichs-Lewy)

Intuitively, it implies that your discretization scheme not propagate information faster than the physical propagation speed of the problem.



The surprising fact that an apparently innocuous change in discretization can render a scheme unconditionally unstable underlines the fact that discretizing PDEs is as much an art as it is science!

To see better what happened, let us rewrite Lax's scheme in a way that it resembles the FTCS scheme, plus an extra term,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) + \frac{1}{2}\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta t}\right)$$

Now we can reinterpret this equation as the FTCS discretization of the following equation,

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2\Delta t}\nabla^2 u$$

The extra term in the equation (if applied to the equations of a fluid) would correspond to a viscous term. We have introduced, via our discretization scheme, what is called "numerical viscosity". This viscosity has a stabilizing effect on the scheme!

The effect of the viscosity can be seen in the amplification factor we computed. Unless vΔ t=Δx exactly, the amplification factor is smaller than one and therefore dies off in time.

But isn't this undesirable? Why is this dissipation better than the amplification we had in the FTCS scheme (apart from the fact that one blows up the code and the other one doesn't). Aren't both behaviors equally bad at the time of getting the real solution (which neither dies off nor blows up)?

In practice, one is interested in a regime in which kΔx<<1 (meaning the spatial discretization is much smaller than the wavelength of the solution. In such situation the amplification factor is very close to unity,

$$\xi = \cos k\Delta x - i\frac{v\Delta t}{\Delta x}\sin k\Delta x$$

But for such scales, isn't the amplification factor of FTCS also close to unity?

$$\xi(k) = 1 - i\frac{v\Delta t}{\Delta x}\sin k\Delta x$$

The answer is affirmative. However, in numerical simulation one always has, in addition to the physical modes of the solution, which are long wavelength with respect to the discretization scale, numerical noise which has wavelengths as small as the discretization scheme.

These physically uninteresting modes are killed by the Lax scheme (and we don't care). However, they are amplified until they blow up things by the FTCS method. That is what really differentiates both methods.

In general, viscosity has that tendency: it kills high frequency modes. As long as what one wishes to model is a low frequency effect (and it always is, in the sense we are using here, otherwise the discretization errors would be huge), adding viscosity does not change the physics but quenches out the high frequency numerical noise.

Some people add viscous terms to the physical equations to ensure that the discretized scheme will have this property. Such technique is called "artificial viscosity".

If one has more than one equation, the von Neumann stability analysis leads to a system of linear equations. For instance, consider,

$$\frac{\partial}{\partial t}\begin{bmatrix} r \\ s \end{bmatrix} = \frac{\partial}{\partial x}\begin{bmatrix} vs \\ vr \end{bmatrix}$$

Lax scheme

$$r_j^{n+1} = \frac{1}{2}(r_{j+1}^n + r_{j-1}^n) + \frac{v\Delta t}{2\Delta x}(s_{j+1}^n - s_{j-1}^n)$$

$$s_j^{n+1} = \frac{1}{2}(s_{j+1}^n + s_{j-1}^n) + \frac{v\Delta t}{2\Delta x}(r_{j+1}^n - r_{j-1}^n)$$

Mode analysis,

$$\begin{bmatrix} r_j^n \\ s_j^n \end{bmatrix} = \xi^n e^{ikj\Delta x}\begin{bmatrix} r^0 \\ s^0 \end{bmatrix}$$

Leads to the coupled equations,

$$\begin{bmatrix} (\cos k\Delta x) - \xi & i\frac{v\Delta t}{\Delta x}\sin k\Delta x \\ i\frac{v\Delta t}{\Delta x}\sin k\Delta x & (\cos k\Delta x) - \xi \end{bmatrix} \cdot \begin{bmatrix} r^0 \\ s^0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Which only have a solution if the determinant is zero, leading to the two solutions.

$$\xi = \cos k\Delta x \pm i\frac{v\Delta t}{\Delta x}\sin k\Delta x$$

And we see that both roots imply stability.

Other types of errors:

Up to now we have concerned ourselves with errors in the amplitude of the solution.

Errors in phase occur due to the fact that the formulas we derived for the amplification factors are k-dependent. Therefore a wave packet composed of various Fourier component will see the weight of the various components changed and as a consequence errors in phase can arise. If the phase of the solution is something of consequence, these errors need to be monitored.

Non-linear instabilities are ignored by the von Neumann method. The way these arise is in a feedback mechanism of the non-linear terms of the equations that can imply transfer of energy from long wavelength modes to short wavelength modes. Since numerically one has a cutoff given by discretization, energy piles up in the shortest mode, that grows in amplitude until the code blows up.

Since viscosity dissipates energy selectively, concentrating on high frequency modes, sometimes it can handle non-linear instabilities.

However, there exist physical situations where this instability is for real. For instance in fluids, the non-linear terms of the Navier Stokes equations imply such a feedback: it is the causal of “shock waves”. In these cases other techniques are needed to handle the problem since viscosity simply damps out the effect one wishes to observe.

For advective equations *transport errors* are a problem. In the Lax scheme, a disturbance in the variable u at the point j propagates to the point j-1 and j+1 in the next timestep. But of course physically if one has a problem with velocity v that is positive, only the point j+1 should be affected.

A way to handle this problem is “upwind differencing”,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v_j^n \begin{cases} \dfrac{u_j^n - u_{j-1}^n}{\Delta x}, & v_j^n > 0 \\ \dfrac{u_{j+1}^n - u_j^n}{\Delta x}, & v_j^n < 0 \end{cases}$$

This scheme is first order in space. How could it be better? The answer is the usual: order does not imply accuracy, or in this case, physical reasonableness in the behavior of the discretization scheme!

For this scheme the amplification factor is,

$$\xi = 1 - \left|\frac{v\Delta t}{\Delta x}\right| (1 - \cos k\Delta x) - i\frac{v\Delta t}{\Delta x}\sin k\Delta x$$

$$|\xi|^2 = 1 - 2\left|\frac{v\Delta t}{\Delta x}\right| \left(1 - \left|\frac{v\Delta t}{\Delta x}\right|\right) (1 - \cos k\Delta x)$$

And therefore the scheme is stable given the Courant condition, as before.

Summary

- The first task when dealing with PDE's is to identify the type of equation one is dealing with.
- For evolution equations, check stability of your scheme using Von Neumann criterion.