Lecture 20

From last time, we introduced overrelaxation as a variation of the finite difference or Jacobi method

Recall that iteration is

$$\phi'(x,y) = \phi(x,y) + \Delta\phi(x,y)$$

Idea for overrelaxation is

$$\phi_\omega(x,y) = \phi(x,y) + (1+\omega)\Delta\phi(x,y)$$

w/ $\omega > 0$

For Laplace equation solution from before, this translates to

$$\phi_\omega(x,y) = (1+\omega)\frac{1}{4}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right] - \omega\,\phi(x,y)$$

Gauss-Seidel method (GS)

In previous method, we need an old array & new array & ~~update~~ use all terms of old array to make updates

When doing this we have to scan elements one-by-one & process

Idea for GS is to simply use one array & use newest values for updating

So the method looks like this

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for x in grid
    for y in grid
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$$\phi(x,y) \leftarrow \frac{1}{4}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right]$$

can then combine GS w/
overrelaxation to have update be

$$\phi(x,y) \leftarrow \frac{1+\omega}{4}\left[\phi(x+a,y)+\dots\right] - \omega\,\phi(x,y)$$

advantage of GS is that it uses less memory

GS ~~is~~ w/ overrelaxation is stable
but overrelaxation alone is not.
method is proven stable w/ $\omega < 1$

Initial Value Problems

giving starting conditions, goal is to predict future behavior.

Example: diffusion equation

$$\frac{\partial\phi}{\partial t} = D\frac{\partial^2\phi}{\partial x^2}$$ where D is diffusion constant

used to calculate motion of diffusing gases & liquids & flow of heat in thermal conductors

PDE w/ 2 variables, but divide spatial dimension into a line of points along the x axis (use evenly spaced points) spacing is "a"

then write

$$\frac{\partial^2 \phi}{\partial x^2} \approx \frac{\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)}{a^2}$$

$$\Rightarrow \frac{d\phi}{dt} \simeq \frac{D}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

try to solve

this now gives a set of simultaneous ordinary diff. eq.'s in $\phi(x,t)$, $\phi(x+a,t)$, $\phi(x-a,t)$ which we can solve using the methods from before!

Which method should we use?

- Actually makes sense to use Euler method here. This is b/c the approx. to the second-derivative given above has a second order error. So doesn't make sense to use more computationally intensive Runge-Kutta which has input w/ higher error.
- Euler method is second-order error which is comparable to error introduced by approx. to 2^{nd} derivative.

Recall Euler method is for solving

$$\frac{d\psi}{dt} = f(\psi, t)$$

Taylor expand $\psi(t)$ about time t

$$\psi(t+h) \simeq \psi(t) + h\frac{d\psi}{dt} =$$

$$\psi(t) + h\, f(\psi, t)$$

Applying this to our case gives

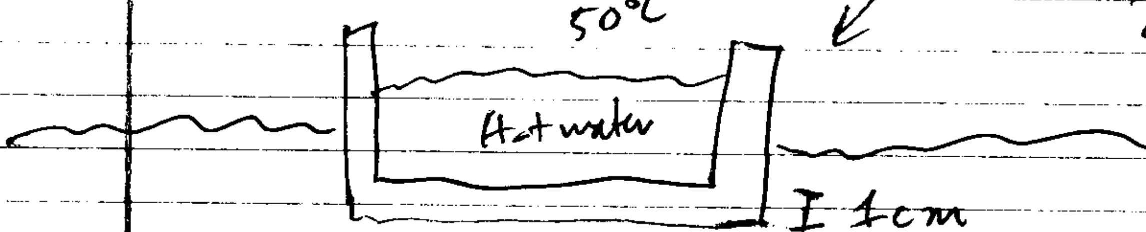
$$\phi(x, t+h) = \phi(x,t) + h\frac{D}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

This method is called <u>forward</u> <u>time</u> <u>centered</u> ~~difference~~ <u>space</u> (FTCS)

Knowing every grid value @ a given time allows us to predict all the next times.

Example: Calculate the temperature profile of a container made of stainless steel + submerged in 2 different baths

initially @ temp 20°C



Cold water 0°C

What is temp profile? function of distance + time

Thermal conduction governed by heat equation

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

make a grid + solve

thermal diffusivity $D = 4.25 \times 10^{-6}\ m^2 \cdot s^{-1}$

Bring up 1-heat.py

Starting out, profile is biased but then becomes more & more linear as time goes on.

