Differential eduation Lec-2:-

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Range Kutta Method:- (RK4).

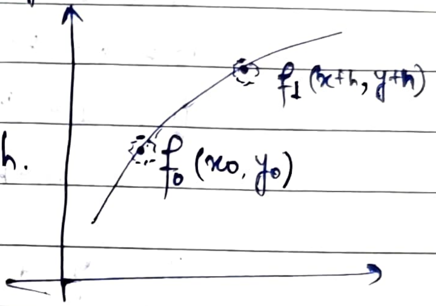
Acuracy $= (dx)^4$

can take longer step size without compromising Accuracy.

$$\frac{dy}{dx} = f(x,y)$$

$dx = h.$

$$y_2 = y_1 + \frac{f_0 + f_1}{2} \times h$$



RK4: improved ~~slope~~ estimate of the average slope over the interval of h.

(x_0, y_0) = Initial pt

→ calculate

$f_0(x_0, y_0)$.

$y\text{-temp-1} = y_0 + f_0(x_0, y_0) \cdot h/2$

calculate

$f_1(x + h/2,\ y_0 + h/2\, f_0)$

$y\text{-temp-2} = y_0 + h/2\, f_1$.

→ $f_2\ (x + h/2,\ y_0 + h/2\, f_1)$

→ $y\text{-temp-3} = y_0 + h\, f_2$

→ Calculate $f_3\ (x_0 + h,\ y_0 + h f_2)$

$$y(x_0 + h) = y_0 + h/6\,(f_0 + 2f_1 + 2f_2 + f_3)$$

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$x_0 = 0,\ y_0 = 0$

$h = 0.02$; write (21, *) x_0, y_0

do i = 1, n-iter

$f_0 = 1 + y_0^2$,

$x_1 = x_0 + h/2$. y-temp-1 = $y_0 + h/2\, f_0$

$f_1 = 1 + (\text{y-temp-1})^2$

$x_2 = x_0 + h/2$; y-temp-2 = $y_0 + h/2\, f_1$

$f_2 = 1 + (\text{y-temp-2})^2$,

$x_3 = x_0 + h$; y-temp-3 = $y_0 + h f_2$

$y_0 = y_0 + h/6\,(f_0 + 2f_1 + 2f_2 + f_3)$

$x_0 = x_0 + h$.

write (21, *) x, y0),

end do

Error:-

Euler method: In each step error goes as h^2

calculated by Euler $y_n - y_n(x_n) = h^2 \frac{d^2y}{dx^2}$,

Actual.

as we neglect the terms of h^2, (Local truncation error).

we neglect this order term

local error goes as $= h^2$

Global truncation error:

$$= \sum_{i=1}^{N} h^2 \frac{d^2y}{dx^2}\Big|_i \approx (x_N - x_0)\, h \left|\frac{d^2y}{dx^2}\right|.$$

value of derivative at ith step.

of h (error reduced by $\frac{1}{2}$)

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Improved Euler:-

Error in each step → Local truncation error h^3.

Global truncation error $\approx h^2$.

Runge Kutta (RK4):

Local truncation error h^5.

Global " " h^4.

Terms of h^5 ignored in the taylor expansion.

Lec-3:-

2nd order Diff eqn : Simple Harmonic oscillator

$$m\frac{d^2x}{dt^2} = -Kx \qquad \frac{d^2x}{dt^2} = -\frac{K}{m}x.$$

2nd order diff. eqn

⇓

2 first order diff eqn.

$$\Rightarrow \frac{dv}{dt} = -K/m\, x, \qquad \frac{dx}{dt} = v$$

for time $t=0$ $\qquad K=1, m=1.$

$x_0 = 0$

$v_0 = 0.1$

$T=20$, $h=0.2$, n-iterations = n-iter $= \frac{20}{0.02}$

$= 1000$

Energy will be constant in SHM

do i = 1, n_iter

$f_0 = v_0$; x_temp_1 = $x_0 + f_0 h/2$

$f_{0v} = -K/m\, x_0$, v_tem_1 = $v_0 + f_{0v} h/2$

calculate f_1, f_{1v}, x_temp_2, v_temp_2,

f_2, f_{2v}, x_temp_3, v_temp_3,

→ f_3, f_{3v},

$x_0 = x_0 + \frac{h}{6}[f_0 + 2f_1 + 2f_2 + f_3]$;

$v_0 = v_0 + \frac{h}{6}[f_{0v} + 2f_{1v} + 2f_{2v} + f_{3v}]$.

write(10, *) h * dfloat(i), x0, v0

as we use dt = 0.02, we get error that energy is not const.

dt = 0.001, energy const

error goes as h,

in RK error goes as h^3,

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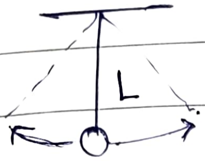
Lec-4:-

$$m\frac{d^2x}{dt^2} = -Kx.$$

$$\frac{d^2x}{dt^2} = -x, \quad K=1,\ m=1.$$



$$\frac{d^2\theta}{dt^2} = -g/L \sin\theta.$$

For small θ.

