Finite difference method

$$\begin{cases} u_t = k u_{xx}, & 0<x<L,\ 0<t<T \\ u(x,0) = u_0(x) \\ \text{B.C.} \end{cases}$$

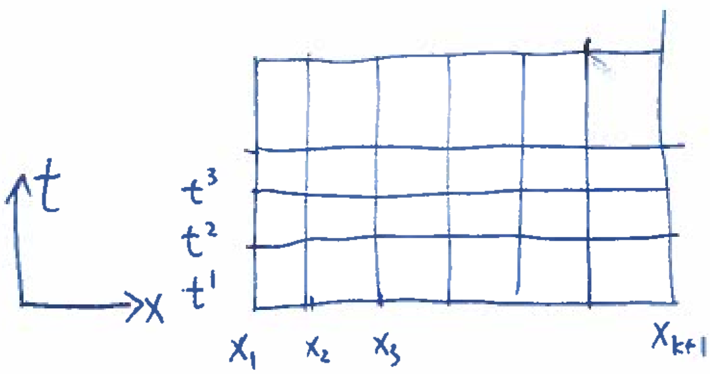
discretize space and time $\quad \underbrace{\Delta x = \frac{L}{k}}_{\text{mesh size}}, \quad \underbrace{\Delta t = \frac{T}{m}}_{\text{time step}}$

Spatial points $\quad x_1,\ x_2,\ x_3,\ \cdots\ x_{k+1} \qquad (x_j) \quad 1 \le j \le k+1$

$x_1 = 0, \quad x_j = (j-1)\Delta x, \quad x_{k+1} = L$

temporal points $\quad t^1,\ t^2,\ \cdots\ t^{m+1} \qquad (t^n) \quad 1 \le n \le m+1$

$t^1 = 0, \quad t^{m+1} = T$



$t^{n+1} - t^n = \Delta t$

$x_{j+1} - x_j = \Delta x$

So instead of solving $u(x,t) \quad 0 \le x \le L,\ 0 \le t \le T,$

we solve $\quad u(x_j, t^n) \quad 1 \le j \le k+1,\ 1 \le n \le m+1$

$\quad\quad\quad\quad\quad \| $

$\quad\quad\quad\quad\quad u_j^n \qquad$ basic idea: $\quad$ Know $(u_j^n)_{j=1}^{k+1}$

$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad$ Find $(u_j^{n+1})_{j=1}^{k+1}$

Forward difference $\quad u_x \approx \dfrac{u_{j+1}^n - u_j^n}{\Delta x} \qquad u_t \approx \dfrac{u_j^{n+1} - u_j^n}{\Delta t}$

backward difference $\quad u_x \approx \dfrac{u_j^n - u_{j-1}^n}{\Delta x} \qquad u_t \approx \dfrac{u_j^n - u_j^{n-1}}{\Delta t}$

Centered difference $\quad u_x \approx \dfrac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = $ (average of forward and backward)

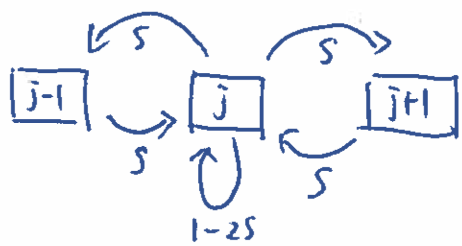
$$u_{xx} \approx \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}$$

Now diffusion equation $u_t = k\,u_{xx}$ (forward in t, centered in xx)

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = k \cdot \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \longrightarrow \text{discrete diffusion equation}$$

Let $s = \dfrac{k\Delta t}{(\Delta x)^2}$. Then $u_j^{n+1} - u_j^n = s\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)$

$$u_j^{n+1} = s\,u_{j+1}^n + (1-2s)\,u_j^n + s\,u_{j-1}^n$$



Example $\quad$ initial condition

$$\begin{array}{ccccccc} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac14 & \frac12 & \frac14 & 0 & 0 \\ 0 & \frac1{16} & \frac14 & \frac38 & \frac14 & \frac1{16} & 0 \end{array}$$

