

# CFD in Python Lecture -1

Tuesday, July 9, 2024 12:11 PM

## Forward differencing Method

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} + O(h)$$

$h \rightarrow$  grid spacing

$$|h < 1|$$

First order estimate

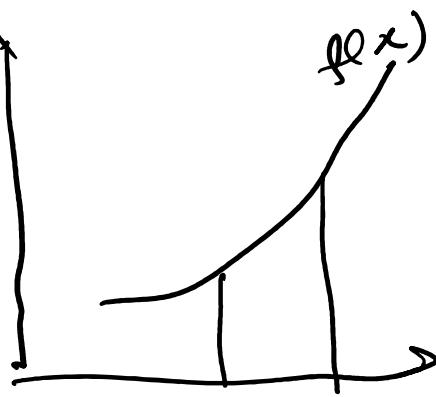
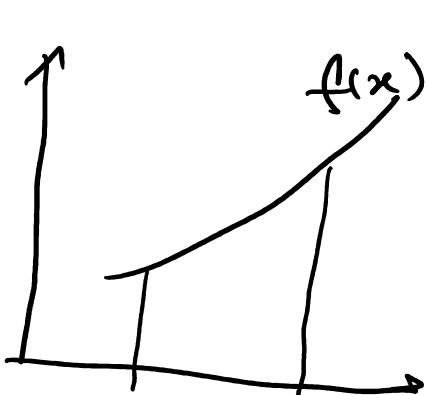
Approximation value