For small oscillation problem we use that. $$\frac{d^2\theta}{dt^2} = -g/L\,\theta.$$

Take $g/L = 1$. $L = 9.8m$

$$\frac{d^2x}{dt^2} = -\sin x.$$

$$\frac{dx}{dt} = v \Rightarrow \boxed{\frac{dv}{dt} = -\sin x.}$$

use Runge Kutta as usual.

$$F = -\frac{dV}{dx} = -\sin(x)$$

$$V = \int \sin(x)\,dx$$

$$= -\cos x$$

$$\boxed{E = \frac{1}{2}mv^2 + \frac{1}{2}Kx^2 \quad \text{(Spring)}}$$

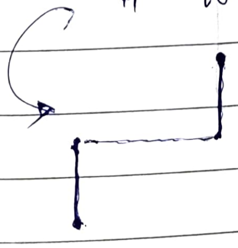
$$\frac{d^2x}{dt^2} = F = -\sin x$$

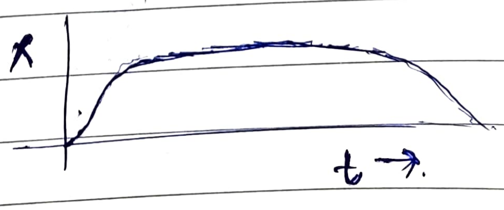
$V_1 = 1.8$

$$\boxed{E = \frac{1}{2}mv^2 - \cos x}$$

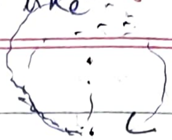
$V_0 = 1.99$ Energy should be conserved.

$V_3 = 2$ — If we gave enough velocity to it it will go to a position.





if we go. further velocity it will go like



Now To look at a slightly more complex problem:-

$$\frac{dy_i}{dt} = v_i,$$

$$\frac{dv_i}{dt} = -\frac{K}{m}\left[(y_{i+1} - y_i) + (y_{i-1} - y_i)\right]$$

$$= -\frac{K}{m}\left[y_{i+1} + y_{i-1} - 2y_i\right]$$

$$\frac{dv_{i+1}}{dt} = -\frac{K}{m}\left[(y_{i+2} + y_i - 2y_{i+1})\right]$$

If you have 20 particles: solve 40 coupled diff edn. bec → 2nd order diff edn → 2 first order diff.

→ Assume periodic boundary conditions

$$\frac{dv_L}{dt} = -\frac{K}{m}\left[y_1 - y_L + y_{L-1} - y_L\right]$$

$$\frac{dv_1}{dt} = -\frac{K}{m}\left[y_2 - y_1 + y_L - y_1\right]$$

Initial conditions:

$$\left.\begin{array}{ll} \text{20 values} & y_0^1 \; y_0^2 \; \cdots \; y_0^L \\ \text{20 values} & v_0^1 \; v_0^2 \; \cdots \; v_0^L \end{array}\right]$$

40 first order diff edn.
40 initial conditions.

let us $y_0^1 = 0.3,$

$$\left.\begin{array}{l} y_0^2 \cdots y_0^L = 0 \\ v_0^1 \cdots v_0^L = 0 \end{array}\right]$$

only the first particle dispeared.

as the particles are coupled all the particle will move.

The main thing to remember is calculate f_0 f_1 f_2, f_3 & f_{0v} f_{1v} f_{2v} f_{3v}.

Arrays:-

$f_0(20)$ $f_1(20)$ $f_2(20)$ $f_3(20)$

$f_{0v}(20)$ $f_{1v}(20)$ $f_{2v}(20)$ $f_{3v}(20)$.

& similarly $y(20)$ & $v(20)$.

Moreover

x_temp1	→	y1 (20)
x_temp_2	→	y2 (20)
x_temp_3	→	y3 (20)

Similarly for:

v_temp_1	v1 (20)
v_temp_2	v2
v_temp_3	v3.

