ODE-BVP

→ Boundary condition's types : 1. Dirichlet BC

$y(x_0) = \beta_1$

$y(x_M) = \beta_2$

2 → Neumann BC

$\left.\dfrac{dy}{dx}\right|_{x_0} = \beta$ [ex. no flux condition impermeable membrane]

3 → Robin BC.

$\beta_1 \left.\dfrac{dy}{dx}\right|_{x_0} + \beta_2 y(x_0) = \beta_3$ --m-- combinatⁿ of 1 & 2

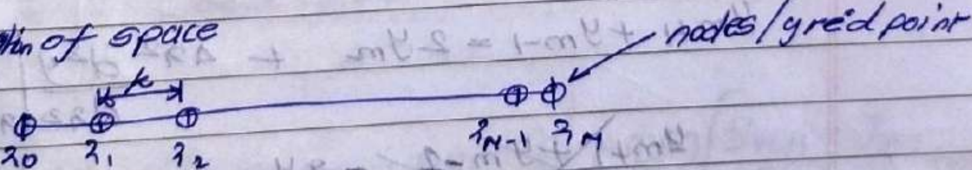
→ Methods:

- Finite difference method
- Initial value method (shooting method)
- Finite element method.
- Orthogonal Collocation

→ FDM:

An approximation of a derivative made in terms of values ~~m~~ at a discrete set of points is called finite difference approximation. The method which is used to perform this approxⁿ is called as FDM.

1. Discretisation of space



$x_M = x_0 + mk.$

$m = 0, 1, 2, 3, \text{----} M$

$k = \dfrac{x_M - x_0}{M}$ [Mesh size or spatial increment]

total nodes $= M+1$

Derivation:

$$y_{m+1} = y(x_m + \Delta x) = y_m + \Delta x\, y'(x_m) + \frac{\Delta x^2}{2} \frac{d^2y}{dx^2}\Big|_{x=x_m} + O(\Delta x^3) \quad \text{--- (1)}$$

$$y_{m+1} = y_m + k \frac{dy}{dx}\Big|_{x=x_m} + O(k^2)$$

$$\frac{dy}{dx}\Big|_{x=x_m} = \frac{y_{m+1} - y_m}{k} + O(k)$$ --- Forward diff. eq^n / 2 point Forward diff method.

- 1 order accurate

$$y_{m-1} = y(x_m - \Delta x) = y_m - \Delta x \frac{dy}{dx}\Big|_{x=x_m} + \frac{\Delta x^2}{2} \times \frac{d^2y}{dx^2}\Big|_{x=x_m} + O(\Delta x^3) \quad \text{--- (2)}$$

$$y_{m-1} = y(x_m - \Delta x) = y_m - \Delta x\, dy/dx\Big|_{x=x_m} + O(k^2)$$

$$\frac{dy}{dx}\Big|_{x=x_m} = \frac{y_m - y_{m-1}}{k} + O(k)$$ --- Backward difference eq^n

- 1 order accurate

(1) − (2)

$$y_{m+1} - y_{m-1} = 2\Delta x\left(dy/dx\Big|_{x=x_m}\right) + O(\Delta x^3)$$

$$\frac{y_{m+1} - y_{m-1}}{2k} + O(k^2) = dy/dx\Big|_{x=x_m}$$ --- Central difference method for 1st order derivative

- 2 order accurate

(1) + (2)

$$y_{m+1} + y_{m-1} = 2y_m + \Delta x^2 \frac{d^2y}{dx^2}\Big|_{x=x_m} + O(\Delta x^4)$$

$$\cancel{\frac{y_{m+1} + y_{m-1} - 2y_m}{k^2}}$$

$$\frac{d^2y}{dx^2}\Big|_{x=x_m} = \frac{-2y_m + y_{m+1} + y_{m-1}}{k^2} + O(k^2)$$

--- central difference for 2nd order derivative

$x_0, x_M \Rightarrow$ Boundary nodes

$x_1, x_2, \ldots x_{M-1} \rightarrow$ internal / interior nodes

$x_0 \quad x_1 \quad x_2 \quad \ldots \quad x_{M-1} \quad x_M$

$\rightarrow$ Algorithm:

Step 1: Spatial discretisation

Step 2: Discretize ODE [ODE $\rightarrow$ set of AE (algebraic eqn)]

no. of AE $= \boxed{M-1}$

Pb: $P(x)\dfrac{d^2y}{dx^2} + q(x)\dfrac{dy}{dx} = r(x)$

BCs: $y(x_0) = y_a \qquad y(x_M) = y_b$

Step 3: Dirichlet BC. $y(m=0)$, $y(m=M)$ @ given

Other: 2AEs ; @ $M+1$ AE

(ODE) $\hookrightarrow$ discretise them ; $M+1$ unknowns $(y_0, y_1, \ldots y_M)$

Remarks: system (ODE) @ non-linear then transformed AEs @ non-linear

$\Rightarrow$ system: $P(x)\dfrac{d^2y}{dx^2} + q(x)\,dy/dx = r(x)$

use central difference method.

$$\left.\frac{dy}{dx}\right|_{x=x_m} = \frac{y_{m+1} - y_{m-1}}{2k} + O(k^2)$$

$$\left.\frac{d^2y}{dx^2}\right|_{x=x_m} = \frac{2y_m - y_{m+1} - y_{m-1}}{k^2} + O(k^2)$$

$$\therefore P(x)\left[\frac{2y_m - y_{m+1} - y_{m-1}}{k^2} + O(k^2)\right] + q(x)\left[\frac{y_{m+1} - y_{m-1}}{2k} + O(k^2)\right] = r(x)$$

$$y_{m-1}\left[\frac{P(x)}{k^2} - \frac{q(x)}{2k}\right] + \left[\frac{2P(x)}{k^2}\right]y_m + y_{m+1}\left[\frac{+P(x)}{k^2} + \frac{q(x)}{2k}\right] + O(k^2) = r(x)$$

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$$\left[\frac{P(x_m)}{h^2}-\frac{q(x_m)}{2h}\right]y_{m-1}+\left[\frac{-2P(x_m)}{h^2}\right]y_m+\left[\frac{+P_m}{h^2}+\frac{q_m}{2h}\right]y_{m+1}+O(h^2)=r_m$$

$$\left[2P_m-q_m h\right]y_{m-1}+\left[-4P_m\right]y_m+\left[2P_m+q_m h\right]y_{m+1}+O(h^4)=r_m\times 2h^2$$

$m=1,2,\ldots,M-1$

$$(2P_1-q_1 h)y_0+\left[-4P_1\right]y_1+\left[2P_1+q_1 h\right]y_2=r_1\times 2h^2$$

$$(2P_2-q_2 h)y_1+\left[-4P_2\right]y_2+\left[2P_2+q_2 h\right]y_3=r_2\times 2h^2$$

$\vdots$

$$(2P_{M-1}-q_{M-1}h)y_{M-2}+\left[-4P_{M-1}\right]y_{M-1}+\left[2P_{M-1}+q_{M-1}h\right]y_M=r_{M-1}\times 2h^2$$

$$\underbrace{\begin{bmatrix}-4P_1 & [2P_1+q_1h] & 0 & \cdots & & \\ (2P_2-q_2h) & [-4P_2] & [2P_2+q_2h] & 0 & \cdots & \\ & & & & & \\ \cdots & & 0 & (2P_{M-1}-q_{M-1}h) & (-4P_{M-1}) & \end{bmatrix}}_{M-1\times M-1}\underbrace{\begin{bmatrix}y_1\\ y_2\\ y_3\\ \vdots\\ y_{M-1}\end{bmatrix}}_{M-1\times 1}=\underbrace{\begin{bmatrix}r_1 2h^2-(2P_1-q_1h)y_0\\ r_2\times 2h^2\\ \vdots\\ r_{M-1}\times 2h^2-y_N[2P_{M-1}+q_{M-1}h]\end{bmatrix}}_{M-1\times 1}$$

$\longrightarrow$ Homework: $\frac{d^2 y}{dx^2}=2$, $x\in[0,1]$

center difference

$M=6$

$y(x=0)=0$

$y(x=1)=0$

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$x_M - x_0 / M$

$k = \frac{1-0}{6} = 1/6$

$$\frac{y_{m+1} + y_{m-1} - 2y_m}{k^2} = \left.\frac{d^2y}{dx^2}\right|_{x=x_m}$$

$\therefore U_{m+1} + U_{m-1} - 2U_m = -2k^2$

$U_{m-1} - 2U_m + U_{m+1} = -2k^2$

$m \in 1, \dots, M-1$

$$\underbrace{\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{M-1 \times M-1} \underbrace{\begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{bmatrix}}_{M-1 \times 1} = \underbrace{\begin{bmatrix} -2k^2 - U_0 \\ -2k^2 \\ -2k^2 \\ -2k^2 \\ -2k^2 - U_6 \end{bmatrix}}_{M-1 \times 1}$$

solving above matrix we get,

$U_1 = 0.1389$

$U_2 = 0.2222$

$U_3 = 0.2500$

$U_4 = 0.2222$

$U_5 = 0.1389$

→ BVP with Neumann BC.

• cooling fin

fin model eqn :

$$\frac{d^2\theta}{d\varepsilon^2} = H^2\theta \qquad \varepsilon \in [0,1]$$

$M = 4$

$\theta(\varepsilon = 0) = 1 \qquad H = 4.$

$$\left.\frac{d\theta}{d\varepsilon}\right|_{\varepsilon=1} = 0 \qquad \text{center difference.}$$

$\xi_0 = 0$ $\quad\quad$ $\xi_4 = 1$ $\quad$ | $H = 4$

0 $\quad$ 0.25 $\quad$ 0.5 $\quad$ 0.75 $\quad$ 1

$k = \frac{\xi_H - \xi_0}{4}$

$k = 0.25$

$$\frac{-2\theta_m + \theta_{m+1} + \theta_{m-1}}{k^2} = H^2 \theta_m$$

$$-2\theta_m + \theta_{m+1} + \theta_{m-1} = H^2 \theta_m k^2$$

$$\theta_{m-1} + \theta_m(-2 - H^2 k^2) + \theta_{m+1} = 0$$

$$\theta_{m-1} + \theta_m(-3) + \theta_{m+1} = 0$$

$$[1, -3, 1] \quad ; \quad m \in 1, 2, 3$$

$$\cancel{\begin{bmatrix} -3 & 1 & 0 & \cancel{0} \\ \cancel{1} & \cancel{-3} & \cancel{1} & \\ 1 & -3 & 1 & \\ 0 & \cancel{13} & -3 & \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} \cancel{0}-1 \\ 0 \\ 0 \end{bmatrix}}$$

$$\cancel{\frac{\theta_{m+1} - \theta_{m-1}}{2k} = \left.\frac{d\theta}{d\xi}\right|_{x = x_m}}$$

$$\cancel{m \in 1, \ldots, 3}$$

$$\cancel{\frac{\theta_4 - \theta_3}{0.5} =}$$

$$\begin{bmatrix} -3 & 1 & 0 \\ 1 & -3 & 1 \\ 0 & 1 & -3 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ -\theta_4 \end{bmatrix}$$

$-3\theta_1 + \theta_2 = -1$ $\quad$ | $\frac{\theta_5 - \theta_3}{0.5} = 0$ --- (1)