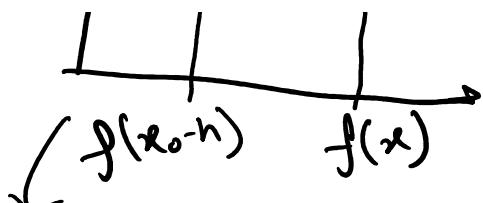
Truncation error

leading term is the order of  $h$   
 $(\frac{h}{2!} f''(x_0) + \dots)$

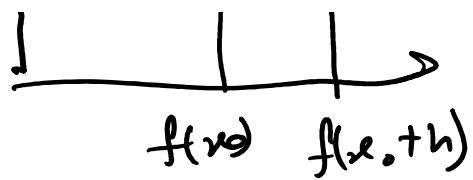
## Backward differencing Method

$$f'(x_0) = \frac{f(x_0) - f(x_0-h)}{h} - O(h)$$





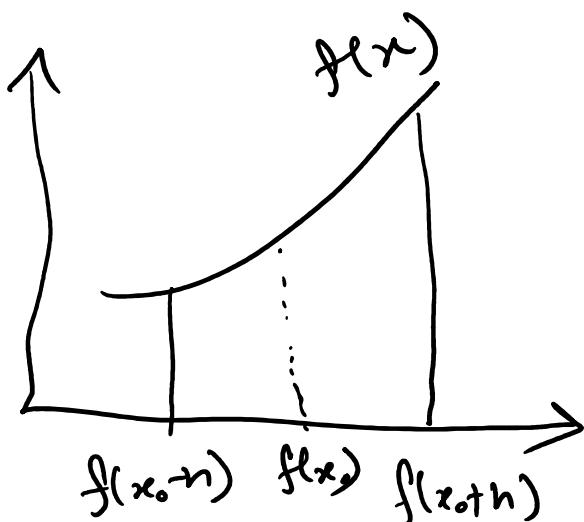
For backward differencing method



forward differencing method

## Central Differentiating Method

$$f'(x_0) = \frac{f(x_0-h) - f(x_0+h)}{2h} - \frac{o(h^2)}{\square}$$



Truncation error  
is in the order  
of  $h^2$

Central differencing method

Solve: 
$$\boxed{-4x^5 + 7x^3 - 3x + 9}$$
 → Polynomial to solve using

Given,  $x_0 = 0$

forward, backward

Given,  $x_0 = 0$

$$h = 0.25$$

Grid spacing

=====

using  
forward, backward  
backward and central  
differencing  
method

## Second Order Derivative

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - O(h^2)$$

Second derivative with second order accuracy

Central differencing

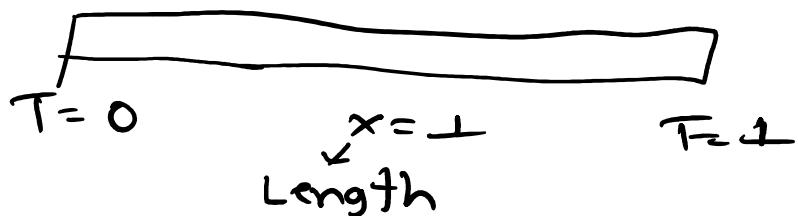
Forward differencing

$$f''(x_0) = \frac{f(x_0+2h) - 2f(x_0+h) + f(x_0)}{h^2}$$

Backward differencing

$$f''(x_0) = \frac{f(x_0) - 2f(x_0-h) + f(x_0-2h)}{h^2}$$

# One dimensional Problem

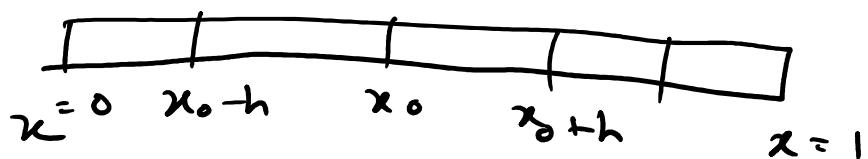


1-D diffusion equation,

$$\frac{d^2T}{dx^2} = 0$$

Initially  $T(t=0, x < 1) = 0$  and  
 $T(t=0, x=1) = 1$

Dividing the geometry in computational mesh



Converging solution,

criterion

$$\sum_{x=x_s} |T_{\text{new}} - T_{\text{old}}| \leq \epsilon$$

↓  
tolerance number

$$T |T_{\text{new}} - T_{\text{old}}| \leq \epsilon$$

↑ ↗

$$\sum_x |T_{\text{new}} - T_{\text{old}}| < \epsilon$$

$\left( \frac{T_{\text{new}} - T_{\text{old}}}{T_{\text{old}}} \right) < \epsilon$

**Exercise:** 1D convection diffusion equation

$$U \frac{dT}{dx} + \frac{d^2T}{dx^2} = 0$$

$$\text{Now, } \frac{dT}{dx} = T'(x)$$

$$T''(x) = \frac{T(x_0+h) - 2T(x_0) + T(x_0-h)}{h^2}$$

[using central  
differenceing  
method]

Given that,

$$\frac{dT}{dx} = T'(x) = 0$$

Therefore,

$$0 = T(x_0+h) - 2T(x_0) + T(x_0-h)$$

. . . . .  $\perp T(x_0+h) - T(x_0-h)$

$$\Rightarrow T(x_0) = \frac{1}{2} (T(x_0+h) + T(x_0-h))$$

Using Forward differencing scheme,

$$T''(x) = \frac{T(x_0+2h) - 2T(x_0+h) + T(x_0)}{h^2}$$

$$T(x_0) - 2T(x_0+h) + T(x_0+2h) = 0$$

$$\Rightarrow T(x_0) = 2T(x_0+h) - T(x_0+2h)$$

Using Backward differencing scheme,

$$T''(x) = \frac{T(x_0) - 2T(x_0-h) + T(x_0-2h)}{h^2}$$

$$\Rightarrow T(x_0) - 2T(x_0-h) + T(x_0-2h) = 0$$

$$\Rightarrow T(x_0) = 2T(x_0-h) - T(x_0-2h)$$

For exercise problem,

$$0 - \frac{dT}{dx} \rightarrow \frac{dT}{dx} = 0$$

taking  $v$  as constant,

using central differencing method,

using central difference

$$\Rightarrow \text{U}_x \frac{T(x_0+h) - T(x_0-h)}{2h} + \frac{T(x_0+2h) - 2T(x_0) + T(x_0-2h)}{2h} = 0$$

$$\Rightarrow \frac{\text{U}_h(T(x_0+h) - T(x_0-h)) + 2T(x_0+h) - 4T(x_0) + 2T(x_0-h)}{2h^2} = 0$$