$\underline{K=6}$ $\quad s = \frac14$

$$u_j^{n+1} = \frac14 u_{j+1}^n + \frac12 u_j^n + \frac14 u_{j-1}^n$$

$$\begin{array}{ccccccc} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac34 & -\frac12 & \frac34 & 0 & 0 \\ 0 & \frac9{16} & -\frac58 & \frac{11}8 & -\frac58 & \frac9{16} & 0 \end{array}$$

$s = \frac34$

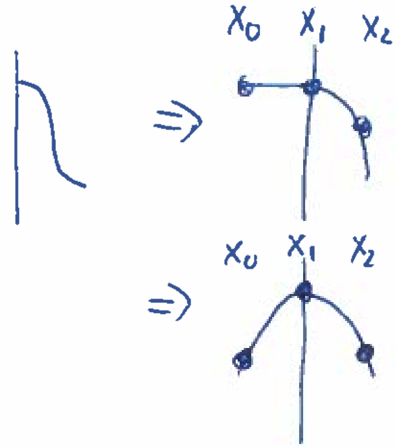
$$u_j^{n+1} = \frac34 u_{j+1}^n - \frac12 u_j^n + \frac34 u_{j-1}^n$$

boundary condition

Dirichlet $u=0 \Rightarrow u_1^n = 0$, $u_{k+1}^n = 0$, $\forall n$

Newmann ① $u_x = 0$

create a phantom point x_0



x_0

$u_0^n = u_1^n \rightarrow$ Neumann 1

$u_0^n = u_2^n \rightarrow$ Neumann 2

Full Algorithm: $[u^{n+1}] = A \cdot [u^n]$ $\qquad u^n = \begin{bmatrix} u_1^n \\ \vdots \\ u_{k+1}^n \end{bmatrix}$

$n=4$ Dirichlet $A_D = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ s & 1-2s & s & 0 & 0 \\ 0 & s & 1-2s & s & 0 \\ 0 & 0 & s & 1-2s & s \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

Neumann 1 : $A_{N1} = \begin{pmatrix} 1-s & s & 0 & 0 & 0 \\ s & 1-2s & s & 0 & 0 \\ 0 & s & 1-2s & s & 0 \\ 0 & 0 & s & 1-2s & s \\ 0 & 0 & 0 & s & 1-s \end{pmatrix}$

Neumann 2

$A_{N2} = \begin{pmatrix} 1-2s & 2s & 0 & 0 & 0 \\ & & \text{———} & & \\ & & \text{———} & & \\ & & \text{———} & & \\ 0 & 0 & 0 & 2s & 1-2s \end{pmatrix}$

same $\leftarrow$

at boundary $\quad u_1^{n+1} = s u_0^n + (1-2s) u_1^n + s u_2^n$ $\overset{\text{Neumann 1}}{=} (1-s) u_1^n + s u_n^2$

$u_1^{n+1} = \text{—————————} = (1-2s) u_1^n + 2s u_n^2$

Forward finite difference method

① given $[u^1]$

② $[u^{n+1}] = A \cdot [u^n]$

Periodic B.C.

$A_p = \begin{pmatrix} 1-2s & s & 0 & 0 & s \\ & & \text{———} & & \\ & & \text{———} & & \\ & & \text{———} & & \\ s & 0 & 0 & s & 1-2s \end{pmatrix}$

cylic matrix

Is the algorithm correct?

$$[u^{n+1}] = A \cdot [u^n] \Rightarrow [u^{n+1}] = A^n [u^1].$$

Solution should be bounded. Suppose $[u^1]$ be an eigenvector of A

$$A[u^1] = \lambda[u^1] \Rightarrow [u^{n+1}] = \lambda^n [u^1]. \quad \text{bounded } |\lambda^n| \le 1$$

$\Leftrightarrow |\lambda| \le 1$. So this numerical algorithm is stable if $|\lambda| \le 1$ for all eigenvalues of A.

$A = [\, s \;\; 1-2s \;\; s \,]$ $\quad A \geq 0$ $\quad$ (if $[U^n]$ is positive then $[u^{n+1}] \geq 0$)

$0 \le s \le \frac{1}{2}$ $\quad$ Theorem: if $0 < s < \frac{1}{2}$, then all eigenvalues $|\lambda_i| \le 1$.