$\theta_1 - 3\theta_2 + \theta_3 = 0$ $\quad$ |

[Ghost-point method] $\theta_2 - 3\theta_3 = -\theta_4$ $\quad$ | $\theta_5 = \theta_3$

for $m = 4 \Rightarrow \theta_3 - 3\theta_4 + \theta_5 = 0$

$\xi_5 \rightarrow$ fictitious node [Note: BD not used bcoz it is 1st order accurate]

$-3\theta_1 + \theta_2 \cancel{+0\theta_3 + 0\theta} = -1$

$\theta_1 - 3\theta_2 + \theta_3 = 0$

$\theta_2 - 3\theta_3 + \theta_4 = 0 \longrightarrow -1 + 3\theta_1 - 3\theta_3 + \frac{2\theta_3}{3} = 0$

$2\theta_3 - 3\theta_4 = 0$

$\theta_2 = -1 + 3\theta_1$

$\theta_1 - 3(-1 + 3\theta_1) + \theta_3 = 0$

$\theta_1 + 3 - 9\theta_1 + \theta_3 = 0$

$-8\theta_1 + \theta_3 = -3$

$3\theta_1 - \frac{7\theta_3}{3} = 1$

$\theta_1 = 0.3829787$

$\theta_3 = 0.06382979$

$\theta_2 = -1 + 3\theta_1$
$= 0.1489361$

$\theta_4 = \frac{2\theta_3}{3}$

$\theta_4 = 0.04255319$

$\theta_1 = 0.3830$

$\theta_2 = 0.1489$

$\theta_3 = 0.0638$

$\theta_4 = 0.0426$

Analytical sol^n

$$\frac{d^2\theta}{d\varepsilon^2} = H^2\theta.$$

$D^2 - H^2\theta = 0.$

$\theta = A\sinh 4\varepsilon + B\cos 4\varepsilon$

$\boxed{1 = B}$

$\frac{d\theta}{d\varepsilon} = 4A\cos 4\varepsilon - B \times 4 \times \sin 4\varepsilon$

$0 = 4A \times \cos 4 - 4\sin 4.$

$\cancel{4}\sin 4 = \cancel{4}A\cos 4$

$\boxed{A = 1.1578213}$

$\theta = 1.1578213\sin(4\varepsilon) + \cos(4\varepsilon).$

$$\frac{d^2\theta}{d\varepsilon^2} = H^2\theta = 16\theta$$

$$\theta = Ae^{4\varepsilon} + Be^{-4\varepsilon}$$

$$1 = Ae^{0} + Be^{0} \quad \text{--- (1)} \qquad A+B=1$$

$$\frac{d\theta}{d\varepsilon} = 4Ae^{4\varepsilon} - 4Be^{-4\varepsilon}$$

$$0 = 4Ae^{4} - 4Be^{-4}$$

$$0 = Ae^{4} - Be^{-4} \quad \text{--- (2)} \qquad Ae^{4} - Be^{-4} = 0$$

$$A = 0.0003354$$
$$B = 0.9996646$$

$$\therefore \boxed{\theta = 0.0003354\, e^{4\varepsilon} + 0.9996646\, e^{-4\varepsilon}}$$

ε	θ_N	θ_A
0	1	1
0.25	0.3829	0.3686678
0.5	0.1489	0.1377682
0.75	0.0638	0.0565071
1.00	0.0426	0.0366217

→ Remarks:
1. Ghost point method. @ ficticious node
2. CD(system) + BD(BC) but there is inconsistency in accuracy
3. to avoid concern in 1 & 2 we use 3 point FDM
4. Mesh refinement. ($k\downarrow$)

→ Mesh refinement:

old grid: $\xi = 0$ … $\xi = 1$; points 0, 0.25, 0.5, 0.75, 1 — 5 grid points, $M = 4$

new grid: 0 … 1 — 9 grid points, $M = 8$

new grid pts = 2 × (old grid points) − 1

$m=1 \quad -2.25\theta_1 + \theta_2 = -1$

$m=2 \quad \theta_1 - 2.25\theta_2 + \theta_3 = 0$

$m=3 \quad \theta_2 - 2.25\theta_3 + \theta_4 = 0$

$m=4 \quad \theta_3 - 2.25\theta_4 + \theta_5 = 0$

$m=5 \quad \theta_4 - 2.25\theta_5 + \theta_6 = 0$

$m=6 \quad \theta_5 - 2.25\theta_6 + \theta_7 = 0$

$m=7 \quad \theta_6 - 2.25\theta_7 + \theta_8 = 0$

$m=8 \quad \theta_7 - 2.25\theta_8 + \theta_9 = 0$

$$\frac{\theta_9 - \theta_7}{2(1/8)} = 0$$

$\theta_9 = \theta_7$

$\theta_7 = 0.0429$

$\theta_9 = 0.0429$

$\theta_8 = 0.0381$

$\theta_6 = -\theta_8 + 2.25\times\theta_7$

$\theta_6 = 0.0584$

$\theta_6 = 0.0885$

~~$\theta_4 =$~~

$\theta_2 = -1 + 2.25\theta_1$

$\theta_1 + 22.5 - 5.0625\theta_1 + \theta_3 = 0$

$-4.0625\theta_1 + \theta_3 = 2.25$

$-1 + 2.25\theta_1 - 2.25\theta_3 + \left(\frac{\theta_3+\theta_5}{2.25}\right) = 0$

$2.25\theta_1 - 1.80536\theta_3 = 0.9607$

	ξ	θ_A	$\theta_N (M=4)$	$\theta_N (M=8)$
θ_0	0	1	1	1
θ_1	0.125	0.6069		0.61
θ_2	0.25	0.3687	0.3829	0.3725
θ_3	0.375	0.2246		0.2281
θ_4	0.5	0.1378	0.1489	0.1407
θ_5	0.625	0.0861		0.0885
θ_6	0.75	0.0565	0.0638	0.0584
θ_7	0.825	0.0460		0.0429
θ_8	1	0.0366	0.0426	0.0381

→ 3 point FDM

$y(x_m+k) = y_{m+1} = y_m + k\frac{dy}{dx}\Big|_{x=x_m} + \frac{k^2}{2!}\frac{d^2y}{dx^2}\Big|_{x=x_m} + O(k^3)$

$y(x_m+2k)\ y_{m+2} = y_m + 2k\frac{dy}{dx}\Big|_{x=x_m} + \frac{(2k)^2}{2!}\, d^2y/dx^2\Big|_{x=x_m} + O(k^3)$

$\boxed{y_{m+2} - 4y_{m+1}}$

$= (y_m - 4y_m) + \frac{dy}{dx}\Big|_{x=x_m}(2k - 4k) + \frac{d^2y}{dx^2}(2k^2 - 2k^2) + O(k^3)$

$y_{m+2} - 4y_{m+1} = -3y_m - 2k\frac{dy}{dx}\Big|_{x=x_m} + O(k^3)$

$\frac{4y_{m+1} - y_{m+2} - 3y_m}{2k} + O(k^2) = \frac{dy}{dx}\Big|_{x=x_m}$

$\frac{dy}{dx}\Big|_{x=x_m} = \frac{-3y_m + 4y_{m+1} - y_{m+2}}{2k} + O(k^2)$

--- 2nd order accurate.

--- 3 point f.d.

$\boxed{y_{m-2} - 4y_{m-1}} = ?$

$y_{m-1} = y(x_m - k) = y_m - k\frac{dy}{dx}\Big|_{x=x_m} + \frac{k^2}{2!} y''_m + O(k^3)$

$y_{m-2} = y(x_m - 2k) = y_m - 2k y'_m + 2k^2 y''_m + O(k^3)$

$y_{m-2} - 4y_{m-1}$
$= (y_m - 4y_m) + y'_m(-2k + 4k) + 0 + O(k^3)$

$\frac{y_{m-2} - 4y_{m-1} - y_m + 4y_m}{2k} + O(k^2) = y'_m$

$y'_m = \frac{y_{m-2} - 4y_{m-1} + 3y_m}{2k} + O(k^2)$

--- 3 point BD

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θ(prev)	θ_N
θ_0	1
θ_1	0.3824
θ_2	0.1471
θ_3	0.0588
θ_4	0.0294

with 3point

$$-3\theta_1+\theta_2=-1 \rightarrow \theta_1=\frac{+1}{3}+\frac{\theta_2}{3}$$

$$\theta_1-3\theta_2+\theta_3=0 \rightarrow \frac{1}{3}+\frac{\theta_2}{3}-3\theta_2+\theta_3=0$$

$$\theta_2-3\theta_3+\theta_4=0$$

$$0=\frac{\theta_2-4\theta_3+3\theta_4}{2\times 1/4} \qquad -\frac{8}{3}\frac{\theta_2}{\cancel{3}}+\theta_3=-1/3$$

$$\theta_2-4\theta_3+3\theta_4=0$$

$$\theta_2-3\theta_3+\theta_4=0$$

$$-\frac{8}{3}\theta_2+\theta_3+0\theta_4=-1/3$$

$$\therefore \boxed{\begin{array}{l}\theta_2=0.1471 \quad \theta_1=0.3824\\ \theta_3=0.0588\\ \theta_4=0.0294\end{array}}$$

→ BVP with Robin BC

$$p(x)\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x) \text{ --- system}$$

$$x \in [a, b]$$

$a_0 y(a) + b_0 y'(a) = C_0$ 3 pt FD

$a_1 y(b) + b_1 y'(b) = C_1$ 3 pt BD

S1: $k = \frac{b-a}{M}$

S2: $p(x) \times [$ discretize ODE

$$[2P_m - q_m k] y_{m-1} + [-4P_m] y_m + [2P_m + q_m k] y_{m+1} = r_m \times 2k^2 \text{ --- (1)}$$

$m \in 1, 2, 3, \ldots, M-1$

$$y'_m = \frac{-3y_m + 4y_{m+1} - y_{m+2}}{2k}$$

$$y'(a) = \frac{-3y(a) + 4y_1 - y_2}{2k} \text{ --- 3Pt FD}$$

$$2ka_0 y_0 - 3b_0 y_0 + 4b_0 y_1 - b_0 y_2 = 2kC_0$$

$$y_0(2ka_0 - 3b_0) + 4b_0 y_1 - b_0 y_2 = 2kC_0 \text{ --- (2)}$$

$$y'_m = \frac{y_{m-2} - 4y_{m-1} + 3y_m}{2k}$$

$$y'(b) = y'_M = \frac{y_{M-2} - 4y_{M-1} + 3y_M}{2k}$$

$$2ka_1 y_M + b_1 y_{M-2} - b_1 4 y_{M-1} + 3b_1 y_M = C_1 2k$$

$$b_1 y_{M-2} - 4b_1 y_{M-1} + y_M(3b_1 + 2ka_1) = 2kC_1 \text{ --- (3)}$$

$$\begin{bmatrix} (2ka_0 - 3b_0) & b_0' & -b_0 & 0 & \cdots & 0 \\ -4P_m & 2P_m + q_m k & 0 & 0 & \cdots & 0 \\ & & & & & \\ & & & & & \end{bmatrix}_{M+1 \times M+1} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{M-1} \\ y_M \end{bmatrix}_{M+1 \times 1} = \begin{bmatrix} 2kC_0 \\ r_m \times 2k^2 - \cancel{\ } \\ \\ \\ \\ \\ \end{bmatrix}_{M+1 \times 1}$$

$$\begin{array}{c|c} m= & \\ 0 & \\ 1 & \\ 2 & \\ \vdots & \\ M & \end{array} \begin{bmatrix} (2ka_0 - 3b_0) & 4b_0 & -b_0 & 0 & 0 & \cdots & 0 \\ 2P_m - q_m k & -4P_m & 2P_m + q_m k & 0 & 0 & \cdots & 0 \\ 0 & 2P_2 - q_2 k & -4P_2 & 2P_m + q_m k & 0 & \cdots & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \cdots & 0\ \ b_1 & -4b_1 & 3b_1 + 2ka_1 \end{bmatrix}_{M+1 \times M+1} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_M \end{bmatrix}_{M+1 \times 1} = \begin{bmatrix} 2kC_0 \\ 2k^2 r_1 \\ 2k^2 r_2 \\ \\ \\ 2kC_1 \end{bmatrix}_{M+1 \times 1}$$