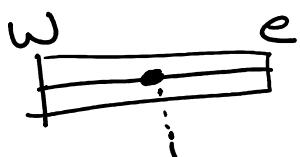
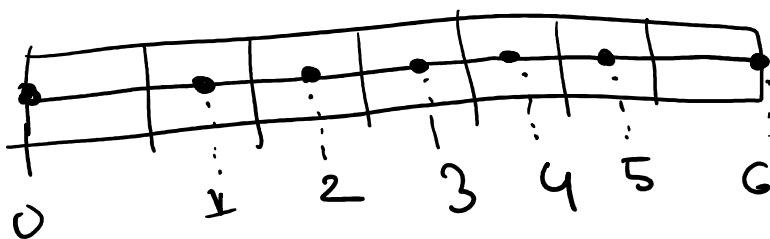
$$\Rightarrow \text{U}_h(T(x_0+h) - T(x_0-h)) + 2T(x_0+h) - 4T(x_0) + 2T(x_0-h) = 0$$

$$\Rightarrow T(x_0+h) \{ \text{U}_h + 2 \} + T(x_0-h) \{ 2 - \text{U}_h \} = 4T(x_0)$$

$$\Rightarrow T(x_0) = \frac{1}{4} \left[ (\text{U}_h + 2)T(x_0+h) + (2 - \text{U}_h)T(x_0-h) \right]$$

1. 1 r. 1 volume

# Generalized Finite Volume Method

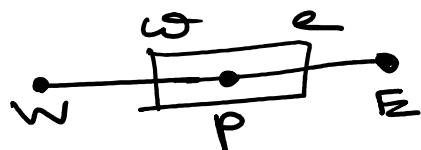


$$\frac{dT}{dx}|_c - \frac{dT}{dx}|_w = 0$$

Heat conduction governing equation

Generalized  $\rightarrow \frac{d}{dx} \left( k \frac{dT}{dx} \right) = 0$  [At first we consider  $k = \text{const}$ ]

$k \rightarrow$  Thermal conductivity



Now employing Gauss divergence theorem.

$$\oint \frac{d}{dx} \left( k \frac{dT}{dx} \right) dV = 0$$

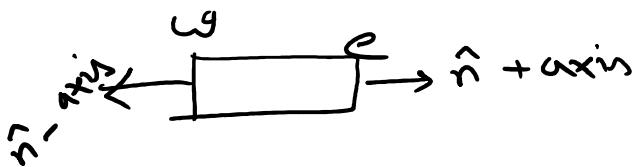
$$\int \frac{d}{dx} \left( k \frac{dT}{dx} \right) dV = 0$$

$$\int \hat{n} \cdot \left( k \frac{dT}{dx} \right) dA = 0 \quad [\hat{n} \rightarrow \text{Normal vector}]$$

Let  
 $\hat{n} \rightarrow +x\text{ axis at E}$   
 $\hat{n} \rightarrow -x\text{ axis at W}$

Now,

$$k_A \frac{dT}{dx} \Big|_C - k_A \frac{dT}{dx} \Big|_W = 0$$



$$k_e A_e \left( \frac{T_E - T_p}{h_{pE}} \right) - k_w A_w \left( \frac{T_p - T_w}{h_{wP}} \right) = 0$$

$k_e \rightarrow$  Thermal conductivity at 'e' face

$k_w \rightarrow$   $\sim$  at 'w' face.

$T_E \rightarrow$  Temperature at E

$T_w \rightarrow$  Temperature at W

$T_p \rightarrow$  Temperature at P

$h_{pE} \rightarrow$  Spacing between P and E

1      r      .      .      L      o      .      .

$h_{PE} \rightarrow$  Spacing between P and E

$h_{PW} \rightarrow$  Spacing between P and W

$$\text{Now, } \alpha_e = \frac{k_e A_e}{h_{PE}} \quad \left. \begin{array}{l} \alpha_p = \frac{k_e A_e + k_w A_w}{h_{PE}} \\ \alpha_w = \frac{k_w A_w}{h_{PW}} \end{array} \right\}$$

