CS 101

Numerical Geometric Integration

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Partial Differential Equations

Multivariate fcts, come in many types

- most common: second order equations

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu = 0$$

- encodes various basic phenomena

$$b^2 - 4ac = \begin{cases} < 0 & \rightsquigarrow \text{ Elliptic equation} \\ = 0 & \rightsquigarrow \text{ Parabolic equation} \\ > 0 & \rightsquigarrow \text{ Hyperbolic equation} \end{cases}$$

Canonical Equations

To each type, its flagship equation

- elliptic:
  Poisson equation $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = g$$
- parabolic:
  heat equation $$\frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2}$$
- hyperbolic:
  wave equation $$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

Initial value problems

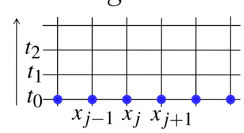
Let's Jump Right In

Wave equation made simpler

- generic scalar transport equation

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x}$$

- how to discretize and integrate this?
  - $x_j = x_0 + j\Delta x$
  - $t_n = t_0 + n\Delta t$
  - $u_j^n = u(x_j, t_n)$



Finite Differences

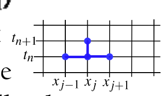
Taylor to the rescue again...

$$\frac{\partial u}{\partial t}\Big|_{j,n} = \frac{u_j^{n+1} - u_j^n}{\Delta t} \qquad \frac{\partial u}{\partial x}\Big|_{j,n} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

Discrete transport equation leads to:

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

- called FTCS, and is explicit
  - forward time, centered space



- oh, btw: does not work *at all*; why?

Stability Analysis

Von Neumann method

- eigenmode $u_j^n = \xi(k)^n\, e^{ikj\Delta x}$ (Amplification factor)
- plug it into FTCS

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

- alas, $|\xi(k)| > 1$
  - all frequencies get amplified
  - unconditionally unstable

Enter Lax (the man, not the airport)

Slight change to discrete update

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

- same space-time dependency
- but now, $|\xi(k)| < 1$ iff $\frac{|v|\Delta t}{\Delta x} < 1$
- Courant (CFL) condition
  - quite general for PDEs
    - never skip a point…
    - or you won't get convergence

But… Why Did It Work?

Rewrite Lax method, you'll get:

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

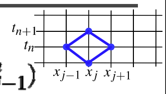
So the "real" PDE we try to integrate is:

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

- Second-order term: diffusion, killing high frequencies
- Called **numerical viscosity**
- Good, but bad… (high frequencies don't overpower low ones)

Other Variants

From Lax, to Leapfrog



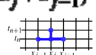
$$u_j^{n+1} = u_j^{n-1} - \frac{v\,\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n)$$

- CTCS
- second-order accurate in space and time

Lax-Wendroff

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

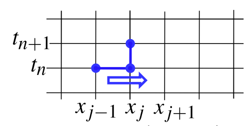
- second-order accurate (Taylor)



Gone With The Wind

We *know* we're dealing w/ transport

- so information "flows" with the wind

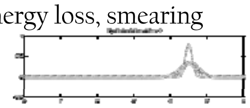


$$\frac{\partial u}{\partial x}\Big|_{j,n} = \frac{u_{j\cancel{+1}}^n - u_{j-1}^n}{\cancel{2}\Delta x}$$

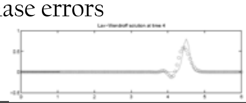
- "upwind" methods $\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} + \frac{1}{2}v\Delta t(1 - \frac{v\Delta x}{\Delta t})\frac{\partial^2 u}{\partial x^2}$
- only first order, but better! (CFL still)

Frequent Types of Num. Errors

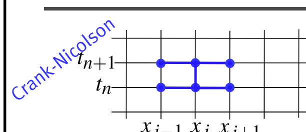
- dissipation (Lax, upwind)
  - energy loss, smearing

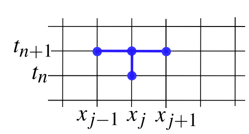


- dispersion (Lax-Wendroff)
  - phase errors



Plenty of Other Stencils





- fully implicit: CFL no longer needed
  - but massive damping for large time steps
- smaller stencils nicer if non-smooth u
  - sparser, less Gibbs oscillations near fast changes

Heat Equation? $\frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2}$

Schemes discussed above apply

- well, not upwind...
- and CFL no longer relevant
- ex: FTCS $u_j^{n+1} = u_j^n - \frac{\lambda \Delta t}{(\Delta x)^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$
  - Von Neumann says: $\xi(k) = 1 - 4\frac{\lambda \Delta t}{(\Delta x)^2}\sin^2(\frac{k\Delta x}{2})$
  - $\frac{4\lambda\Delta t}{(\Delta x)^2} < 1$ is new condition for stability

Elliptic Equations $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = g$

Should be obvious by now

$$\frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{(\Delta x)^2} = g_{i,j}$$

- boundary conditions need work
- less relevant for this class
  - no time step!

More To Life Than F. Differencing

Long list of numerical methods

- spectral, finite element, finite volume, ...
  - finite elements for elliptic equations
    - arbitrary spatial discretization
    - basis functions to provide discrete fct space
    - based on minimization on that space
    - easier handling of boundary conditions
  - finite volume also quite versatile
- and mix of thereof

Discrete vs. Differential

Facts that will come back again & again

- numerical integration not perfect
  - variety of issues can pop up
  - may have to pick the least bad...
- discrete scheme may integrate a **nearby** differential equation
- stability always the delicate thing

Yeay, Homework!

Due next monday

- closer look at ODEs
- implementation
  - second order ODE
    - separates into 2
  - meet with Patrick if (really) necessary
  - send solutions & notebooks by email
    - derivations on paper if you prefer