$\rightarrow$ Shooting method: $\boxed{BVP}$

$$\left\{ \begin{array}{l} \text{ODE (2nd or higher order)} \Rightarrow \text{Convert to a set of first order ODE} \ \ (\text{IVP}) \\ \text{BCs} \end{array} \right.$$

Pb - $\dfrac{d^2y}{dx^2} = f(x, y, dy/dx)$ --- ODE

$$\left. \begin{array}{l} y(x=0) = \alpha \\ y(x=a) = \beta \end{array} \right\} BC$$

IVP
$$\left| \begin{array}{l} y = y_1 \\ \dfrac{dy_1}{dx} = y_2 \\ \dfrac{dy_2}{dx} = f(x, y_1, y_2) \\ y_1(x=0) = \alpha \\ y_2(x=0) = r \text{ (assumed)} \end{array} \right.$$

$\cancel{dy/dx = \theta_1}$

$\cancel{\dfrac{d\theta_1}{dx} = f(x, y, \theta_1)}$

$\cancel{\dfrac{d\theta_1}{dx} = \theta_2}$

$\cancel{\theta_2 = f(x, y, \theta_1)}$

Step-2:

$y_1(x=h)$, $y_1(x=2h)$, $y_1(3h)$ --- $y_1(x=a)$

$y_2(x=h)$, $y_2(2h)$, $y_2(3h)$ --- $y_2(x=a)$

Step-3:

$$|y_1(a)-\beta| \le tol$$

reassume $y_2(x=0)$??

Remarks: ① linear interpolation to assume $y_2(0)$

② It is analogus to a procedure of firing object at stationary target.

example: $\frac{d^2y}{dx^2} = 5y + 10x(1-x)$

$y = y_1$

$\frac{dy_1}{dx} = y_2$ --- ①

$\frac{dy_2}{dx} = 5y_1 + 10x(1-x)$ --- ②

$y(0)=0$

$y(9)=0$

$M=3$

$tol = 10^{-6}$

~~y_2~~ Explicit Euler,

$k = \frac{9-0}{3}$

$y_2^{(k+1)} = y_2^k + h(5y_1^k + 10x^k(1-x^k))$

$k = h = 3$

$y_2(3) = y_2(0) + 3\times(5\times0 + 10\times0)$

$y_2(3) = 4$

$x_0 = 0$

$x_1 = 3$

$x_2 = 6$

$x_3 = 9$

$y_1^{k+1} = y_1^k + h y_2^k$

$y_1(3) = 0 + 3\times(4)$

$y_2^0(\text{assumed}) = 4$

$y_1(3) = 12$

$y_2^{(6)} = y_2(3) + 3\times(5y_1(3) + 10\times 3\times -2)$

$y_2^{(6)} = 4 + 3\times(5\times 12 - 60)$

$y_2^{(6)} = 4.$

$y_1^{(6)} = y_1(3) + h\,y_2(3)$

$= 12 + 3\times 4$

$y_1^{(6)} = 24.$

$y_2^{(9)} = (5y_1(6) + 10\times 6\times -5)\times 3 + y_2(6).$

$= 4 + 3\times(5\times 24 - 300)$

$y_2^{(9)} = -536.$

$y_1^{(9)} = y_1(6) + 3\,y_2(6)$

$= 24 + 3\times 4$

$y_1^{(9)} = 24+12 = 36.$

$\therefore$ ~~tot~~ $|36-0|$ is not less than tolerance.

$y_2(0) = -2$ (new assumed.)

$y_1^{(k+1)} = y_1^{(k)} + h y_2^{(k)}$

$y_2^{(k+1)} = y_2^{(k)} + h(5y_1^{(k)} + 10x^k(1-x^k))$

~~$y_2^{(k+1)}$~~

$y_{11} = y_{10} + 3\times y_{20}$

$= 0 + 3\times -2$

$y_{10} = 0 \qquad \boxed{y_{11} = -6}$

$y_{21} = y_{20} + 3(5y_{10} + 10\times 0)$

$y_{21} = -2 + 15\times 0 = -2$

$y_{21} = -2.$

$y_{12} = y_{11} + 3\times y_{21} = -6 + 3\times -2$

$y_{12} = -12$

$y_{22} = -2 + 3\times(5\times -6 + 3 + 10\times 3\times -2)$

$y_{22} = -272.$

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$y_{13} = y_{12} + 3 \times y_{22}$

$y_{13} = -12 + 3 \times -272$

$= \cancel{-12 - 6} \quad -828$

$\cancel{= -18}$

$|y_{13} - 0| \nleq tol$.

Interpolating

$4 \longrightarrow 36$

$q \quad 0$

$-2 \quad -828$

$$\frac{-828 - 36}{-2 - 4} = \frac{0 - 36}{q - 4}$$

$q = 3.75$.

$y_2(0) = 3.75$.

$y_{11} = y_{10} + h y_{20}$

$= 0 + 3 \times 3.75$

$\boxed{y_{11} = 11.25}$

$y_{21} = y_{20} + h(5y_{10} + 10x_0(1 - x_0))$

$= 3.75$.

$y_{12} = y_{11} + 3 \times y_{21}$

$= 22.5$.

$y_{22} = y_{21} + h(5y_{12} + 10x_1(1 - x_1))$

$y_{22} = 161.25$.

$y_{13} = y_{12} + 3 \times y_{22}$

$|y_{13} - 0| = 0 \leq tol$

Non-linear BVP.

$$\frac{d^2y}{dx^2} + y\frac{2dy}{dx} = 0 \qquad y(0)=1 \quad y(4)=0.2 \qquad x \in [0,4]$$

$n = 4$

$k = 1$

$x_0 = 0, \ x_1 = 1, \ x_2 = 2, \ x_3 = 3, \ x_4 = 4.$

$$\frac{y_{m+1} + y_{m-1} - 2y_m}{k^2} + \cancel{2} \times \left(y_m \frac{y_{m+1} - y_{m-1}}{\cancel{2}k}\right) = 0$$

$y_{m+1} + y_{m-1} - 2y_m + y_m k y_{m+1} - y_m k y_{m-1} = 0$

$\cancel{\boxed{y_{m-1}(1-k) - 2y_m + y\,y_{m+1}(k+1) = 0}}$

$\cancel{-2y_m + 2y_{m+1} = 0}$

$\cancel{y_m + y_{m+1} = 0}$

$\cancel{m \in 1, 2, 3}$

$$\cancel{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \ \end{bmatrix}}$$

$y_{m+1} + y_{m-1} - 2y_m + k y_m y_{m+1} - k y_m y_{m-1} = 0$

$y_{m-1}(1 - k y_m) - 2y_m + y_{m+1}(1 + k y_m) = 0$

$m \in 1, 2, 3.$ $\qquad y_0 = 1$

$\qquad y_4 = 0.2$

$y_0(1 - y_1) - 2y_1 + y_2(1 + y_1) = 0$

$1 - y_1 - 2y_1 + y_2 + y_2 y_1 = 0$

$1 - 3y_1 + y_2 + y_1 y_2 = 0 \ ---- (1).$

$y_1 \times (1 - y_2) - 2y_2 + y_3(1 + y_2) = 0$

$y_1 - y_1 y_2 - 2y_2 + y_3 + y_2 y_3 = 0 \ --- (2)$

$m = 3$

$0.2(1+y_3) - 2y_3 + y_2(1-y_3) = 0$

<u>NR:</u>

$$Y^{k+1} = Y^k - J_H^{-1} \times G^k$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}^{k+1} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}^{k} - J_H^{-1} \times \begin{bmatrix} g_1 \\ g_2 \\ g_3 \end{bmatrix}^{k}$$

$$J_H = \begin{bmatrix} \frac{\partial g_1}{\partial y_1} & \frac{\partial g_1}{\partial y_2} & \frac{\partial g_1}{\partial y_3} \\ \frac{\partial g_2}{\partial y_1} & \frac{\partial g_2}{\partial y_2} & \frac{\partial g_2}{\partial y_3} \\ \frac{\partial g_3}{\partial y_1} & \frac{\partial g_3}{\partial y_2} & \frac{\partial g_3}{\partial y_3} \end{bmatrix}$$

$$\boxed{Y^{k+1} = Y^k - J_k^{-1} F_k}$$

$$J_k^{-1} = \begin{bmatrix} -3 + y_2^k & 1 + y_1^k & 0 \\ 1 - y_2^k & -2 + y_3^k - y_1^k & 1 + y_2^k \\ 0 & 1 - y_3^k & -1.8 - y_2^k \end{bmatrix}^{-1}$$

$$F_k = \begin{bmatrix} 1 - 3y_1 + y_2 + y_1 y_2 \\ y_1 - 2y_2 + y_3 + y_2 y_3 - y_2 y_1 \\ 0.2 + y_2 - 1.8 y_3 - y_3 y_2 \end{bmatrix}^k$$

$$Y^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad Y^2 = \begin{bmatrix} 0.466667 \\ 0.4 \\ 0.333331 \end{bmatrix}$$

$$Y^3 = \begin{bmatrix} 0.49982 \\ 0.330612 \\ 0.251701 \end{bmatrix}$$

$$Y^4 = \begin{bmatrix} 0.500001 \\ 0.333336 \\ 0.249999 \end{bmatrix}$$

$$Y^5 = \begin{bmatrix} 0.5 \\ 0.333333 \\ 0.25 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.333333 \\ 0.25 \end{bmatrix}$$

→ ~~Par~~

11/10/23

→ Partial Differential equation

its an eqⁿ which consists of 1 ~~or~~ more dependent variable wrt more than 1 independent variable.

$$\cancel{A\frac{\partial^2 y}{\partial x^2} + B\frac{\partial^2 y}{\partial x \partial y} + C\frac{\partial^2 y}{\partial y^2} + E\frac{\partial y}{\partial t} + Fy = G}$$

Reference eqⁿ

$$\boxed{A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + FU = G}$$

$A, B, C, D, E, F, G \Rightarrow$ coefficients

$$AU_{xx} + BU_{xy} + CU_{yy} + DU_x + EU_y + FU = G$$

ODE	PDE
1. Independent variable	1. >1 independent variable
2. IVP: IC BVP: BC	2. Boundary conditions or IC + BC [Initial Boundary Value Problem]
3.	3. Calculate at different nodes
4. Solution plot looks like a curve	4. Solution plot looks like a surface.