(can be proved through matrix theory)

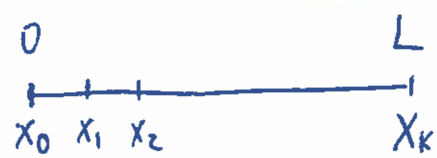
"PDE solution" $\quad u_j^{n+1} = s u_{j+1}^n + (1-2s) u_j^n + s u_{j-1}^n$

$$u_j^n = X_j T^n \quad \Rightarrow \frac{T^{n+1}}{T^n} = 1 - 2s + s\frac{X_{j+1} + X_{j-1}}{X_j} = \xi$$

$$T^{n+1} = \xi^n T^1, \quad s\frac{X_{j+1} + X_{j-1}}{X_j} + 1 - 2s = \xi. \quad \text{we need } |\xi| \le 1$$

~~Solution $X_j = A\cos j\theta + B\sin j\theta$~~ $\boxed{\theta = \Delta x}$

Dirichlet B. C. $\quad X_j = \sin j\theta$



Eigenvalue Problem $\quad (X_j)$ $\quad 1 \le j \le K+1$, $\quad 0 \le j \le K$

$$\begin{cases} s X_{j+1} + (1-2s) X_j + s X_{j-1} = \xi X_j \\ X_0 = X_K = 0 \end{cases} \Rightarrow \xi = ?$$

Solution $\quad X_j = \sin(j\theta)$ $\quad X_0 = \sin 0 = 0$ $\quad K\theta = m\pi$

$X_K = \sin(K\theta) = 0$ $\quad \theta = \frac{m\pi}{K}$.

So $x_j = \sin\left(j \cdot \frac{m\pi}{K}\right) \qquad \theta = \frac{m\pi}{K}$

$= \sin(j\theta)$

$$s \cdot \sin((j+1)\theta) + (1-2s)\sin j\theta + s\sin(j-1)\theta = \xi \cdot \sin j\theta$$

$$\sin(j\theta \pm \theta) = \sin j\theta \cos\theta \pm \cos j\theta \sin\theta$$

$$\Rightarrow \quad 2s\sin j\theta\cos\theta + (1-2s)\sin j\theta = \xi \sin j\theta$$

$$\Rightarrow \quad \xi = 1-2s+2s\cos\theta$$

$$|\xi| \le 1 \Rightarrow -1 \le 1-2s+2s\cos\theta \le 1 \quad \Rightarrow -1 \le 1-4s \le 1 \le 1$$

$$\Rightarrow \quad 4s \le 2 \Rightarrow s \le \frac{1}{2}$$

So stability condition $\quad k\frac{\Delta t}{(\Delta x)^2} = s \le \frac{1}{2}$.

Backward finite difference

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

matrix form $\quad [u^n] = B \cdot [u^{n+1}] \quad$ or $\quad [u^{n+1}] = B^{-1}[u^n]$

<u>Dirichlet</u>

$$B_D = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ -s & 1+2s & -s & 0 & 0 \\ - & - & & - & \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$B_N = \begin{array}{c} \begin{matrix} 1+2s & -2s \end{matrix} \\ \begin{pmatrix} \boxed{1+s \quad -s} & 0 & 0 & 0 \\ -s & 1+2s & -s & 0 & 0 \\ 0 & -s & 1+2s & -s & 0 \\ 0 & 0 & -s & 1+2s & -s \\ 0 & 0 & 0 & \boxed{-s \quad 1+s} \end{pmatrix} \\ \begin{matrix} & & & -2s & 1+2s \end{matrix} \end{array}$$

$$B_p = \begin{pmatrix} 1+2s & -s & 0 & 0 & -s \\ & & \vdots & & \\ -s & 0 & 0 & -s & 1+2s \end{pmatrix}$$

Crank-Nicolson scheme

$$\frac{u_j^{n+1}-u_j^{n}}{\Delta t} = (1-\theta)k\underbrace{\frac{u_{j+1}^{n}-2u_j^{n}+u_{j-1}^{n}}{(\Delta x)^2}}_{\text{forward}} + \theta k\underbrace{\frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{(\Delta x)^2}}_{\text{backward}}$$

$\theta = 0 \Rightarrow$ forward, $\theta = 1 \Rightarrow$ backward, $0<\theta<1 \Rightarrow$ mix.

