Overview of slides 08

Boundary and initial value problems

We looked at boundary value problems, which may be solved in a similar way to boundary-value odes.

Now: initial value problems.
Start with diffusion equation in 1+1 dimension:

Diffusion equation

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

Identical to heat equation.
Similar to Schroedinger equation in 1+1 dimension.

Initial value problems for pdes

Diffusion equation in 1+1 dimension:

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

Discretise space & time.

Using grid spacings $\Delta x = a$ in space, Δt in time, we write

$$u(x_i, t_n) = u(x_0 + ia, t_0 + n\Delta t) \equiv u_i^{(n)} .$$

Take forward derivative in time, and symmetric second derivative in space: Forward Time, Centred Space

$$\frac{\partial u}{\partial t} = \frac{u_j^{(n+1)} - u_j^{(n)}}{\Delta t} = D \frac{\partial^2 u}{\partial x^2} = \frac{D}{a^2}\left(u_{j-1}^{(n)} - 2u_j^{(n)} + u_{j+1}^{(n)}\right) \quad (1)$$

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

It is straightforward to iterate this forward in time from $n = 0$.

Stability issues

- Discretization of time-dep PDE's often leads to instabilities ☹
  - If discretization scheme is unstable, small errors blow up with time evolution.
  - Origin of errors? E.g., machine precision
  - Error in each step can be, e.g., of order $\Delta t(\Delta x)^2$
    Instability is due to continued time evolution, not single-step error

- Think of $u^{(m)}$ as a vector at each timestep.
  Explicit schemes like FTCS: $u^{m+1} = Au^m$
  Scheme is stable if A has $|\text{eigenvalues}| < 1$.
  Alternative analysis: von Neumann stability analysis

- Later: implicit schemes: $Bu^{m+1} = Au^m$

Stability analysis

von Neumann analysis

Fourier transform in space: $u(x) = \sum_k e^{ikx} u(k)$
Each $u(k)$ evolves independently in time
(at least for linear problems with constant coeffs)
This gives the eigenmode evolution

$$u_k^{(n+1)} = \xi_k u_k^{(n)} \quad \Longrightarrow \quad u_j^{(n)} = u_0^{(0)} (\xi_k)^n e^{ikja} \tag{2}$$

To find amplification factor ξ_k, substitute (2) into finite difference equation

$$|\xi_k| \quad \begin{cases} > 1 & \text{exponential growth, instability} \\ < 1 & \text{exponential damping, stability} \\ = 1 & \text{more detailed analysis needed} \end{cases}$$

von Neumann stability: $|\xi_k| \leq 1 \quad \forall k$ (for ALL k)

Stability for FTCS

Inserting the eigenmode evolution (2) into the FTCS equation (1) gives

$$\frac{\xi_k^{n+1} e^{ijka} - \xi_k^n e^{ijka}}{\Delta t} = \frac{D}{a^2} \xi_k^n \left(e^{ik(j-1)a} - 2e^{ikja} + e^{ik(j+1)a} \right)$$

$$\xi_k = 1 + \frac{D\Delta t}{a^2} \left(e^{-ika} - 2 + e^{ika} \right) = 1 - \frac{4D\Delta t}{a^2} \sin^2 \frac{ka}{2}$$

This is always ≤ 1 $\implies$ stability requires $\xi_k \geq -1$

$$\implies \frac{4D\Delta t}{a^2} \sin^2 \frac{ka}{2} \leq 2\,.$$

'Worst case': $\sin^2(ka/2) = 1$

Stability condition: $\displaystyle \frac{\Delta t}{a^2} \leq \frac{1}{2D}$

An example

The python file `ftcs_driver.py` solves the diffusion equation with the initial distribution

$$u_0(x) = u(x, t_0) = e^{-x^2/4Dt_0}\,, \quad -5 \le x \le 5\,, t_0 = 0.1\,,$$

and boundary conditions

$$u(\pm x_0, t) = \sqrt{\frac{t_0}{t}} e^{-x_0^2/4Dt}\,, \quad x_0 = 5\,.$$

The grid spacing in the x direction has been set to $a = 0.05$, and the diffusion constant $D = 1$.

`ftcs_driver(dt,t)` plots the solution for time step `dt` at time(s) `t`.

Run this with `dt=0.0012` and see what you get.
Then run with `dt=0.0013` and see what happens.