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

IC at $t=0$

BC at $x=a$

$x=b$

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$x_{n+1} = x_n - \frac{f_n}{f_n'}$

$x_1^{n+1} = x' - J_n^{-1}$

Numerical methods:

1. FDM
2. FEM
3. FVM (Finite volume method)

- FDM:
  - → Leap-frog
  - → Method of lines
  - → Lax-friedrichs
  - → Dufort-Frankel
  - → Crank-Nicholson

CD

$$\left(\frac{\partial u}{\partial x}\right)_m = \frac{U_{m+1} - U_{m-1}}{2k} + O(k^2)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_m = \frac{U_{m-1} - 2U_m + U_{m+1}}{k^2} + O(k^2)$$

FD

$$\left.\frac{\partial u}{\partial x}\right|_m = \frac{U_{m+1} - U_m}{k} + O(k), \quad \left(\frac{\partial^2 u}{\partial x^2}\right)_m = \frac{U_{m+2} - 2U_{m+1} + U_m}{k^2} + O(k)$$

BD

$$\left(\frac{\partial u}{\partial x}\right)_m = \frac{U_m - U_{m-1}}{k} + O(k) \qquad \left(\frac{\partial^2 u}{\partial x^2}\right)_m = \frac{U_m - 2U_{m-1} + U_{m-2}}{k^2} + O(k)$$

Algorithm:

S1: Discretise surface regime into grid of nodes.

S2: Use FDM to discretise PDE.

S3: BC's and IC's to get sol^n.

ex – one-way wave eq^n:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad a>0 \quad a=\text{const}$$

$t \in (0,\infty)$

$x \in (0,1)$

$$t_n = t_0 + nh$$

$h = \Delta t$

$n \in 0,1,2,\dots N$

$$x_m = x_0 + mk$$

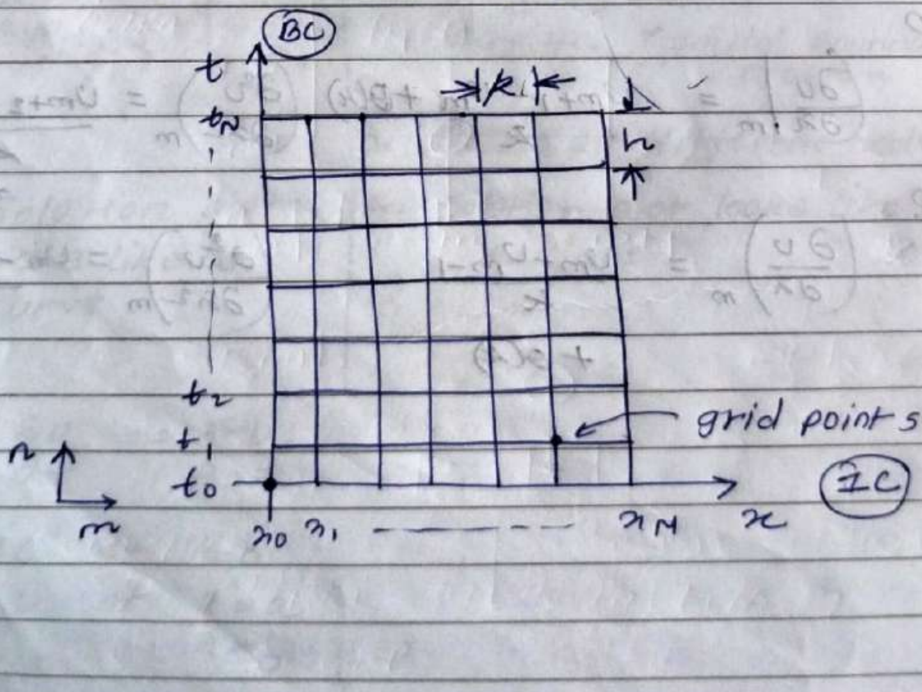
$k = x_M - x_0 / M$

$m \in 0,1,2,\dots M$

follow: $U(\text{space}, \text{time})$

IC $U(x,0)$ $\cancel{= U(0,0)}$ $x \in [0,1]$

BC $U(0,t)$ $\cancel{= g(t)}$ $t \in [0,\infty)$



→ Forward in time and forward in space (FTFS)

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$$\frac{\partial u}{\partial t} = U_t(x_m, t_n) = \frac{U_{m,n+1} - U_{m,n}}{h} + O(h)$$

---- Forward difference

$$\frac{\partial u}{\partial x} = U_x(x_m, t_n) = \frac{U_{m+1,n} - U_{m,n}}{k} + O(k)$$

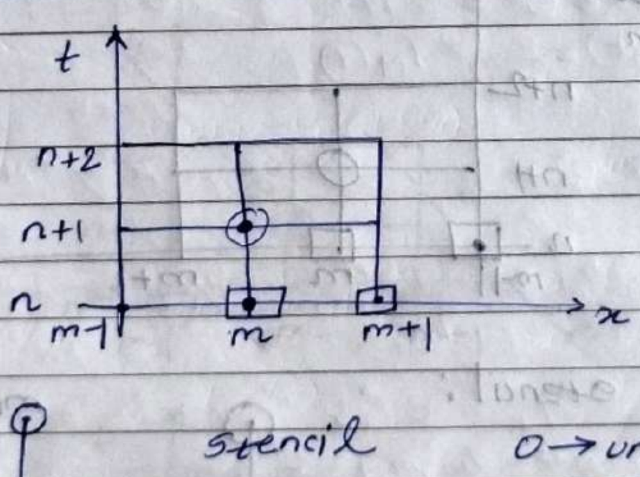
---- Forward difference

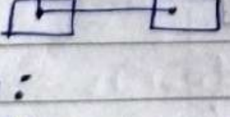
$$\frac{U_{m,n+1} - U_{m,n}}{h} + \frac{a}{k}\left(\frac{U_{m+1,n} - U_{m,n}}{1}\right) = 0$$

$$+ O(k, h)$$

$$U_{m,n+1} = -\frac{ah}{k}(U_{m+1,n} - U_{m,n}) + U_{m,n} + \cancel{O(k, h^2)}$$

$$\boxed{U_{m,n+1} = -\frac{ah}{k} U_{m+1,n} + U_{m,n}\left(1 + \frac{ah}{k}\right)}$$ --- FTFS





stencil

O → unknown

□ → known

Remarks:

1. 1st order accurate in both space and time.
2. One-step

- Forward in time and backward in space [FTBS]

$$\frac{\partial u}{\partial t} = u_t(x_m, t_n) = \frac{U_{m,n+1} - U_{m,n}}{h} + O(h)$$

$$\frac{\partial u}{\partial x} = u_x(x_m, t_n) = \frac{U_{m,n} - U_{m-1,n}}{k} + O(k)$$

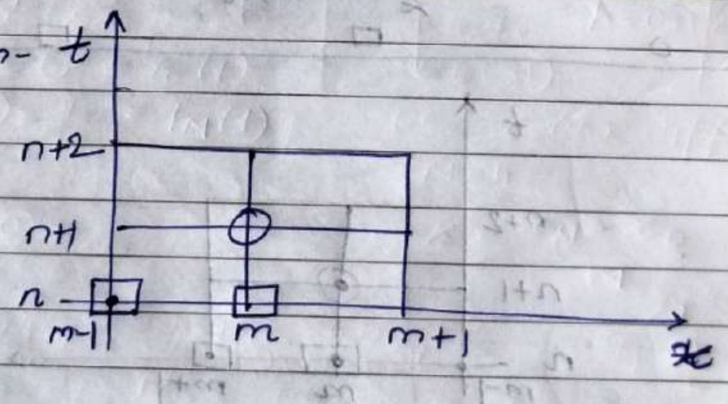
$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$$\frac{U_{m,n+1} - U_{m,n}}{h} + a\left[\frac{U_{m,n} - U_{m-1,n}}{k}\right] + O(h,k) = 0.$$

$$U_{m,n+1} = +\frac{ah}{k} U_{m-1,n} + U_{m,n}\left[\frac{-ah}{k} + 1\right].$$

$$\boxed{U_{m,n+1} = U_{m,n}\left(1 - \frac{ah}{k}\right) + \frac{ah}{k} U_{m-1,n} + O(h,k)}$$

graphical represen-tation



stencil:

$m = 1, 2, \ldots M-1$

Remarks:

1. 1st order accurate in both space and time
2. One-step.

- central in time and central in space : [Leap frog Method]

$$\frac{\partial u}{\partial t} = u_t(x_m, t_n) = \frac{U_{m,n+1} - U_{m,n-1}}{2h} + O(h^2)$$

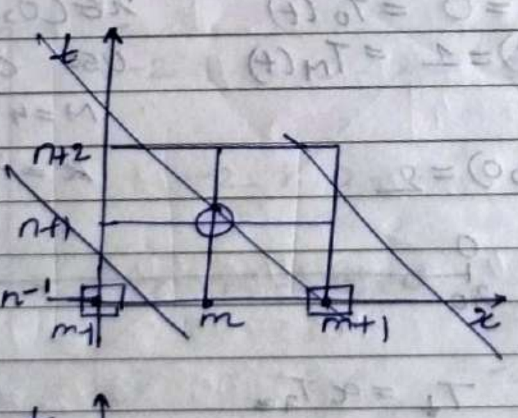
$$\frac{\partial u}{\partial x} = u_x(x_m, t_n) = \frac{U_{m+1,n} - U_{m-1,n}}{2k} + O(k^2)$$

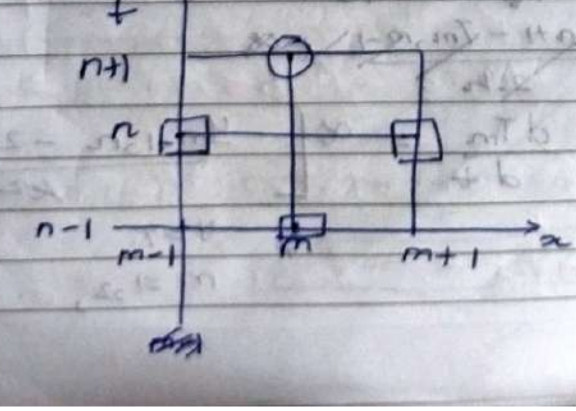
$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$$\frac{U_{m,n+1} - U_{m,n-1}}{2h} + \frac{a}{2k}\left[U_{m+1,n} - U_{m-1,n}\right] + O(k^2, h^2) = 0$$

$$U_{m,n+1} = \frac{-a}{2k} \times 2h\left[U_{m+1,n} - U_{m-1,n}\right] + U_{m,n-1} + O(k^2, h^2)$$

$$U_{m,n+1} = -\frac{ah}{k}U_{m+1,n} + \frac{ah}{k}U_{m-1,n} + U_{m,n-1} + O(k^2, h^2)$$





stencil :

Remarks:

1. Second order accurate in ~~time~~ space & time.
2. ~~one~~ step (information required in n & $n-1$)

→ Method of lines:

PDE → (ODE) (IVP)

Algorithm:

S-1: Discretise spatial domain $x_0, x_1, \ldots, x_M$

S-~~2~~: $M+1 \Rightarrow$ nodes

S-2: PDE → ODE @ spatial

S-3: Solve the set of ODE's

$\boxed{h = \frac{x_M - x_0}{M}}$

→ Ex

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

[1-Dimensional heat conduction]

$h = 0.025$.