Lastly

$$\frac{dv_i}{dt} = -\frac{K}{m}\left[y(i+1) + y(i-1) + y(i)\right]$$

$$= f_{0v}(i)$$

What about PBC

$$\boxed{\begin{aligned} v1i &= v(i) + f_{0v}(i)\, h/2 \\ y1(i) &= y(i) + f_0(i)\, h/2. \end{aligned}}$$

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Now In the case of array we have to calculate $f_0(20)$, $f_1(20)$,

~~calculate f_0 for 20 particles.~~
~~$f_1(20) \rightarrow$ for 20 particles.~~
~~$f_2(20) \rightarrow$ for 20 particles ——~~
~~$f_{0V}(20)$, $f_{1V}(20)$: 20 particles.~~

To calculate

$f_{1V}(i) \rightarrow$ you need $y1(i)$ & $y1(i+1)$ & $y1(i-1)$

So the ALGO SHOULD BE

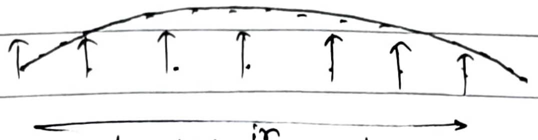
```
do i = 1, n-iter
do KK = 1, no. of particles
calculate f0 & f0v -> for all particles
end do.
do KK = 1, no. of particles
calculate x1 & v -> for all particles
end do
do KK = 1, no. of particles
calculate f1 & f1v
end do
do KK = 1, no. of particles
calculate y2 & v2 -> for all particles
end do
end do,
```

Take care of PBC

$\boxed{\text{Incorporate PBC}}$

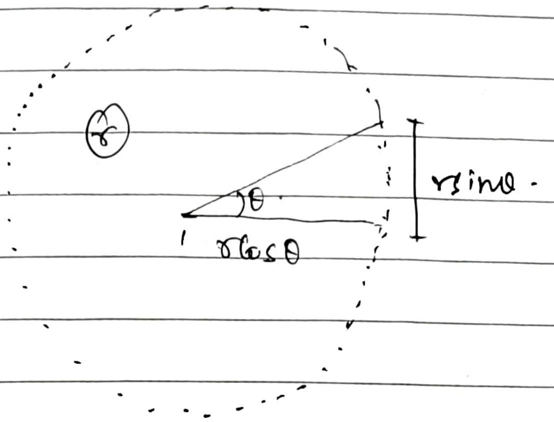
Assignment-4.

→ Lec-5:-



particle in xz plane.

So this particle will vibrate along y direction.



Lec-6 : Boundary value problems

: Finite Difference method:

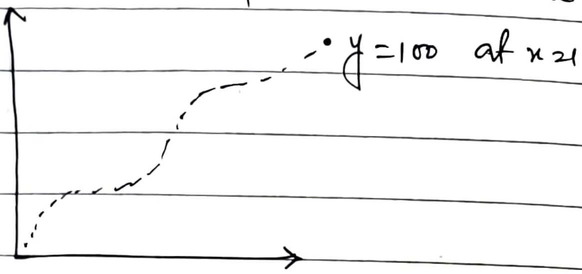
$$\frac{d^2y}{dx^2} - 5\frac{dy}{dx} + 10y(x) = 10x.$$

$$y'' - 5y' + 10y = 10x.$$

Boundary Conditions

$y(0) = 0$, $y(1) = 100$

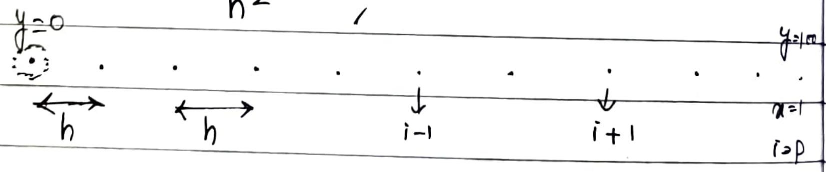
Find the solution from $x = 0$ to $x = 1$



$$y'_i(x) = \frac{y_{i+1} - y_{i-1}}{h}$$

$$y(x) = y_0(x) + \frac{dy}{dx} \times h,$$

$$y''_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2},$$



$$p = \frac{x_f - x_i}{h}$$

nop = int(p)

$i = 1, 2, 3, 4, 5, \ldots, p$

If $h = 0.1$ $x_1 = 0$ $x_2 = 0.1$ $x_3 = 0.2$ - -

If $h = 0.05$ $x_1 = 0$ $x_2 = 0.05$ $x_3 = 0.1$, ...

$y_1 = 0$, $y_i = ?$ $y_p = 100$.