FTCS in 2+1 dimension

Our Ansatz is now

$$u_{jl}^{(n)} = u_0 \xi_k^n e^{ik_x j\Delta x} e^{ik_y l\Delta y} \tag{3}$$

For $\Delta x = \Delta y = a$ the FTCS scheme is

$$\frac{u_{jl}^{(n+1)} - u_{jl}^{(n)}}{\Delta t} = \frac{D}{a^2}\left(u_{j-1,l}^{(n)} + u_{j,l-1}^{(n)} + u_{j+1,l}^{(n)} + u_{j,l+1}^{(n)} - 4u_{jl}^{(n)}\right)$$

Inserting (3) gives

$$\begin{aligned}\xi_k &= 1 + \frac{D\Delta t}{a^2}\left(e^{-ik_x a} + e^{-ik_y a} + e^{ik_x a} + e^{ik_y a} - 4\right)\\ &= 1 - \frac{4D\Delta t}{a^2}\left(\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}\right)\end{aligned}$$

$$|\xi_k| \leq 1 \quad \forall k \qquad \Longrightarrow \quad \frac{\Delta t}{a^2} \leq \frac{1}{4D}$$

Improving stability (want to use larger Δt)

Stability condition is quite severe

- We want to model features at large scales $\lambda \gg a$
  Typical diffusion time is $\tau \sim \lambda^2/D$
  $\rightarrow$ need $n = \frac{\tau}{\Delta t} \sim \frac{\lambda^2}{a^2}$ time steps

- We want to improve accuracy by reducing a
  But if $a \rightarrow a/2$ then $\Delta t \rightarrow \Delta t/4$
  $\rightarrow$ 8 times as much cpu time!

Can we improve on this?

Second order time derivative?

FTCS is first-order accurate in time, second order in space

What about using second-order differencing in time?

Centred Time Centred Space

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

von Neumann

$$\xi_k - \frac{1}{\xi_k} = -\frac{8D\Delta t}{a^2}\sin^2\frac{ka}{2}$$

$$\Longrightarrow \xi_k = -\frac{4D\Delta t}{a^2}\sin^2\frac{ka}{2} \pm \sqrt{1 + \left(\frac{4D\Delta t}{a^2}\sin^2\frac{ka}{2}\right)^2}$$

The $(-)$ mode is unstable for all k and Δt!

CTCS is unconditionally unstable

Implicit schemes: BTCS

Explicit scheme: $\frac{\partial^2 u}{\partial x^2}$ evaluated at t

Implicit scheme: evaluate at $t + \Delta t$

Backward Time, Centred Space

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

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

We get a sparse matrix equation for $u^{(n+1)}$.

von Neumann analysis

$$\frac{\xi - 1}{\Delta t} = \frac{\xi}{a^2}\left(e^{ika} - 2 + e^{-ika}\right) \quad \implies \xi = \frac{1}{1 + \frac{4\Delta t}{a^2}\sin^2\frac{ka}{2}}$$

$\xi < 1$ for all $k, \Delta t$: BTCS is unconditionally stable

Crank–Nicolson

BTCS is stable, but only first-order accurate in time.
How can we get second-order accuracy?

Average FTCS and BTCS!
(the same as taking a centred time derivative around $t + \Delta t/2$)

$$\frac{u_j^{(n+1)} - u_j^{(n)}}{\Delta t} = \frac{1}{2a^2}\Big[\underbrace{u_{j+1}^{(n+1)} - 2u_j^{(n+1)} + u_{j-1}^{(n+1)}}_{BTCS} + \underbrace{u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)}}_{FTCS}\Big]$$

Crank-Nicolson

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

Stability of Crank-Nicolson

von Neumann analysis

$$\xi\left(1 - \frac{-4\Delta t}{2a^2}\sin^2\frac{ka}{2}\right) = 1 + \frac{-4\Delta t}{2a^2}\sin^2\frac{ka}{2}$$

$$\Longrightarrow \quad \boxed{\xi = \frac{1 - \frac{2\Delta t}{a^2}\sin^2\frac{ka}{2}}{1 + \frac{2\Delta t}{a^2}\sin^2\frac{ka}{2}}} \quad = \frac{1 - b^2}{1 + b^2}$$

The modulus of the numerator is always smaller than the denominator

Crank-Nicolson is unconditionally stable

Price of stability

BTCS and Crank-Nicholson are stable, but

implicit methods: need to solve linear set of equations at each step

$Bu^{(m+1)} = Au^{(m)}$ $\longrightarrow$ pre-factorize B (LU or Cholesky)

Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar}{2m}\nabla^2\Psi + V(\vec{x})\Psi$$

This can be discretised in the same way as diffusion equation

Important constraint

Time evolution is unitary $\iff$ Total probability is conserved

Formally: $\Psi(t) = e^{-iH(t-t_0)/\hbar}\Psi(t_0)$

FTCS for Schrödinger equation

$$\Psi^{(n+1)} = \Psi^{(n)} - \frac{i\Delta t}{\hbar}H\Psi^{(n)} = \left(1 - \frac{i\Delta t}{\hbar}H\right)\Psi^{(n)}$$

This is unconditionally unstable, and not unitary!

BTCS is stable, but still not unitary.

A unitary evolution operator

Use the Cayley form for $\exp(iH)$,

$$e^{iH\Delta t} \approx \frac{1 - \frac{1}{2}iH\Delta t}{1 + \frac{1}{2}iH\Delta t}$$

This gives us

$$\left(1 + \frac{1}{2}iH\Delta t\right)\Psi^{(n+1)} = \left(1 - \frac{1}{2}iH\Delta t\right)\Psi^{(n)}$$

This is Crank–Nicolson again!
Stable, second-order accurate and unitary.

Schrödinger equation

Widely used methods

- Crank-Nicholson type methods
  Price: solving linear system at each step

- Spectral methods with time splitting

$$\psi(t+\epsilon) = e^{-(i/\hbar)(\hat{T}+\hat{V})\epsilon}\psi(t) \approx e^{-(i/\hbar)\hat{T}\epsilon/2}e^{-(i/\hbar)\hat{V}\epsilon}e^{-(i/\hbar)\hat{T}\epsilon/2}\psi(t)$$

  Evolve with $\hat{T}$ in Fourier space, evolve with $\hat{V}$ in real space.
  Price: Fourier and inverse Fourier transforms at each step.

Wave equation

Examples too numerous to list...

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

has formal solution

$$u(x,t) = F(x - ct) + G(x + ct)\,, \quad \text{any } F, G$$

The equation can be discretised directly (using staggered leapfrog scheme) or transformed to two coupled first-order equations,

$$\frac{\partial v}{\partial t} + c\frac{\partial w}{\partial x} = 0\,, \qquad \frac{\partial w}{\partial t} + c\frac{\partial v}{\partial x} = 0$$

$$\text{with} \qquad v(x,t) = \frac{\partial u}{\partial t}\,, \qquad w(x,t) = -c\frac{\partial u}{\partial x}$$

Courant–Friedrichs–Lewy condition

Any explicit discretisation scheme for wave or advection equation requires

$$\Delta t < c\Delta x$$

Relaxation methods for static boundary value problems

We want to sove $\mathcal{L}\Phi = \rho$, $\mathcal{L} =$ elliptic operator, eg. ∇^2

Start with initial guess, let system 'relax' $\longrightarrow$ solution of pde

Diffusion in computer time

$$\frac{\partial \Phi}{\partial t} = \mathcal{L}\Phi - \rho \qquad \mathcal{L} = \text{elliptic operator, eg. } \nabla^2$$

$\rightarrow$ stationary (late time) solution fulfils $\mathcal{L}\Phi = \rho$

We converted the problem to initial value PDE

Applying PDE techniques to solving ODE BVP!!

Relaxation methods for static boundary value problems

Common example: time-independent Schrödinger equation

$\hat{H}\Psi(x, y) = E\Psi(x, y)$ can be solved for smallest E by evolving

$$\frac{\partial}{\partial t}\Psi(x, y, t) = \hat{H}\Psi(x, y, t) \text{ to late times}$$

$\longrightarrow$ propagation in imaginary time

Summary

- von Neumann stability criterion for time evolution equations:
  1. Fourier transform in space
  2. Find amplification factor ξ_k for each mode k
  3. Stability $\Longleftrightarrow \xi_k \leq 1$
- Forward Time, Centred Space:
  Explicit, stable for $\Delta t \leq a^2/2dD$ (1+d dim)
- Backward Time, Centred Space:
  Implicit, unconditionally stable
- Both FTCS and BTCS are first order in time
- Crank–Nicolson: Average FTCS and BTCS.
  Second order in time, unconditionally stable, widely used
- Relaxation: applying PDE techniques to ODE BVP's