Dirichlet BC's.

$T(0,t) = 0 = T_0(t)$

$T(1,t) = 1 = T_M(t)$

$x \in (0,1)$

Use center difference

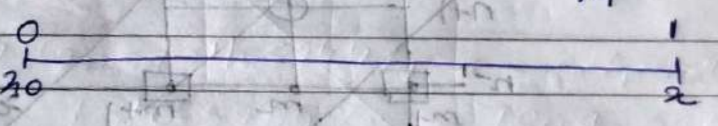
IC;

$M = 4$

$T(x,0) = 2$

$$h = \frac{x_M - x_0}{M}$$

S1 :



S-2 :

$$T_t = \alpha T_{xx}$$

$$\cancel{\frac{T_{m,n+1} - T_{m,n-1}}{2h} = \alpha}$$

$$\frac{dT_m}{dt} = \alpha \left[\frac{y_{m-1,n} - 2y_{m,n} + y_{m+1,n}}{h^2} \right]$$

$y = T$.

$m = 1, 2, \ldots M-1$

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$$\frac{dT_m}{dt} = \alpha\left[\frac{T_{m-1}^{(t)} - 2T_m^{(t)} + T_{m+1}(t)}{k^2}\right]$$

s-s.

$m=1 \quad \frac{dT_1}{dt} = \frac{\alpha}{k^2}\left[T_0 - 2T_1 + T_2\right]$

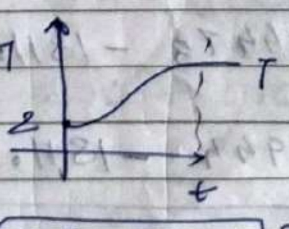
$m=2 \quad \frac{dT_2}{dt} = \frac{\alpha}{k^2}\left[T_1 - 2T_2 + T_3\right]$

$\vdots$

$m=M-1 \quad \frac{dT_{M-1}}{dt} = \frac{\alpha}{k^2}\left[T_{M-2} - 2T_{M-1} + T_M\right]$

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \\ 0 & 0 & 0 & 0 & 0 \cdots & -2 & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ \vdots \\ \vdots \\ \vdots \\ T_{M-1} \end{bmatrix} = \begin{bmatrix} \frac{k^2}{\alpha}\frac{dT_1}{dt} - T_0 \\ \\ \vdots \\ \\ \frac{k^2}{\alpha}\frac{dT_{M-1}}{dt} - T_M \end{bmatrix}$$

$$\underset{M-1\times 1}{\begin{bmatrix} \frac{k^2}{\alpha}\frac{dT_1}{dt} - 0 \\ \frac{k^2}{\alpha}\frac{dT_2}{dt} \\ \vdots \\ \frac{k^2}{\alpha}\frac{dT_{M-1}}{dt} - 1 \end{bmatrix}} = \underset{M-1\times M-1}{\begin{bmatrix} -2 & 1 & 0 & 0 & - & - & 0 \\ 1 & -2 & 1 & 0 & - & - & 0 \\ 0 & 1 & -2 & 1 & 0 & - & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & -2 \quad 1 \end{bmatrix}} \times \underset{M-1\times 1}{\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_{M-1} \end{bmatrix}}$$



$\boxed{M=4}$

$\alpha = 0.00138$

$k = 0.25$

$\frac{k^2}{\alpha} = 45.28986$

$\boxed{\text{soln at s.s.}}$??

$$T_1 = T_0 + h\left(\frac{dT_0}{dt}\right)_{t=t_0}$$

Using Euler:

$$T_1 = T_1 + h\frac{dT_1}{dt} \Rightarrow 40T_2 - 40T_1$$

$$T_2 = T_2 + h\frac{dT_2}{dt} \Rightarrow 40T_3 - 40T_2$$

$$T_3 = T_3 + h\frac{dT_3}{dt} \Rightarrow 40 - 40T_3$$

$$\frac{x^2}{\alpha} = 45.28986$$

$M = 4$

$$\begin{bmatrix} 45.28986 \times [40T_2 - 40T_1] \\ 45.28986 \times [40T_3 - 40T_2] \\ 45.28986\,[40 - 40T_3] - 1 \end{bmatrix} = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}$$

$45.28986 \times 40 = \boxed{1811.5944}$

$$1811.5944\,T_2 - 1811.5944\,T_1 = -2T_1 + T_2$$

$$1810.5944\,T_2 = 1809.5944\,T_1$$

$$\boxed{1.000553\,T_2 = T_1}$$

$$1811.5944\,T_3 - 1811.5944\,T_2 = T_1 - 2T_2 + T_3$$

$$1811.5944 - 1811.5944\,T_3 - 1 = T_2 - 2T_3$$

$$\boxed{1810.5944 = T_2 + 1809.5944\,T_3}$$

$0 = T_1 + 1809.5944 T_2 - 1810.5944 T_3$

$T_1 - 1.000553 T_2 + 0 T_3 = 0$

$0 \cdot T_1 + 1809.5944 T_2 - 1810.5944 T_3 = 0$

$0 \times T_1 + T_2 + 1809.5944 T_3 = 1810.5944$

$T_1 = 1.00055$
$T_2 = 0.99999$
$T_3 = 1$

$T_{10}, T_{20}, T_{30} = 2$

Using Backward difference method,

$$T_{mn} = T_{mn-1} + h \frac{dT_{mn}}{dt}$$

$$\frac{T_{mn} - T_{m(n-1)}}{h} = \frac{dT_{mn}}{dt}$$

$$-T_{1n-1} = 0.000552(\overset{0}{\cancel{T_{0n}}} - 2T_{1n} + T_{2n}) + T_{1n}$$

$$-T_{1n-1} = -1.001104 T_{1n} + 0.000552 T_{2n}$$

Similarly

$$-T_{2n-1} = 0.000552 T_{1n} - 1.001104 T_{2n} + 0.000552 T_{3n}$$

$$T_{3n} - T_{3n-1} = 0.000552(T_{2n} - 2T_{3n} + T_{4n})$$

$$-T_{3n-1} - 0.000552 = -2.000552 = 0 + 0.000552 T_{2n} - 1.001104 T_{3n}$$

$$\begin{bmatrix} -T_{1\,n-1} \\ -T_{2\,n-1} \\ \left(\begin{matrix}-T_{3\,n-1} \\ -0.00052\end{matrix}\right) \end{bmatrix} = \begin{bmatrix} -1.001104 & 0.000552 & 0.000000 \\ 0.000552 & -1.001104 & 0.000552 \\ 0 & 0.000552 & -1.001104 \end{bmatrix} \begin{bmatrix} T_{1n} \\ T_{2n} \\ T_{3n} \end{bmatrix}$$

$$\downarrow P_{n-1} \qquad \downarrow A \qquad 3\times3 \qquad \downarrow P_n$$

$$A\, P_n = P_{n-1}$$
$$P_n = A^{-1} P_{n-1}$$

iterating we get, $\qquad$ tolerance $=10^{-6}$

at steady state

$T(0) = 0$

$T(0.25) = 0.2531$

$T(0.5) = 0.5044$

$T(0.75) = 0.7531$

$T(1) = 1$

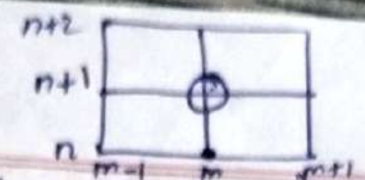
→ Lax-friedrichs method:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

FTCS

$$\frac{U_{m,n+1} - U_{m,n}}{h} + a\left[\frac{U_{m+1,n} - U_{m-1,n}}{2k}\right] = 0$$

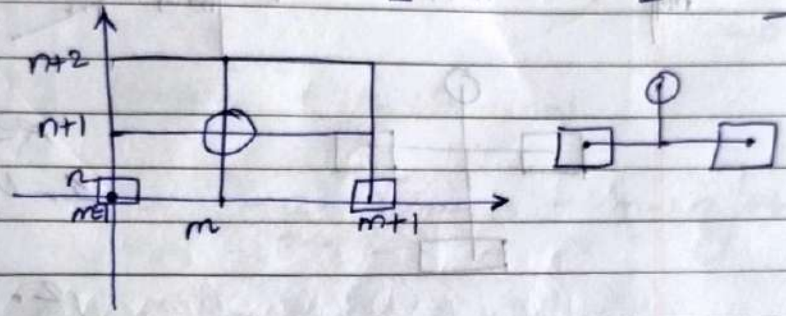
$$\frac{U_{m,n+1} - U_{m,n}}{h} = -a\left[\frac{U_{m+1,n} - U_{m-1,n}}{2k}\right] + O(k^2, h)$$



$$U_{m,n} = \frac{1}{2}\left(U_{m+1,n} + U_{m-1,n}\right)$$

$$U_{m,n+1} = -\frac{ha}{2k}\left[U_{m+1,n} - U_{m-1,n}\right] + \frac{1}{2}\left(U_{m+1,n} + U_{m-1,n} + O(h,k^2)\right)$$

$$U_{m,n+1} = U_{m+1,n}\left[\frac{1}{2} - \frac{ha}{2k}\right] + U_{m-1,n}\left[\frac{1}{2} + \frac{ha}{2k}\right]$$



Remarks:

→ Unconditionally unstable

→ one step.

→ Bounded $sol^n \equiv \left|\frac{ah}{k}\right| \leq 1$

- Dufort-frankel

$$\frac{\partial U}{\partial t} = \alpha \frac{\partial^2 U}{\partial x^2}$$

CTCS,

$$\frac{U_{m,n+1} - U_{m,n-1}}{2h} = \alpha\left[\frac{U_{m-1,n} - 2U_{m,n} + U_{m+1,n}}{k^2}\right] + O(h^2,k^2)$$

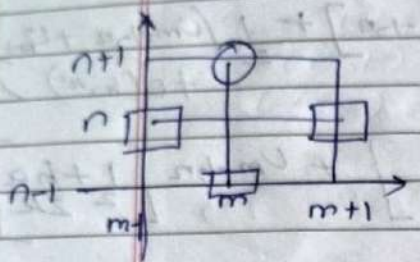
$$U_{m,n} = \frac{1}{2}\left(U_{m,n+1} + U_{m,n-1}\right), \quad \frac{h\alpha}{k^2} = r$$

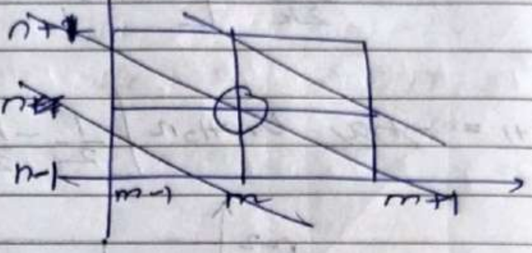
$$U_{m,n+1} = \frac{2h\alpha}{k^2}\left[U_{m-1,n} - \frac{2}{2}\left[U_{m,n+1} + U_{m,n-1}\right] + U_{m+1,n}\right] + U_{m,n-1}$$