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$$y''(x) - 5y' + 10y = 10x$$

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} - 5\,\frac{y_{i+1} - y_{i-1}}{2h} + 10y_i = 10x_i,$$

$$y_{i+1} - 2y_i + y_{i-1} - \frac{5}{2}h\,(y_{i+1} - y_{i-1}) + 10h^2 y_i = 10x_i h^2$$

$$y_i = \frac{1}{2-10h^2}\left[\left(1-\frac{5h}{2}\right)y_{i+1} + \left(1+\frac{5h}{2}\right)y_{i-1} - 10h^2 \cdot x_i\right]$$

Now this becomes algebric eqn.

Now from this eduation if you know the value of y_{i+1} & y_{i-1} Then you can calculate Improved (more accurating) values of y_i.

$x_3 = 0.1$

$x_1 = 0$ $x_2 = 0.05$ $x_4 = 0.15$

$i = p$ = no. of pts.

NOTE → $y(1)$ $y(nop)$ | cal- y (nop)

NOT updated | = initial values of y_i for all values of i, i.e. at each values of x_i.

Boundary points

Imp.

$y(2) =$ ____, $y(3) =$ ____. $y(4) =$ ____

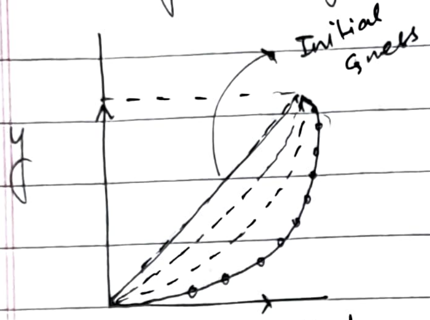
$y(nop-1) =$ ____ -

new improved value of the solution $y(x)$ available.

$y\text{-old} = y$ for all i.

* calculate new improved values of y

$y\text{-old} = y$ for all i



$y\text{-old} = 0 y$ for all i

$y = y_{init}$

do

$y\text{-old} = y;\ ll = ll + 1$

do i = 2, nop − 1

$$y(i) = \frac{1}{(2 - 10h^2)}\left[d_1\, y\text{-old}(i+1) + d_2\, y\text{-old}(i-1) - d_3\, x(i)\right]$$

end do

$x = 0$ $\qquad$ $x = 1$

$y = 0$ at $x = 0$, $\qquad$ $y = 100$ at $x = 1$

$d_1 = \left(1 - \frac{5h}{2}\right)$

$d_2 = \left(1 + \frac{5h}{2}\right)$

$d_3 = 10h^2$

* condition for exit ?

Cond = 1

If (Cond = 1) THEN Exit

end do

If

$y(i) - y\text{-old}(i) < 10^{-3}$ for all values of i then Cond = 1

Convergence criteria

Cond = 1.

do i = 2, nop − 1

if ($y(i) - y\text{-old}(i)$ g.e. 10^{-3}) Cond = 0

end

If (cond. eq. 1) exit

Jacobi method :-

$$y' = \frac{y_{i+1} - y_{i-1}}{2h}$$

$$y'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$$

error h^3,

will come errors, 10^{-5}. order

error = 0.0025,

So I have to set the limit to be 10^{-8}.

$h = 0.05$,

Gauss Seidal method :-

i=1 i=2 i=3 .... i=4

y_1 y_2 y_3 ------ y_4 - y_p.

in the jacobian method

→ update all values of y_i using Yold (i+1) & y.old (i-1) & then y.old = y.

→ calculate new values of y_i

But $y(i-1)$ updated before $y(i)$

So $y(i) = c_1 [d_1\ y.old(i+1) + d_2\ y(i-1) + d_3\ x(i)]$

÷ Partial Diff equation :-

Finite Difference method.

1. $\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u \rightarrow$ Wave equation.

c is the speed of the wave.

2. $\nabla^2 \phi = 0$ (Laplace eqn)

3. $\nabla^2 \phi = \rho$ (poisson eqn)

$\hookrightarrow$ charge Density.

