Partial Differential Equations

			order t	order x	
wave eqn $c>0$	$\frac{\partial^2 \phi}{\partial t^2} - c^2 \frac{\partial^2 \phi}{\partial x^2} = 0$		2	2	
diffusion $\alpha > 0$	$\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0$		1	2	
schrodinger	$i\hbar \frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t) \right]\psi$		1	2	complex
Poisson's	$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x,y)$			2 (2)	

First 3 involve time evolution from starting point $\Rightarrow$ IVP

Static Poisson $\Rightarrow$ BVP

Diffusion Example

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

α is diffusion coefficient

same form as heat equation

$\phi \equiv \phi(x,t)$

Need $\phi(x,0) = f(x)$ $\quad \phi(0,t) = u \quad \phi(L,t) = v$

Boundary along x at $[0, L]$

Discretize $\quad x_j = j\,\dfrac{L}{n-1} \qquad j = 0, 1, \ldots, n-1$

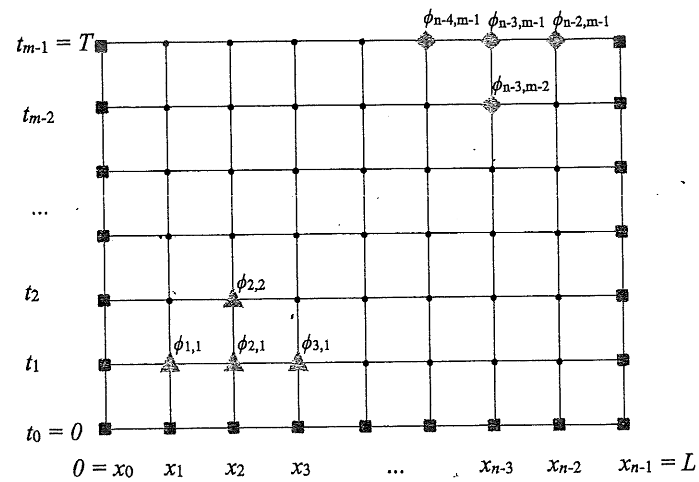
$$t_k = k\,\frac{T}{m-1} \qquad k = 0, 1, \ldots, m-1$$

$j \Rightarrow$ space index $\qquad k \Rightarrow$ time index

$\phi(x,t) \Rightarrow \phi_{j,k}$

x spacing $\quad h_x = \dfrac{L}{n-1}$

t spacing $\quad h_t = \dfrac{T}{m-1}$



$\uparrow k$

$\longrightarrow j \longrightarrow$

$\dfrac{\partial \phi}{\partial t} \Rightarrow$ Forward Diff

$\dfrac{\partial^2 \phi}{\partial x^2} \Rightarrow$ Central diff to 2nd derivative $\quad \left(\begin{array}{c}\text{forward time}\\ \text{centered space}\end{array}\right)$

$$\underbrace{\frac{\phi_{j,k+1} - \phi_{j,k}}{h_t}}_{j \text{ fixed, need } k+1} = \alpha\, \underbrace{\frac{\phi_{j+1,k} - 2\phi_{j,k} + \phi_{j-1,k}}{h_x^2}}_{k \text{ fixed need } j+1,\, j-1} \qquad \text{(FTCS)}$$

$$\phi_{j,k+1} = \gamma\,\phi_{j-1,k} + (1-2\gamma)\,\phi_{j,k} + \gamma\,\phi_{j+1,k}$$

$$\gamma \equiv \alpha\, h_t/h_x^2 \qquad \begin{array}{l} j = 1, 2, \ldots\, n-2 \\ k = 0, 1, \ldots\, m-2 \end{array}$$

Gets us from k to $k+1$, explicit method

Could also start at x_j, t_{k+1} and move backward in time, centered in space BTCS

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$\frac{\partial \phi}{\partial t} \Rightarrow$ Backward Diff

$\frac{\partial^2 \phi}{\partial x^2} \Rightarrow$ Central diff to 2nd deriv (at t_{k+1})

$$\frac{\phi_{j,k+1} - \phi_{j,k}}{h_t} = \alpha \frac{\phi_{j+1,k+1} - 2\phi_{j,k+1} + \phi_{j-1,k+1}}{h_x^2}$$

see diamonds in figure

$$-\gamma \phi_{j-1,k+1} + (1+2\gamma)\phi_{j,k+1} - \gamma \phi_{j+1,k+1} = \phi_{j,k}$$

implicit, harder!