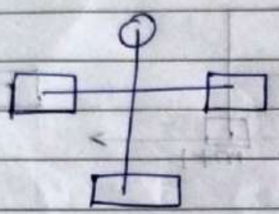
$$U_{m,n+1} = 2r\left[U_{m-1,n} - U_{m,n+1} - U_{m,n-1} + U_{m+1,n}\right] + U_{m,n-1}$$

$$U_{m,n+1} = 2r\left[U_{m-1,n} - U_{m,n+1} + U_{m+1,n}\right] + U_{m,n-1}(1-2r)$$

$$U_{m,n+1} = \frac{2r(U_{m-1,n}+U_{m+1,n}) + U_{m,n-1}(1-2r)}{1+2r}$$





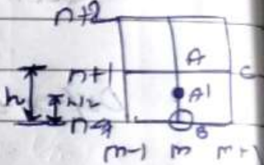


Remarks:

1. Unconditionally stable
2. 2-step method

→ Crank-Nicholson [widely used method]

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad (m, n+1/2)$$



$$U_t(m, n+1/2) = \frac{U_{m,n+1}-U_{m,n}}{2(h/2)}$$

$$U_x(m, n+1/2) = \frac{1}{2}\left[U_x(m,n+1) + U_x(m,n)\right]$$

A' A B

now applying CD

$$U_x(m, n+1/2) = \frac{1}{2}\left[\frac{U_{m+1,n+1}-U_{m-1,n+1}}{2k} + \frac{U_{m+1,n}-U_{m-1,n}}{2k}\right]$$

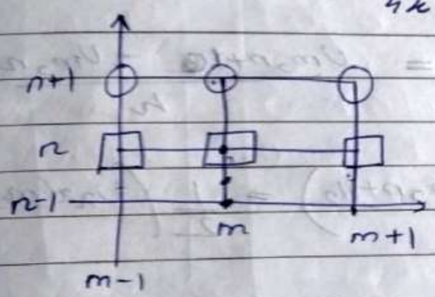
$$\therefore \cancel{U_{m,n+1/2}} \Rightarrow (\quad)\,U_{m-1,n+1} + (\quad)\,U_{m,n+1} + (\quad)\,U_{m+1,n+1}$$

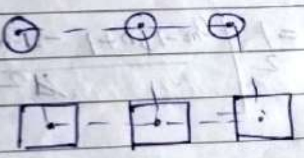
$U(\text{space}, \text{time})$
$k, m \quad h, n$

$$\frac{U_{m,n+1}-U_{m,n}}{h} + \frac{a}{4k}\left[U_{m+1,n+1} - U_{m-1,n+1} + U_{m+1,n} - U_{m-1,n}\right] = 0$$

$$-\frac{a}{4k}U_{m-1,n+1} + \frac{1}{h}U_{m,n+1} + \frac{a}{4k}U_{m+1,n+1} + \frac{a}{4k}\left[U_{m+1,n}-U_{m-1,n}\right] = 0.$$

$$-\frac{ah}{4k}U_{m-1,n+1} + U_{m,n+1} + \frac{ah}{4k}U_{m+1,n+1} = -\frac{ah}{4k}\left[U_{m+1,n} - U_{m-1,n}\right] + U_{m,n}$$





Remark :

1. 2^{nd} order accurate in both space and time
2. Implicit [Unconditionally stable]

16. $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$

BC

$U(0,t) = 0 \rightarrow BC1$

$U(1,t) = 1 \rightarrow BC2$

IC

$U(x,0) = 2$

$x \in (0,1)$ & not $[0,1]$

$$\frac{\partial u}{\partial t} = U_t(m, n+1/2) = \frac{U_{m,n+1} - U_{m,n}}{h}$$

$$\frac{\partial^2 u}{\partial x^2} = U_{xx}(m, n+1/2) = \frac{1}{2}\left(U_{xx}(m,n+1) + U_{xx}(m,n)\right)$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{2}\left[\frac{U_{m-1,n+1} - 2U_{m,n+1} + U_{m+1,n+1}}{k^2} + \frac{U_{m-1,n} - 2U_{m,n} + U_{m+1,n}}{k^2}\right]$$

$$r = \frac{\alpha h}{k^2}$$

$$\frac{(U_{m,n+1} - U_{m,n})}{1} = \frac{\alpha h}{2k^2}\left[U_{m-1,n+1} - 2U_{m,n+1} + U_{m+1,n+1} + U_{m-1,n} - 2U_{m,n} + U_{m+1,n}\right]$$

$$U_{m,n+1} - \frac{r}{2}U_{m-1,n+1} + r U_{m,n+1} - \frac{r}{2}U_{m+1,n+1} = U_{m,n} + \frac{r}{2}\left[U_{m-1,n} - 2U_{m,n} + U_{m+1,n}\right]$$

$$-\frac{r}{2}U_{m-1,n+1} + (1+r)U_{m,n+1} - \frac{r}{2}U_{m+1,n+1} = U_{m,n} + \frac{r}{2}\left[U_{m-1,n} - 2U_{m,n} + U_{m+1,n}\right]$$

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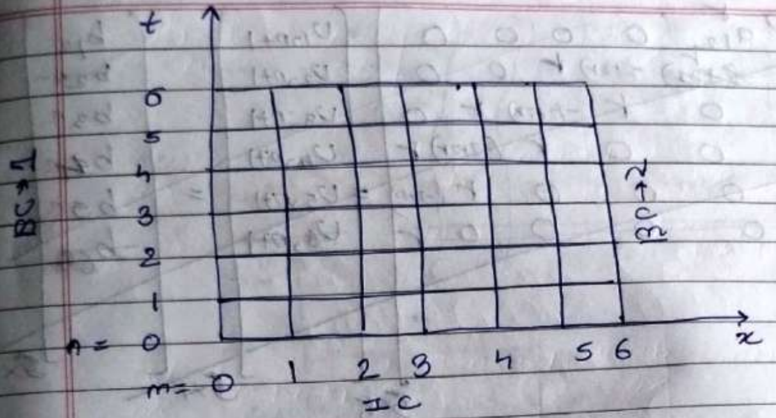


$$\boxed{\begin{matrix} M=6 \\ N=6 \end{matrix}}$$

Knowns: U_{10} U_{20} U_{30} U_{40} U_{50} (IC).

m (space), n (time)

U_{00} U_{01} U_{02} U_{03} U_{04} U_{05} U_{06} (BC1)

U_{60} U_{61} U_{62} U_{63} U_{64} U_{65} U_{66} (BC2)

$\boxed{m = 1, 2, 3, \ldots (M-1)}$

$$-\frac{r}{2} U_{m-1,n+1} + (1+r) U_{m,n+1} - \frac{r}{2} U_{m+1,n+1}$$
$$= U_{m,n}(1-r) + \frac{r}{2} U_{m-1,n} + \frac{r}{2} U_{m+1,n} \text{ (completely known).}$$

Note: If $u(x,0) = 2$ at $x \in [0,1]$

then $U_{00} = \dfrac{u(0,t) + u(x,0)}{2}$

$U_{60} = \dfrac{u(6,t) + u(6,0)}{2}$

needs to be considered in IC,

$m = 1$

$$\cancel{r U_{0,n+1}}^{\,0} - (2+2r) U_{1,n+1} + r U_{2,n+1} = b_1$$

$$a_{11} U_{1,n+1} + a_{12} U_{2,n+1} = b_1$$

$m = 2$

$$r U_{1,n+1} - (2+2r) U_{2,n+1} + r U_{3,n+1} = b_2$$

$$a_{21} U_{1,n+1} - \cancel{(2+2r)}\, a_{22} U_{2,n+1} + a_{23} U_{3,n+1} = b_3$$

$U_{n+1} = A^{-1} B_n$

$= U(0,t) - B(\ldots)$

$$\begin{array}{c} m=1 \\ m=2 \\ m=3 \\ m=4 \\ m=5 \\ m=6 \end{array}
\begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 & 0 \\ 0 & -(2+2r) & r & 0 & 0 & \\ 0 & 0 & r & -(2+2r) & r & 0 \\ 0 & 0 & 0 & r & -(2+2r) & r \\ 0 & 0 & 0 & 0 & r & -(2+2r) \\ 0 & 0 & 0 & 0 & 0 & r \\ & & \cdot & & & \end{bmatrix}_{5\times 5}
\begin{bmatrix} U_{1,n+1} \\ U_{2,n+1} \\ U_{3,n+1} \\ U_{4,n+1} \\ U_{5,n+1} \\ U_{6,n+1} \\ \cdot \end{bmatrix}_{5\times 1}
=
\begin{bmatrix} b_{1n} \\ b_{2n} \\ b_{3n} \\ b_{4n} \\ b_{5n} \\ b_{6n} \\ \cdot \end{bmatrix}_{5\times 1}$$

$$\begin{array}{c} m=1 \\ m=2 \\ m=3 \\ m=4 \\ m=5 \end{array}
\begin{bmatrix} -(2+2r) & r & 0 & 0 & 0 \\ r & -(2+2r) & r & 0 & 0 \\ 0 & r & -(2+2r) & r & 0 \\ 0 & 0 & r & -(2+2r) & 0 \\ 0 & 0 & 0 & r & -(2+2r) \end{bmatrix}_{5\times 5}
\times
\begin{bmatrix} U_{1,n+1} \\ U_{2,n+1} \\ U_{3,n+1} \\ U_{4,n+1} \\ U_{5,n+1} \end{bmatrix}_{5\times 1}
=
\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}_{5\times 1}$$

$\Rightarrow$ Thomas algorithm for solving trigonal matrix.

- Generalised implicit method

$$\frac{\partial U}{\partial t} = \alpha \frac{\partial^2 U}{\partial x^2}$$

$$U_t(m, n+1/2) = \frac{U_{m,n+1} - U_{m,n}}{h}$$

$$U_{xx}(m, n+1/2) = \theta\, U_{xx}(m,n) + (1-\theta)\, U_{xx}(m, n+1)$$

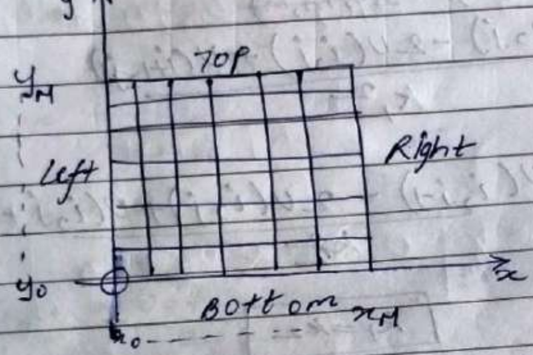
$$U_{xx}(m, n+1/2) \Rightarrow \cancel{\theta}\ U_{m,n+1} - U_{m,n} = \theta \left[\frac{U_{m-1,n} - 2U_{m,n} + U_{m+1,n}}{k^2}\right] + [1-\theta]\left[\frac{U_{m-1,n+1} - 2U_{m,n+1} + U_{m+1,n+1}}{k^2}\right]$$

Elliptic PDE :

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = H(x,y) \quad ---- \left(\frac{\text{system eq}^n}{\boxed{\text{poisson eq}^n}} \right)$$

BC:

$u(x,0) = u_1$ Bottom boundary.