- could have time-varying boundary conditions - straightforward to incorporate

Numerical Stability Analysis

FTCS method fails for wave equation. let's analyze why...

Recall wave equation is

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \phi}{\partial t^2}$$

To solve using FTCS method, divide space into discrete points w/ spacing "a"

$$\frac{d^2\phi}{dt^2} = \frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

Divide this into 2 simultaneous 1st order equations

$$\frac{d\phi}{dt} = \psi(x,t)$$

$$\frac{d\psi}{dt} = \frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

Applying Euler method gives

$$\phi(x,t+h) = \phi(x,t) + h\psi(x,t)$$

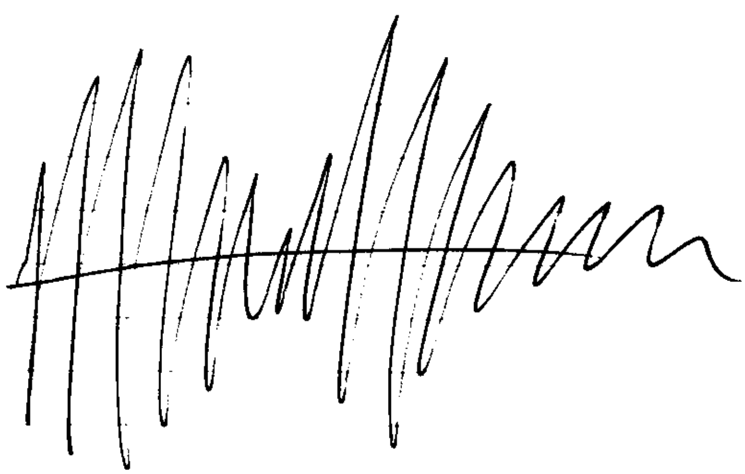
$$\psi(x,t+h) = \psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

idea is then to iterate these equations

What will happen?
after short time

t = 2ms

t = 50ms



t = 100ms

noise

calculation has become
numerically unstable

What's happening?

We can apply a von Neumann stability analysis.

return to diffusion equation for a moment (in FTCS form)

$$\phi(x, t+h) = \phi(x,t) + \frac{hD}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

Assuming spatial region is finite, (of course)

we can express $\phi(x,t)$ w/ a Fourier expansion

$$\phi(x,t) = \sum_k c_k(t)\, e^{ikx}$$

for some wavevectors k + coefficients $c_k(t)$ (time varying)

useful approach b/c diffusion equation is linear

Plug in a single term $c_k(t)\, e^{ikx}$,

we get

$$\phi(x, t+h) = c_k(t)\, e^{ikx} + \frac{hD}{a^2} c_k(t) \left[e^{ik(x+a)} + e^{+ik(x-a)} - 2e^{ikx} \right]$$

$$= c_k(t) e^{ikx} \left[1 + \frac{hD}{a^2} \left[e^{ika} + e^{-ika} - 2 \right] \right]$$

$$= c_k(t) e^{ikx} \left[1 - h \frac{4D}{a^2} \sin^2\left(\frac{ka}{2}\right) \right]$$

where we use $e^{i\theta} + e^{-i\theta} = 2\cos\theta$ &

$$1 - \cos\theta = 2\sin^2\left(\tfrac{1}{2}\theta\right)$$

$\Rightarrow$ each term in Fourier series transforms independently (terms don't couple)

$\Rightarrow$

$$c_k(t+h) = \left[1 - h \frac{4D}{a^2} \sin^2\left(\tfrac{1}{2} ka\right) \right] c_k(t)$$

So now we see that for stability we require that prefactor have magnitude ≤ 1

So we need

$$\left| 1 - \frac{h\,4D}{a^2} \sin^2\left(\frac{ka}{2}\right) \right| \le 1$$

we always have

$$1 - \underbrace{\frac{h\,4D}{a^2} \sin^2\left(\frac{ka}{2}\right)} \le 1$$

b/c is always ≥ 0

we need

$$-1 \le 1 - \frac{h\,4D}{a^2} \sin^2\left(\frac{ka}{2}\right)$$

$$\rightarrow \quad \frac{h\,4D}{a^2} \sin^2\left(\frac{ka}{2}\right) \le 2$$

sufficient to take

$$\frac{h\,4D}{a^2} \le 2 \quad \text{or}$$

$$h \le \frac{2a^2}{4D}$$

if strict inequality holds, then all terms in Fourier series except for

$k>0$ converge exponentially fast to zero.