4. Maxwell equations

$$\vec{\nabla} \cdot \vec{E} = \rho, \quad \vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \mu_0 J + \mu_0 \epsilon_0 \frac{\partial E}{\partial t}$$

Diffusion equation:

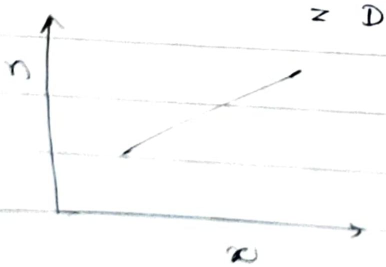
$$\frac{\partial n}{\partial t} = D \nabla^2 n.$$

particle current $\vec{J} = -D \bar{\nabla} n$

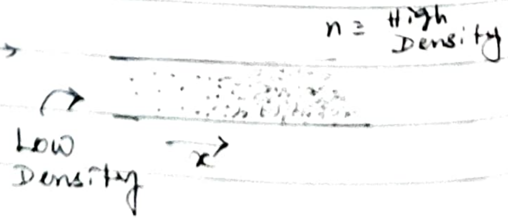
$$\frac{\partial n}{\partial t} = -\vec{\nabla} \cdot \vec{J} \quad \text{(Conservation of mass)}$$

$$\Rightarrow \frac{\partial n}{\partial t} = -\vec{\nabla} \cdot (-D \vec{\nabla} n)$$

$$= D \nabla^2 n (x, y, t)$$



n $\rightarrow$ number Density

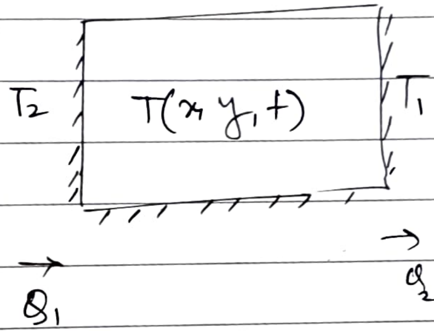


particle current: no. of particle crossing per unit area per unit time.
particle current

Heat conduction through a metalic plate:-

$$\vec{q}(x,y,t) = -\alpha \bar{\nabla} T(x,y,t) \qquad T \to \text{Temp.}$$

$\vec{q}(x,y,t)$ = Heat current
: Magnitude to heat flow at (x,y) at time t ⊥ to the Area. A.



$\alpha \to$ Thermal Conductivity.

Amount of heat passes through unit area per unit time. when $\frac{dT}{dx} = 1$.

Conservation of energy in unit volume

~~when $\frac{dT}{dx} = 1$.~~

$$\frac{\partial Q}{\partial t} = -\vec{\nabla} \cdot \vec{q}$$

$$= \vec{\nabla}(-\alpha \bar{\nabla} T)$$

$$\frac{\partial Q}{\partial T} = \alpha \nabla^2 T$$

$Q \to$ Internal heat energy per unit volume.

Now

$$\frac{\partial Q}{\partial t} = c\rho \frac{\partial T}{\partial t} \qquad T \to \text{temperature} \quad t \to \text{time.}$$

$c \to$ specific Heat capacity. $\qquad \rho \to$ density

Amount of Heat in Joules required to raise the temperature of 1gm of metal by 1 Kelvin.

$c\rho \rightarrow$ Amount of Heat in Joules required to raise the temperature of 1 gm of metal by 1 Kelvin.

$c\rho \rightarrow$ Amn. of heat required to raise temp of unit volume by 1 Kelvin.

Assuming Homogeneous & isotropic material.

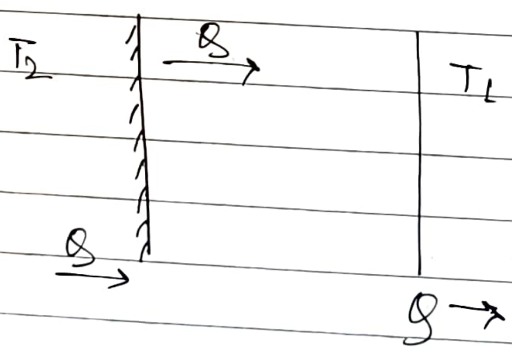
$$c\rho \frac{\partial T}{\partial t} \cancel{dt} = K \nabla^2 T$$

$$\frac{\partial T}{\partial t} = \frac{K}{c\rho} \nabla^2 T.$$

$$\frac{\partial T}{\partial t} = K' \nabla^2 T.$$

$$\frac{\partial n}{\partial t} = D \nabla^2 n.$$

(Diffusion eqn)



When there is no explicit time Dependence i.e. the system (metalic plate) has relaxed to steady state (NOT equilibrium)*

That is there is no time Dependence.

Whatever heat flow from the ~~right~~ left side Coming out from right side

$$\frac{\partial T}{\partial t} = 0$$

$\nabla^2 T = 0$. (Laplace eqn).