To solve for ϕ at $k+1$ use BC $\phi_{0,k+1} = \phi_{0,k} = u$ and $\phi_{n-1,k+1} = \phi_{n-1,k} = v$

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & & & 0 \\ -\gamma & 1+2\gamma & -\gamma & \cdots & & & \\ 0 & -\gamma & 1+2\gamma & \cdots & & & \\ \vdots & & & \ddots & & & \\ & & & & 1+2\gamma & -\gamma & 0 \\ 0 & & \cdots & & -\gamma & 1+2\gamma & -\gamma \\ & & & & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi_{0,k+1} \\ \phi_{1,k+1} \\ \vdots \\ \\ \phi_{n-1,k+1} \end{bmatrix} = \begin{bmatrix} \phi_{0,k} \\ \phi_{1,k} \\ \vdots \\ \\ \phi_{n-1,k} \end{bmatrix}$$

$$A \phi_{k+1} = \phi_k \qquad k = 0, 1, \ldots M-2$$

FTCS easy $\Longleftrightarrow$ BTCS more robust

Poisson's Equation (2D)

Recall Gauss's equation

$$\oint \vec{E} \cdot d\vec{a} = q_{in}/\epsilon_0 \iff \nabla \cdot \vec{E} = \rho_{in}/\epsilon_0$$

ρ = net charge density $[C/m^3]$

$\vec{E} = -\nabla V$

$$\Rightarrow \nabla^2 V = -\rho_{in}/\epsilon_0$$

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = -\rho_{in}/\epsilon_0 \quad \text{in 2D} \quad \rho = f(x,y)$$

Let's use ϕ instead of V

discretize $x_p = p \frac{L_x}{n-1}$ $\quad y_q = q \frac{L_y}{n-1}$ $\quad p,q = 0,1,\ldots n-1$

on rectangular grid with size L_x, L_y

Need boundary conditions

1) ϕ specified on boundary (Dirichlet)
2) $\frac{d\phi}{dn}$ derivative normal to boundary (Neumann)
3) mixed
4) periodic

use central diff approx to 2nd derivative (let $L_x = L_y = L$)

$$\frac{\phi_{p+1,q} - 2\phi_{p,q} + \phi_{p-1,q}}{h^2} + \frac{\phi_{p,q+1} - 2\phi_{p,q} + \phi_{p,q-1}}{h^2} = f_{pq}$$

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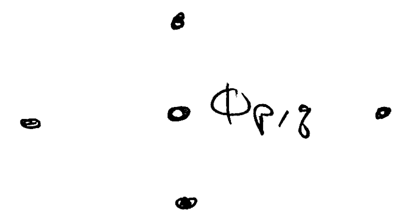
$$\Phi_{p,q} = \frac{1}{4}\left[\Phi_{p+1,q} + \Phi_{p-1,q} + \Phi_{p,q+1} + \Phi_{p,q-1} - h^2 f_{pq}\right]$$

when $f_{pq} = 0$



ϕ is average of nearby values

can form linear algebra solution like

$A\vec{x} = \vec{b}$ (but x is made of $\Phi_{p,q}$ matrix)

can do it one at a time

-or- iterate until $\phi_{p,q}$ is 'not changing'

need bc and initial guess for $\Phi_{p,q}$ everywhere

$\Rightarrow$ relaxation method

update $\phi_{p,q}$ continuously (Gauss-Seidel method)

works but fairly slow

[see code]