Therefore,

$$\boxed{\alpha_e T_E + \alpha_w T_W = \alpha_p T_p}$$

General equation

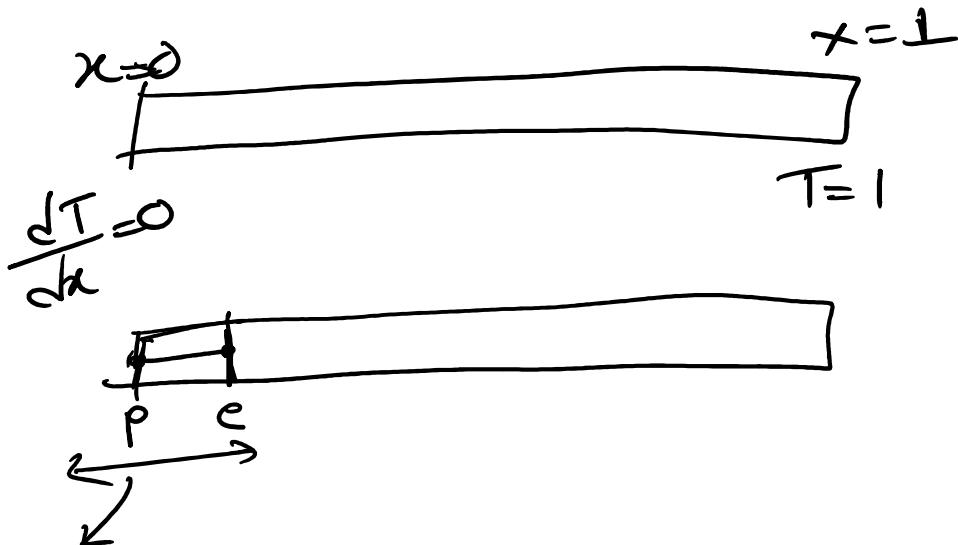
## Dirichlet Boundary Condition

When the value is specified at the boundary. Then it is called Dirichlet Boundary condition

## Neumann boundary condition

When gradient is specified at the boundary then it is called

boundary then it is called  
Neumann boundary condition



$$\int \frac{d}{dx} \left( k \frac{dT}{dx} \right) dV = 0$$

$$\hookrightarrow \int_{\Sigma} \left( k \frac{dT}{dx} \right) dA = 0$$

$$\Rightarrow kA \frac{dT}{dx} \Big|_e - \boxed{kA \frac{dT}{dx} \Big|_p} = 0$$

Given that  $\frac{dT}{dx} \Big|_p = 0$

Then,

$$k_e A_e \left( \frac{T_E - T_p}{h_p F_e} \right) = 0$$

here,  $a_w = 0$

and so,

$$a_E = \frac{k_e A_e}{h_o e}$$

$$\alpha_c = \frac{k_c A_c}{h_{pe}}$$

and  $\alpha_{pf} = \alpha_c T_c$

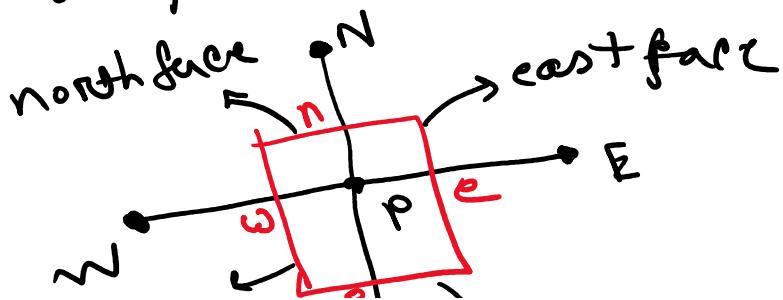
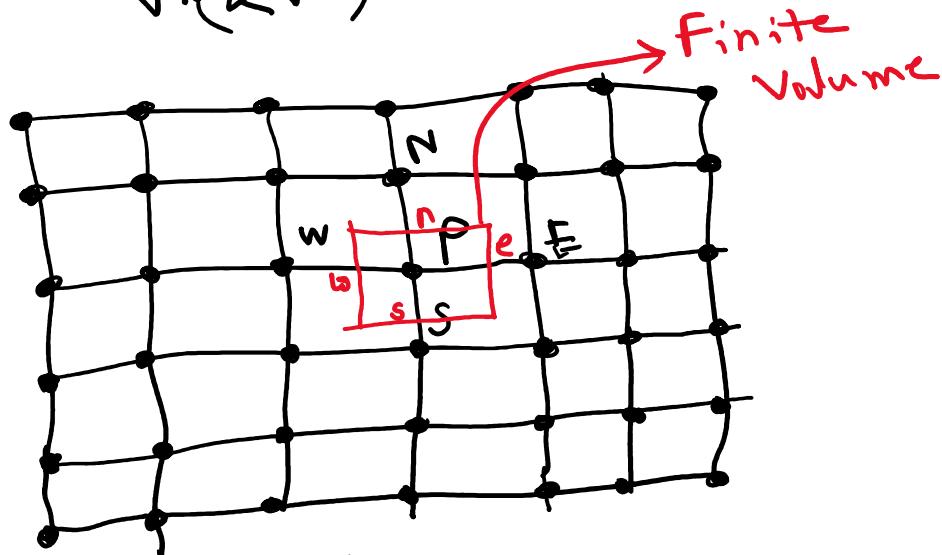
## 2D Heat Diffusion