So we have Laplace equation.

finite in $x, y \rightarrow L_x, L_y$
but no z dependence.

$$\nabla^2 \phi = 0$$

$$\nabla^2 T(x,y) = 0$$

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

0 1 2 3 4 5 6 7 L_x

$\overleftrightarrow{\Delta x}$

Discretising space

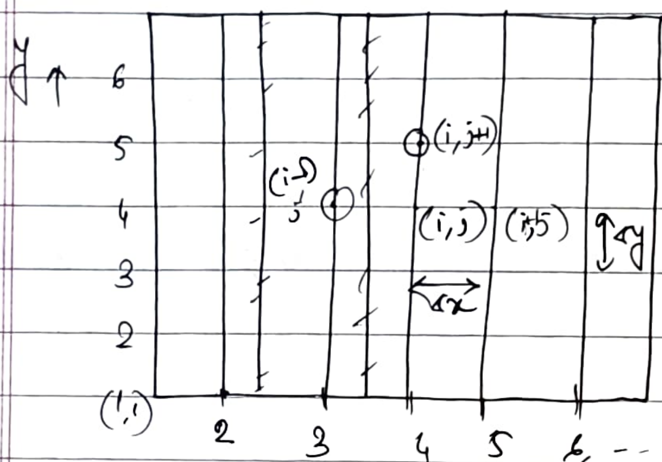
$$\frac{\partial^2 T}{\partial x^2} = \frac{T(x+\Delta x) - 2T(x) + T(x-\Delta x)}{(\Delta x)^2}$$

$$\boxed{\frac{\partial T}{\partial x} = \frac{T(x+\Delta x) - T(x-\Delta x)}{2\Delta x}}$$

$$\frac{T(x+\Delta x, y) - 2T(x,y) + T(x-\Delta x, y)}{(\Delta x)^2}$$

$$+ \frac{T(x, y+\Delta y) - 2T(x,y) + T(x, y-\Delta y)}{(\Delta y)^2} = 0$$

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i+1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j+1}}{(\Delta y)^2} = 0$$



$$T_{i,j} = \frac{(\Delta x)^2 (\Delta y)^2}{2\left[(\Delta x)^2 + (\Delta y)^2\right]} \times \left[\frac{T_{i+1,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} + T_{i,j-1}}{(\Delta y)^2}\right]$$

If $\Delta y = \Delta x$

$$T_{i,j} = \frac{1}{4}\left[T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}\right]$$

In Addition you need Boundary condition.

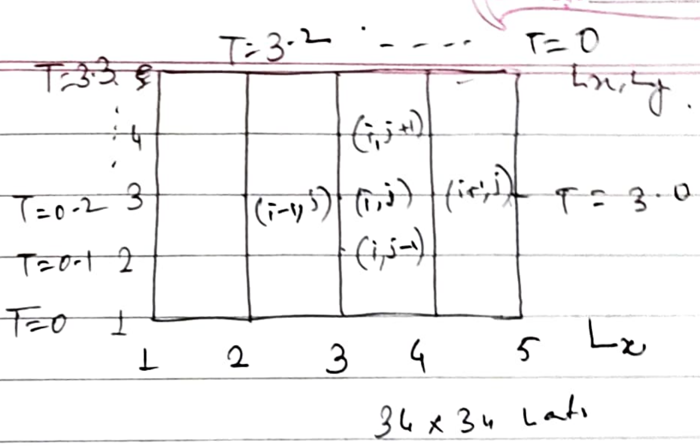
When no explicit t dependence

$$\nabla^2 T = 0, \Rightarrow \frac{\partial^2 T}{\partial x^2} = 0$$

$$\frac{dT}{dx} = C_1 \quad \& \quad T = C_1 x + C_2$$

& B.C. - $T = T_2$ at $x = 0$

$T = T_1$ at $x = L_x$.



Dirichleet Boundary Conditions:-
→ $T(x,y)$ was specified along the Boundaries.

specify:-
$\frac{\partial T}{\partial x}$, or $\frac{\partial T}{\partial y}$ along Boundaries.

This is Neumann Boundary conditions.

$$\vec{q}(x,y,t) = -k\vec{\nabla}T(x,y,t) \rightarrow \text{Fourier law.}$$

$\vec{q}(x,y) = -k\nabla T(x,y)$ If the system reached the steady state.

$$q_x = -k\frac{\partial T}{\partial x}$$

$$q_y = -k\frac{\partial T}{\partial y}$$

If instead of $T(x,y)$ at Boundaries, we specify heat flowing in per unit time.

$q_x = A_0$, $\quad q_y = -C_0$,

→ Neumann B.C.