Implies final solution is uniform in space, which is what we expect for diffusion equation.

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return to wave equation.

Slightly more complicated b/c we have coupled equations.

can expand vector $\begin{bmatrix} \phi(x,t) \\ \psi(x,t) \end{bmatrix}$ in terms of Fourier series,

Consider one term in the expansion

$$\begin{bmatrix} c_\phi(t) \\ c_\psi(t) \end{bmatrix} e^{ikx}$$

Plugging into evolution equations from before give

$$c_\phi(t+h) = c_\phi(t) + h\, c_\psi(t)$$

$$c_\psi(t+h) = c_\psi(t) - h\, c_\phi(t)\, \frac{4v^2}{a^2} \sin^2\left(\frac{ka}{2}\right)$$

Write as a matrix-vector equation

$$\underline{c}(t+h) = \underline{\underline{A}}\, \underline{c}(t)$$

w/ $\underline{c}(t) = \begin{bmatrix} c_\phi(t) \\ c_\psi(t) \end{bmatrix}$

& $\underline{\underline{A}} = \begin{bmatrix} 1 & h \\ -hr^2 & 1 \end{bmatrix}$ w/ $r = \frac{2v}{a} \sin\frac{ka}{2}$

$\Rightarrow$ At each time step, $\underline{c}$ gets multiplied by 2x2 matrix depending only on k.

can write $\underline{c}(t)$ as a linear combination of two eigenvectors of $\underline{\underline{A}}$:

$$\underline{c}(t) = \alpha(t)\, \underline{v}_1 + \beta(t)\, \underline{v}_2$$

$$\Rightarrow \underline{c}(t+h) = A\left(\alpha(t)\, \underline{v}_1 + \beta(t)\, \underline{v}_2\right) = \alpha(t)\, \lambda_1 \underline{v}_1 + \beta(t)\, \lambda_2 \underline{v}_2$$

Repeating this again gives

$$\underline{c}(t+2h) = \alpha(t)\lambda_1^2 \underline{v}_1 + \beta(t)\lambda_2^2 \underline{v}_2$$

& for m steps gives

$$\underline{c}(t+mh) = \alpha(t)\lambda_1^m v_1 + \beta(t)\lambda_2^m \underline{v}_2$$

eigenvalues for A are

$$\lambda = 1 \pm ihr$$

magnitude for both is

$$|\lambda| = \sqrt{1+h^2r^2} = \sqrt{1 + \frac{4h^2v^2}{a^2}\sin^2\left(\frac{ka}{2}\right)}$$

i.e. never less than one!

So this method is unstable for wave equation.

How to solve this problem?

use "implicit" method

Substitute $h \to -h$ in evolution eqn's

leading to

$$\phi(x, t-h) = \phi(x,t) - h\psi(x,t)$$

$$\psi(x,t-h) = \psi(x,t) - h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

tell us how to go back in time

substitute $t \to t+h$ & then rearrange

$$\phi(x,t+h) - h\psi(x,t+h) = \phi(x,t)$$

$$\psi(x,t+h) - h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right] = \psi(x,t)$$

not an explicit expression but we can solve these for future values (will be slower than before but the advantage is numerical stability)

Can rewrite these equations as

$$\underline{\underline{B}}\,\underline{c}(t+h) = \underline{c}(t)$$

$$\underline{\underline{B}} = \begin{bmatrix} 1 & -h \\ hr^2 & 1 \end{bmatrix}$$

$$\Rightarrow \underline{c}(t+h) = \underline{\underline{B}}^{-1}\underline{c}(t)$$

$$= \begin{bmatrix} 1 & h \\ -hr^2 & 1 \end{bmatrix} \frac{1}{1+h^2r^2}$$

eigenvalues are now

$$\lambda = \frac{1 \pm ihr}{1+h^2r^2}$$ w/ magnitude

$$|\lambda| = \frac{1}{\sqrt{1+h^2r^2}}$$ so we have stability

however, unphysical. waves propagate indefinitely but here we have exponential decay...