~~matrix form~~

$$u_j^{n+1}-u_j^{n} = (1-\theta)s\left(u_{j+1}^{n}-2u_j^{n}+u_{j-1}^{n}\right) + \theta s\left(u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}\right)$$

$$\underbrace{-\theta s\, u_{j+1}^{n+1} + (1+2\theta s)u_j^{n+1} - \theta s\, u_{j-1}^{n+1}}_{\text{time } n+1} = \underbrace{(1-\theta)s\, u_{j+1}^{n} + (1-2(1-\theta)s)u_j^{n} + (1-\theta)s\, u_{j-1}^{n}}_{\text{time } n}$$

$$u_j^n = T^n X_j$$

$$T^{n+1}\left(-\theta s X_{j+1} + (1+2\theta s)X_j - \theta s X_{j-1}\right) = T^n\left((1-\theta)s X_{j+1} + (1-2(1-\theta)s)X_j + (1-\theta)s X_{j-1}\right)$$

$$\frac{T^{n+1}}{T^n} = \frac{(1-\theta)s X_{j+1} + (1-2(1-\theta))X_j + (1-\theta)s X_{j-1}}{-\theta s X_{j+1} + (1+2\theta s)X_j - \theta s X_{j-1}} = \xi$$

need $|\xi| < 1$ $\quad X_j = \sin(j\phi)$ $\quad$ Dirichlet B.C

$$\frac{2(1-\theta)s\cdot \sin j\phi\cos\phi + (1-2(1-\theta))\sin j\phi}{-2\theta s\ \sin j\phi\cos\phi + (1+2\theta s)\sin j\phi} = \xi.$$

$$|\xi| = \left|\frac{2(1-\theta)s\cos\phi + (2\theta-1)}{1+2\theta s - 2\theta s\cos\phi}\right| \le 1$$

$$\cancel{-1-2\theta s+2\theta s\cos\phi \underset{②}{\le} 2(1-\theta)s\cos\phi + 2\theta - 1 \underset{①}{\le} 1+2\theta s - 2\theta s\cos\phi}$$

Let $X_j = \sin(j\psi)$ similar to previous case

$$X_{j+1} + X_{j-1} = \sin((j+1)\psi) + \sin((j-1)\psi)$$
$$= 2\sin j\psi \cos\psi$$

So
$$\xi = \frac{2(1-\theta)s\cdot\sin j\psi\cos\psi + (1-2(1-\theta)s)\sin j\psi}{-2\theta s\cdot\sin j\psi\cos\psi + (1+2\theta s)\sin j\psi} = \frac{1-2(1-\theta)s + 2(1-\theta)s\cdot\cos\psi}{1+2\theta s - 2\theta s\cdot\cos\psi}$$

$$= \frac{1-2s(1-\theta)(1-\cos\psi)}{1+2s\theta(1-\cos\psi)}$$

Let $y = 1-\cos\psi$ Then $0 \le y \le 2$.

Define
$$\xi(y) = \frac{1-2s(1-\theta)y}{1+2s\theta y} \qquad 0 \le y \le 2.$$

Then
$$\xi'(y) = \frac{(1+2s\theta y)(-2s(1-\theta)) - (1-2s(1-\theta)y)\cdot 2s\theta}{(1+2s\theta y)^2}$$

$$= \frac{-2s}{(1+2s\theta y)^2} < 0 \quad \text{for } 0 \le y \le 2$$

$$\xi(0) = 1, \quad \xi(2) = \frac{1-4s(1-\theta)}{1+4s\theta} = \frac{1+4s\theta-4s}{1+4s\theta} = 1 - \frac{4s}{1+4s\theta}$$

Thus $|\xi| \le 1$ if and only if $1 \ge 1 = \xi(0) \ge \xi(y) \ge \xi(2) \ge -1$

$1 \ge 1$ is obviously true, $\xi(2) \ge -1 \iff 2 > \dfrac{4s}{1+4s\theta}$

$\iff 2+8s\theta \ge 4s \iff 1+4s\theta \ge 2s \iff 1 \ge 2s(1-2\theta)$

$\iff s \le \dfrac{1}{2(1-2\theta)}$ If $\frac{1}{2} \le \theta \le 1$ then this is always true.

If $0 \le \theta < \frac{1}{2}$, then $|\xi| \le 1$ iff

$$0 < s \le \frac{1}{2(1-2\theta)}.$$