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Cauchy Boundary Condition:-

$T(x, y)$ & $\frac{\partial T}{\partial x}\Big|_{x=1}$ specified for $x=1$ or $x = L_x$.

$$\frac{\partial T}{\partial x} = \frac{T(x+\Delta x) - T(x-\Delta x)}{2\Delta x}$$

$$= \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x}.$$

$$\frac{\partial T}{\partial y} = \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta y}$$

→ Taylor expansion.

2nd order term

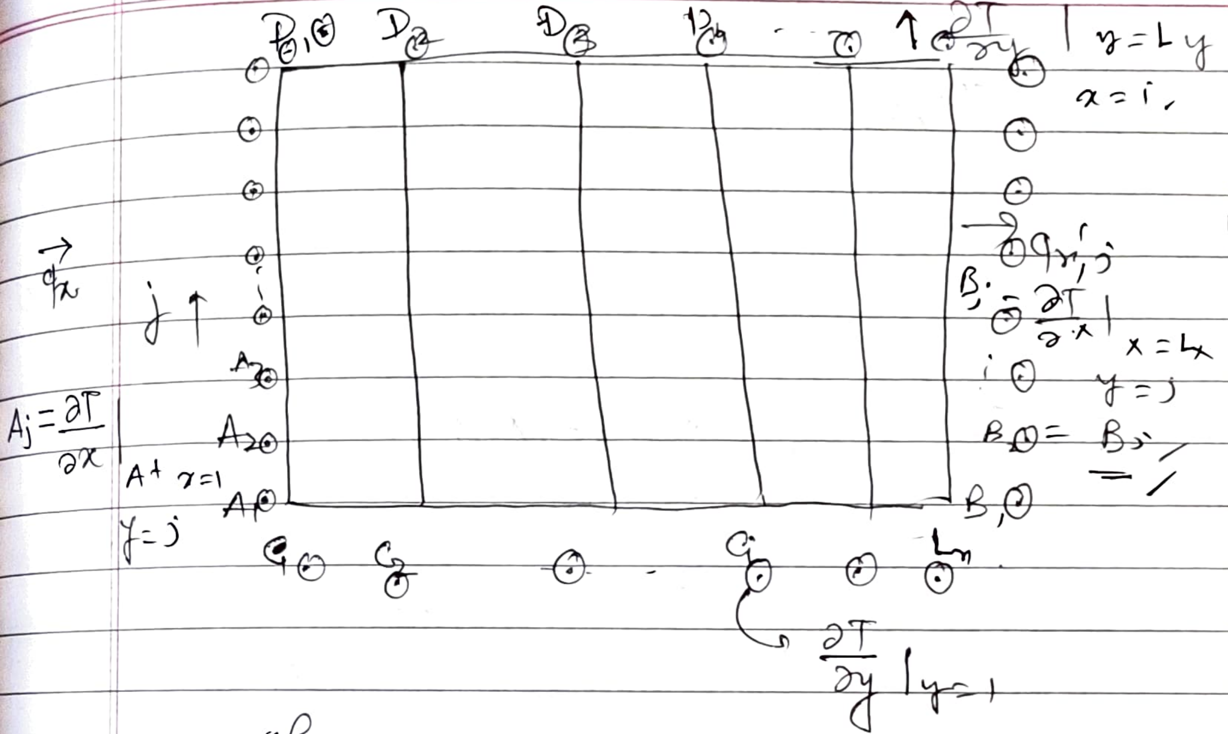
$$\frac{\partial T}{\partial x} = \frac{T(x+\Delta x) - T(x)}{\partial x}$$

keeping first order term for Taylor expansion.

Laplace eqn: $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0.$

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0$$

$i = 1$ & L_x: $T_{0,j}$, T_{L_x+1} | $j = 1, L_y$. $T_{i,0}$, T_{i,L_y+1}.



if you $T_{i,j+1}$ $\quad j = L_y$

T_{i,L_y+1} ↳ But this you not have

$T_{i-1,j}$

$i = 1 \Rightarrow T_{0,j}$ you not have

$$A_j = \frac{\partial T}{\partial x}\Big|_{x=1, y=j} = \frac{T_{2,j} - T_{0,j}}{2\delta x}$$

$$\Rightarrow 2A_j\delta x = T_{2,j} - T_{0,j}$$

$$T_{0,j} = T_{2,j} - 2A_j\delta x$$

$$D_i = \frac{\partial T}{\partial y}\Big|_{y=L_y, x=i} = \frac{T_{i,L_y+1} - T_{i,L_y-1}}{2\delta y}$$