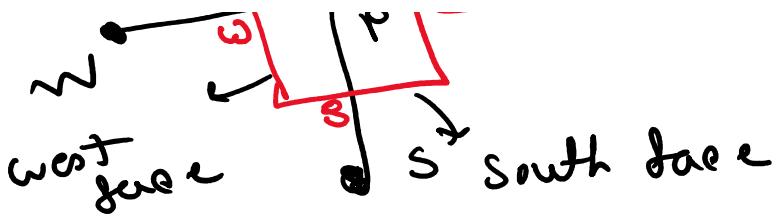
Governing Equation,

$$\text{For 1D} \rightarrow \frac{d}{dx} \left( k \frac{dT}{dx} \right) = 0$$

$$\text{For 2D} \rightarrow \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) = 0$$

$$\nabla \cdot (k \nabla T) = 0$$





Finite Volume,

$$\int \left[ \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) \right] dv = 0$$

Using Gauss divergence theorem,

$$\int_{\hat{V}} \nabla \cdot \left( k \frac{\partial T}{\partial x} + k \frac{\partial T}{\partial y} \right) dA = 0$$

Now considering the four faces.

$$k_A \frac{dT}{dx} \Big|_e - k_A \frac{dT}{dx} \Big|_w + k_A \frac{dT}{dy} \Big|_n - k_A \frac{dT}{dy} \Big|_s = 0$$

$$k_e A_e \left( \frac{T_E - T_P}{h_{PE}} \right) - k_w A_w \left( \frac{T_P - T_W}{h_{WP}} \right) + k_n A_n \left( \frac{T_N - T_P}{h_{PN}} \right) - k_s A_s \left( \frac{T_P - T_S}{h_{PS}} \right) = 0$$

Now we can write,

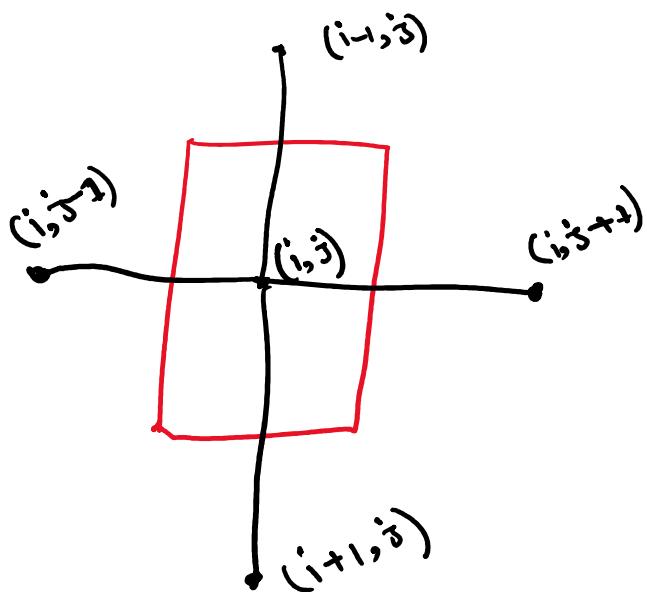
$$\boxed{\alpha_p T_p = \alpha_E T_E + \alpha_W T_W + \alpha_N T_N + \alpha_S T_S}$$