$u(0,y) = u_2$ Left

$u(x,1) = u_3$ Top

$u(1,y) = u_4$ Right

Dirichlet Boundary Condition

Algorithm :

S-1 : Discretise the spatial domain

$$k_1 = \Delta x = x_{i+1} - x_i$$

$$k_2 = \Delta y = y_{i+1} - y_i$$

S2 : ~~Forward~~ Finite difference method is used to discretise PDE

set of algebraic eq^n.

S-3 : Deal with BC $\rightarrow$ AEs (if Dirichlet BC are not given)

S-4 : Solve resulting set of AE's.

unknown ⇒ $(n+1)^2$

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = H(x,y)$$

$$U_{xx} + U_{yy} = H(x,y)$$

$$\cancel{U(m-1,m) - 2U(m,m)}$$

$$\frac{U(i-1,j) - 2U(i,j) + U(i+1,j)}{k_1^2}$$

$$+ \frac{U(i,j-1) - 2U(i,j) + U(i,j+1)}{k_2^2} = H(i,j)$$

$$\boxed{k_1 = k_2}$$

$$U(i-1,j) - 4U(i,j) + U(i+1,j) + U(i,j-1) + U(i,j+1) = k^2 H(i,j)$$

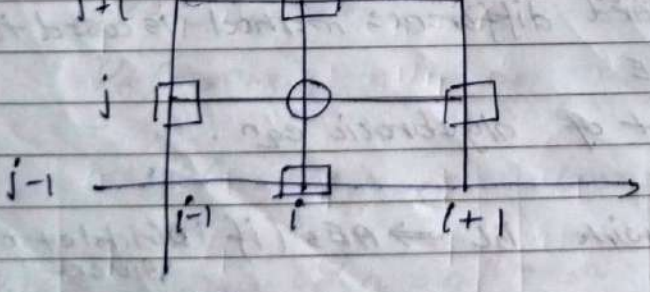
$$U(i,j) = \frac{U(i-1,j) + U(i+1,j) + U(i,j-1) + U(i,j+1) - k^2 H(i,j)}{+4}$$

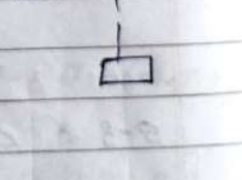
5 point formula,

valid for interior nodes ⇒ $U_{i,j} = \frac{U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - k^2 H(i,j)}{4}$ — (1)

Graphical representation.

for ⇒ H=0





for H=0 [The eq^n converts to laplace eq^n].

$$1 \le i, j \le N-1$$

no. of eq^n from (1),
$(M-1)^2$

BC $\quad U_{i,0} = U_1$ (Bottom) $\quad 1 \le i \le M-1$

$U_{0,j} = U_2$ (L) $\quad 1 \le j \le M-1$

$U_{i,M} = U_3$ (T) $\quad 1 \le i \le M-1$

$U_{M,j} = U_4$ (R) $\quad 1 \le j \le M-1$

eq$^n \Rightarrow 4(M-1)$

$$U_{00} = \frac{U_1 + U_2}{2}$$

$$U_{0,M} = \frac{U_3 + U_2}{2}$$

$$U_{M,M} = \frac{U_3 + U_4}{2} \qquad \text{Eq}^n = 4.$$

$$U_{M,0} = \frac{U_1 + U_4}{2}$$

$\therefore$ total eq^n = $(M-1)^2 + 4(M-1) + 4$
$= (M+1)^2$

Problem :-

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = 0$$

$0 \le x, y \le 1$

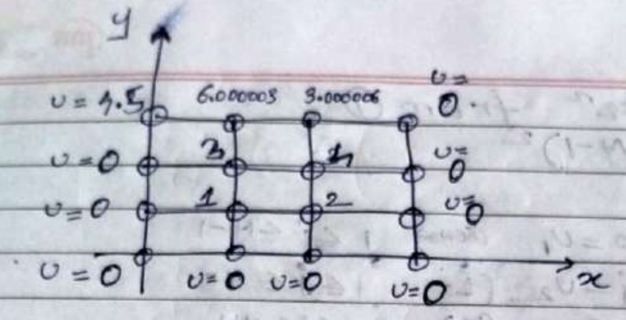
$M = 3$

U_1	B	$U(x,0) = 0$	U_1
U_2	L	$U(0,y) = 0$	U_4
U_3	T	$U(x,1) = 9(1-x)$	
U_4	R	$U(1,y) = 0$	

~~$U_{i,j}^{0} = U_i$~~

x_0	x_1	x_2	x_M / x_3
0	0.333333	0.666666	1

y_0	y_1	y_2	y_M / y_3
0	0.333333	0.666666	1



1, 2, 3, 4 ⇒ nodes

$$U_{i,j} = \frac{U_{i-1,j} + U_{i+1,j} + U_{i,j+1} + U_{i,j-1}}{4}$$

$$1 \le i,j \le M-1$$

$$U_1 = \frac{1}{4}\left[0 + 0 + U_2 + U_3\right]$$

$$U_2 = \frac{1}{4}\left[U_1 + 0 + 0 + U_4\right]$$

$$U_3 = \frac{1}{4}\left[6 + 0 + U_1 + U_4\right]$$

$$U_4 = \frac{1}{4}\left[3 + U_3 + U_2 + 0\right]$$

$$4U_1 - U_2 - U_3 = 0$$
$$-U_1 + 4U_2 - U_4 = 0$$
$$-U_1 + 4U_3 - U_4 = 6$$
$$-U_2 - U_3 + 4U_4 = 3$$

$$\begin{bmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & +4 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 6 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} 4 & -1 & 0 & -1 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \end{bmatrix}$$

$$U_1 = \frac{U_2 + U_4}{4}$$

$$-U_2 - U_4 + 16U_2 - 4U_4 = 0$$

$$15U_2 - 5U_4 = 0$$

$$3\cancel{15}U_2 = \cancel{5}U_4$$

$$U_4 = 3U_2$$

$$-U_2 - U_3 + 12U_2 = 3$$

$$11U_2 - 3 = U_3$$

$$-U_1 + 44U_2 - 12 - 3U_2 = 0$$

$$-\left(\frac{3U_2 + U_2}{4}\right) + 44U_2 = 12$$

$$\therefore \boxed{\begin{aligned} U_1 &= 0.625 \\ U_2 &= 0.5 \\ U_3 &= 2 \\ U_4 &= 1.875 \end{aligned}}$$

Pb - $\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = 0$

BC

$U = 0$ over the edge $x = 0$

$U = 0$ over the edge $y = 0$

$U = 16 - x^2 - y^2$ at the edge $x + y = 4$

Find U at the nodes of the square ~~with~~ region with mesh lenght 1.

solved in ~~Rough~~ next book

Rough work

Backwa → space

forword → time

$$\frac{C_{A\,m,n+1} - C_{A\,m,n}}{h} + v\left[\frac{C_{A\,m,n} - C_{A\,m,n-1}}{k}\right]$$

$$+ k_0 \exp\left[\frac{-\Delta E}{R}\left(\frac{1}{T_{m,n}} - \frac{1}{T_R}\right)\right] = 0$$

$C_{A\,0,n} = 1 \quad T_{0,n} = 500$

$C_{A\,m,n+1}$ $\quad C_{A\,m,0} = 1 \quad T_{m,0} = 500$

$m+1 < M \quad k = 0.025 \quad n \in 0, N-1 \quad h = 0.001$

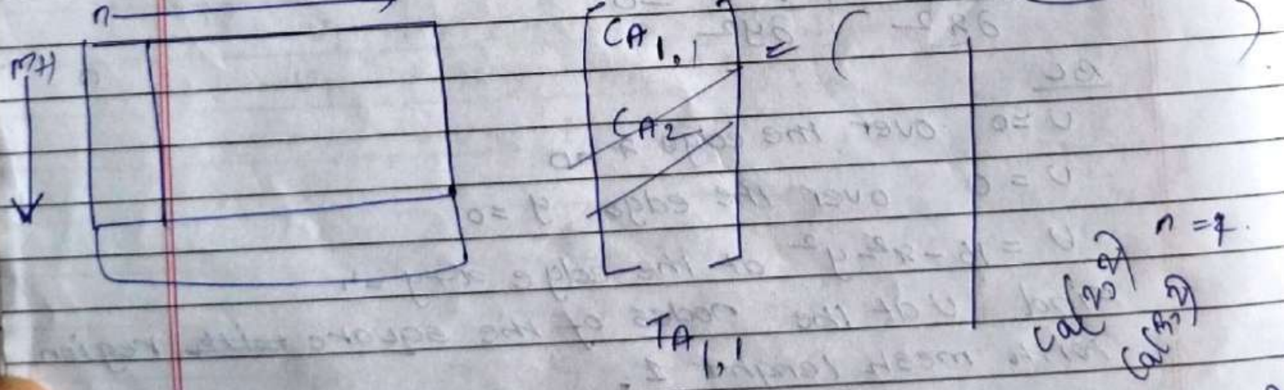
$C_{A\,1,n+1} = f(C_{A\,1,n} ; C_{A\,0,n} ; T_{1,n} ; C_{A\,1,n})$

$C_{A\,1,1} = f(C_{A\,1,0} ; C_{A\,0,0} ; T_{1,0} ; C_{A\,1,0})$

$C_{A\,2,1} = f(C_{A\,2,0} ; C_{A\,1,0} ; T_{2,0} ; C_{A\,2,0})$

C_A / T /

$n = 0.$ $\quad$ $n = 0$

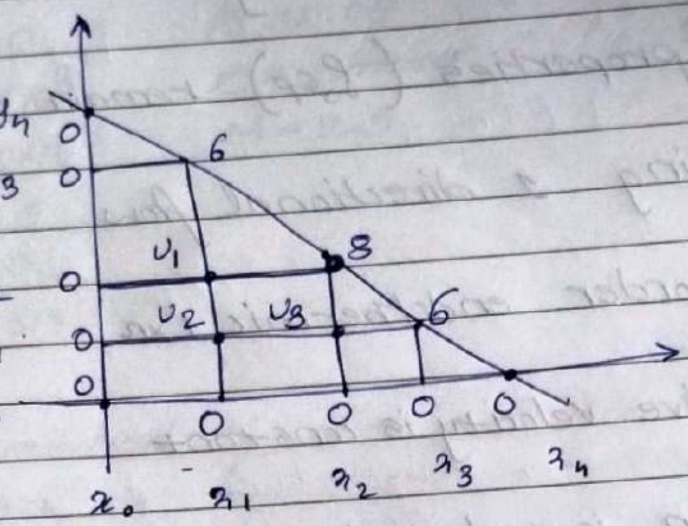


C_A

$C_{A\,1,2} = f(C_{A\,1,1} ; C_{A\,0,1} , T_{1,1} , C_{A\,1,1})$.

continue:

pb. Graphical representation:



(x, y)	$16-x^2-y^2$
(1, 3)	6
(2, 2)	8
(3, 1)	6

$U_1 = \frac{1}{4}[0+6+8+U_2]$ --- ①

$U_2 = 1/4\,[U_1 + U_3 + 0 + 0]$ --- ②

$U_3 = 1/4\,[8+6+U_2+0]$ --- ③

from ①, ② & ③

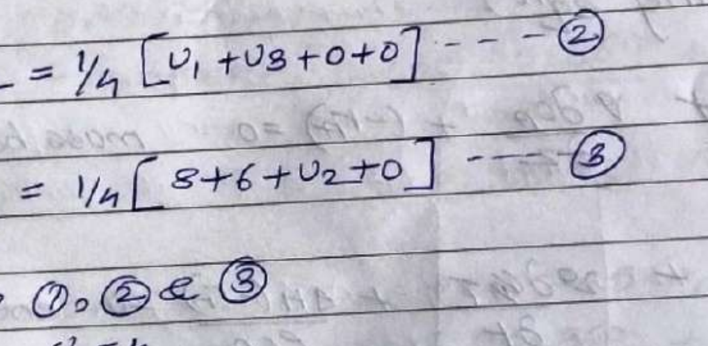
$U_1 = 4$

$U_2 = 2$

$U_3 = 4$

⟹ System with 2 PDE:

PFR:



Assumptions:

1. Perfect mixing (within plug)
2. No variation of conc^n of A and Temp. in radial direct^n

3. Not heat loss [Adiabatic]

4. Physical properties (ρ, c_p) remain constant

5. Considering 1 directional flow.

6. 2nd order endothermic rxn.