$$T_{i,L_y+1} = D_i \, 2\Delta y + T_{i,L_y-1}$$

$$\frac{T_{2,j} - 2T_{1,j} + T_{0,j}}{(\Delta x)^2} + \frac{T_{1,j+1} - 2T_{1,j} + T_{1,j-1}}{(\Delta y)^2} = 0$$

$$\Rightarrow \frac{T_{2,j} - 2T_{1,j} + (T_{2,j} - 2A_j \Delta x)}{(\Delta x)^2} + \frac{T_{1,j+1} - 2T_{1,j} + T_{1,j-1}}{(\Delta y)^2} = 0$$

$$\Rightarrow T_{1,j} = \frac{(\Delta x)^2 (\Delta y)^2}{2[\Delta x^2 + \Delta y^2]} \times \left[\frac{2T_{2,j} - 2\Delta x A_j}{(\Delta x)^2} + \frac{T_{1,j+1} + T_{1,j-1}}{(\Delta y)^2} \right]$$

$$T_{1,j} = \frac{1}{4}\left[2T_{2,j} - 2\Delta x A_j + T_{1,j+1} + T_{1,j-1}\right]$$

for all $j = 1, \dots L_y$ at $x = 1$.

$T_{L_x,j}$

$T_{i,j}$

T_{i,L_y}

can be calculated

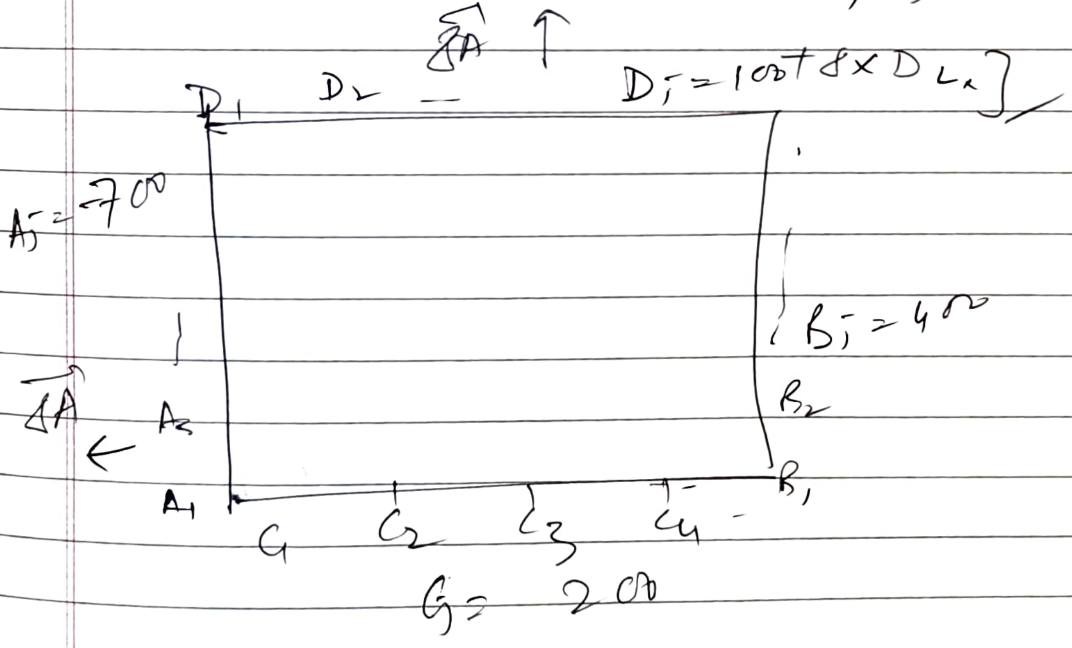
So ~~you~~ using these ~~ghost~~ pts /

$$T_{1,1} = \frac{1}{2}\left[T_{1,2} - \Delta x\, C_1 + T_{2,1} - \Delta x\, A_1\right]$$

$$T_{1,L_y} = \frac{1}{2}\left[T_{1,L_y-1} + \delta x\, D_1 + T_{2,L_y} + \delta x\, A_{L_y}\right]$$

$$T_{L_x,1} = 0.5\left[T_{L_x-1,1} + \delta x\, B_1 + T_{L_x,2} - \delta x\, C_{L_x}\right]$$

$$T_{L_x,L_y} = 0.5\left[T_{L_x-1,L_y} + \delta x\, B_{L_y} + T_{L_x,L_y-1} + \delta x\, D_{L_x}\right]$$



So at steady state

net Incoming flux

= net outgoing flux.