7. Convective velocity is constant

8. ~~axial~~ Diffusion is neglected.

Modelling eqn:

$$\frac{\partial C_A}{\partial t} + \frac{v \partial C_A}{\partial z} + (-r_A) = 0$$ mass balance

$$\frac{\partial T}{\partial t} + \frac{v \partial T}{\partial t} + \frac{\Delta H(-r_A)}{\rho C_p} = 0$$ energy balance.

BC's $C_A(0, t) = 1$

$T(0, t) = 500$

IC's $C_A(z, 0) = 1$

$T(z, 0) = 500$

$-r_A = k C_A^2$

$$k = k_0 \exp\left[\frac{-\Delta E}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)\right]$$

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Data:

$K_0 = 5$ $\quad h = 0.001$ $\quad$ use: BS FT

$T_r = 500$ $\quad k_1 = 0.08$ $\quad$ Backward in space and forward in time.

$\Delta E = 50\times10^3$ $\quad l = 2$ meter

$\Delta H_r = 10\times10^3$ $\quad M = 25$

$\vartheta = 0.5$

$\rho C_p = 1000$

$R = 8.314$

Using method of lines we discretise the differential eq^n

$$T_{m,n+1} = 0.99375\,T_{m,n} + 0.00625\,T_{m-1,n} - 0.05\exp\left[-\frac{6013.952869}{T_{m,n}} + 12.027905\right] C_{A_{m,n}}^2$$

$$n \geq 0 \;;\; m \in [1, M]$$

$$C_{A_{m,n+1}} = 0.99375\,C_{A_{m,n}} + 0.00625\,C_{A_{m-1,n}} - 0.005\exp\left[-\frac{6013.952869}{T_{m,n}} + 12.027905\right] C_{A_{m,n}}^2$$

$$n \geq 0 \;;\; m \in [1, M]$$

know: $C_A(0,n) = 1$ $\quad T(0,n) = 500$

$C_A(m,0) = 1$ $\quad T(m,0) = 500$

first for $m=1$ $n=0$.

$C_{A_{1,1}} = f(C_{A_{1,0}} ; C_{A_{0,0}} ; T_{1,0})$ ✓

$m=2$ $\quad C_{A_{2,1}} = f(C_{A_{2,0}} ; C_{A_{1,0}} ; T_{2,0})$ ✓

⋮

$C_{A_{M,1}}$ ✓

then for $m=1$ $n=0$.

$T_{1,1} = f(T_{1,0} ; T_{0,0} ; C_{A_{1,0}})$ ✓

$m=2$ $\quad T_{2,1} = f(T_{2,0} ; T_{1,0} ; C_{A_{2,0}})$ ✓

⋮

$T_{M,1}$ ✓

for $m=1$; $n=1$

$m=1$ $C_{A_{1,2}} = f(C_{A_{b,1}} ; C_{A_{0,1}} ; T_{1,1})$

$m=2$ $C_{A_{2,2}} = f(C_{A_{2,1}} ; C_{A_{1,1}} ; T_{2,1})$

⋮

$m=M$ $C_{A_{M,2}}$

Same gose for temperature and so on.

S-1: generate function for $C_A(m,n+1)$ & $T(m,n+1)$ computation.

S-2: keeping n same vary m from $1 \rightarrow M$ to find C_A & T at various positions.

S-3: now change n (i.e. go to next time step)
note: after 2^{st} iterations are done start checking tolerance for C_A & T

$$|C_A(m,n+1) - C_A(m,n)| \leq 10^{-6}$$

$$|T(m,n+1) - T(m,n)| \leq 10^{-6}$$

if tolerance cond^n satisfied then
Stop
else

At 5.5

z	T	C_A
1.	500	1
2.	496.692	0.6693
3.	494.9565	0.4957
4.	493.9139	0.3914
5.	493.2489	0.3244
6.	492.5358	0.2809
7.	492.3757	0.2536
8.	492.2891	0.2376
9.	492.2462	0.2289
10.	492.2265	0.2246
11.	492.2183	0.2227
12.	492.2151	0.2218
13.	492.2139	0.2215
14.	492.2135	0.2214
15.	492.2134	0.2214
16.	492.2134	0.2213
17.	492.2133	
18.		
19.		
20.		
21.		
22.		
23.		
24.		
25.		
26.		
27.	492.2133	0.2213

Batch Distillation : [for slow process]
If we use continuous distillation for slow process the residence time required is high.

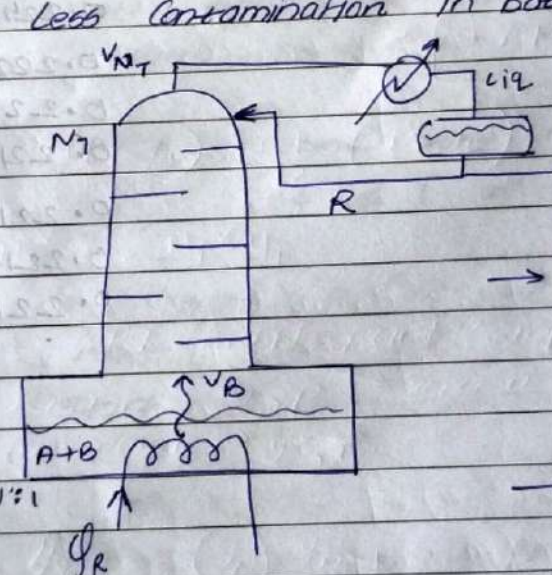
Motivation:

→ To get high valul added product
→ $N_c - 1$ no. of columns for continuous distillation
↓
no. of components

Whereas we can perform some ternary component seperation in batch distillation.

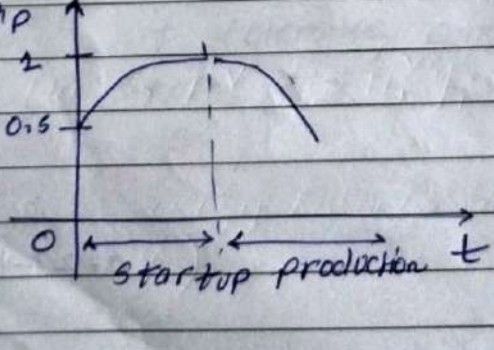
→ ~~Les~~ Less Contamination in batch distillation.

$$V_B = \frac{\varphi_R}{\lambda_B}$$



→ Start up phase:
$D = 0$
Total reflux operation

→ Production phase:
$D \neq 0$
Partial reflux operation



Note: In Batch distillation we are reaching steady state.

Assumptions:

1. - Perfect mixing on the trays.
[and eqn]

2. No heat loss (insulated column)

3. P is constant

4. Tray efficiency is fixed η [in practice $\eta \Rightarrow 40-50\%$]

$$\eta = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}} \quad \text{--- Murphy tray efficiency.}$$

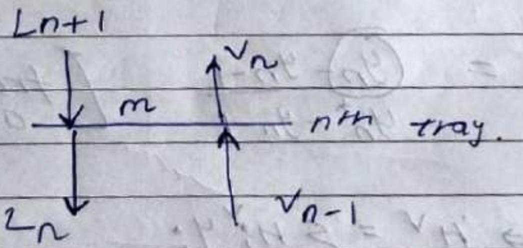
y_n^* ↳ eqm ~~compo~~ vapour composition

$y_n = ??$

5. No vapour hold up [negligible]

6. Liquid hold up is variable

7. Liquid phase is non-ideal but vapour phase is considered ideal.



will give } modelling.

$m \Leftarrow$ total $\Rightarrow$ $L_{n+1} + V_{n-1} - V_n - L_n = \frac{dm_n}{dt}$

$x \Leftarrow$ (component $\Rightarrow$ $x_{n+1} L_{n+1} + y_{n-1} V_{n-1} - x_n L_n - y_n V_n$
$= \frac{d\, x_n m_n}{dt}$

V ← energy balance,
(vapour flow rate)

maxmind®

$L_{n+1} C_{p_L} T_{n+1} + V_{n-1} C_{p_V} T_{n-1} + \lambda V_{n-1}$

energy balance

$$\cancel{\frac{H_n\, dm_n}{dt}} = \cancel{H_{n+1} L_{n+1}} + \cancel{H_{n-1} V_{n-1}} - \cancel{L_n H_n} - \cancel{V_n H_n}$$

$$\frac{d(H_{L_n} m_n)}{dt} = H_{L_{n+1}} \times L_{n+1} + H_{V_{n-1}} V_{n-1} - L_n H_{L_n} - V_n H_{V_n}$$

suppose, $C_p = a + bT + cT^2$

$$H = \int_{T_0}^{T} C_p\, dT = \int_{T_0}^{T} (a + bT + cT^2)\, dT$$

$$= \left[aT + \frac{bT^2}{2} + \frac{cT^3}{3}\right]_{T_0}^{T}$$

$$H = a(T - T_0) + \frac{b}{2}(T^2 - T_0^2) + \frac{c}{3}(T^3 - T_0^3)$$

$$H_n^V = \Sigma H_i^V y_i$$

Steps

1. from BPT (Bubble point temperatue)
   Known → x, P → known from mass balance
   Unknown → y^*, T

2. $$h = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}}$$ [from here calculate actual y]

3. find ⇒ $H^V = \Sigma H_i^V y_i$

4. Use energy balance to find V (vapour flow rate)

→ How to calculate H_L / H^L

$$\boxed{\underset{\text{sat}}{H_i^L} = \underset{\text{sat.}}{H_i^V} - \underset{\text{Latent heat}}{\lambda_i}}$$

$\lambda_i \Rightarrow f(T)$.

∴ Use Clausius Clapeyron eqⁿ

→ To calulate V assume : i. $H_n^L = 0$

ii. $H_n^L \frac{dm_n}{dt}$

iii. $H_n^L \frac{dm_n}{dt} + \dot{m}_n \frac{dH_n^L}{dt}$

→ Francis-weir eqⁿ to calculate liq flowrate

$$L_n = \underbrace{L_{n_0}}_{\text{steady state}} + \frac{m_n - m_{n_0}}{\beta} \rightarrow SS$$

β = hydraulic time constant

3-6 sec

Assume $L_{n_0} = R$ (Reflux flow rate)

→ finally we can calulate V

Note: Reboiler and reflux drums are also 2 stages with 100% efficiency.