$$\alpha_p T_p = \alpha_E T_E + \alpha_w T_w + \alpha_N T_N + \alpha_s T_s$$

$$\alpha_E = \frac{k_e A_e}{h_{pe}} \quad \alpha_N = \frac{A_n K_n}{h_{pn}}$$

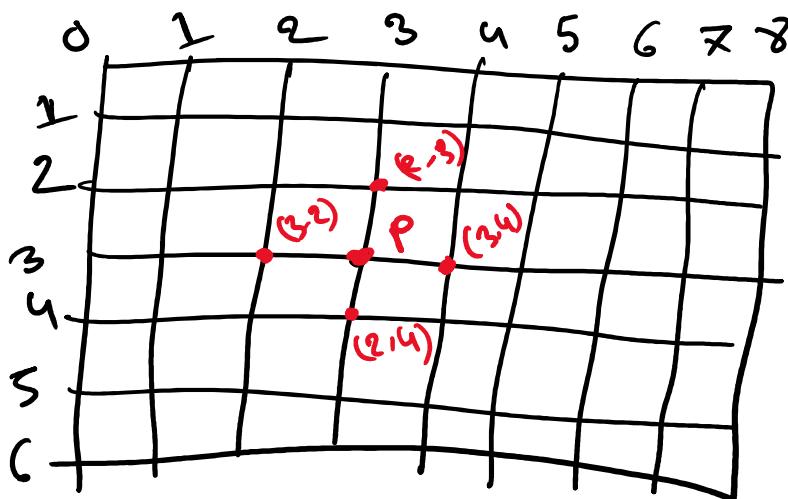
$$\alpha_w = \frac{k_w A_w}{h_{wp}} \quad \alpha_s = \frac{A_s K_s}{h_{ps}}$$

Discretized Governing Equation

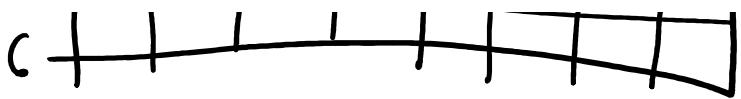


We have,

$$\alpha_p T_p = \alpha_E T_E + \alpha_w T_w + \alpha_N T_N + \alpha_s T_s$$



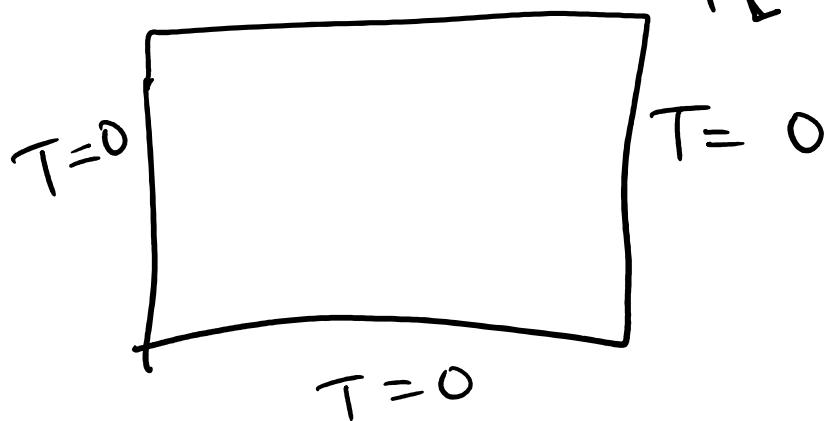
For  $i=3$   
 $j=3$



Now we can write,

$$\alpha_p T_{3,3} = \alpha_E T_{3,4} + \alpha_w T_{3,2} + \alpha_N T_{2,3} + \alpha_S T_{2,4}$$

Problem,  $T = 4 \rightarrow$  can be presented as,  
 $T[0,:] = 1$



## Source Term

Governing equation.

$$\int_V \left[ \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + S \right] dV = 0$$

$$\int \hat{n} \left( k \frac{\partial T}{\partial x} + k \frac{\partial T}{\partial y} \right) dA + \int S dV = 0$$

← Same as previous  
one

$\leftarrow$  Same as P  
one

$$\int s dv = \bar{s} \Delta V$$

$\left\{ \begin{array}{l} \bar{s} \rightarrow \text{Average} \\ \text{value of} \\ \text{source at} \\ \text{control volume} \end{array} \right.$

$\rightarrow$  Constant based source term

$\rightarrow$  Not constant

Source term linearization,

$$\bar{s} \nabla V = S_u + S_p T_p$$

$\swarrow \quad \downarrow$

Constant value      Non constant

Now we can write,

$$k_A \frac{dT}{dx} \Big|_c - k_A \frac{dT}{dx} \Big|_w + k_A \frac{dT}{dy} \Big|_o - k_A \frac{dT}{dy} \Big|_s + S_u + S_p T_p = 0$$

$$\Rightarrow k_e A_c \left( \frac{T_c - T_p}{h_{pe}} \right) - k_w A_w \left( \frac{T_p - T_w}{h_{pw}} \right) + k_n A_n \left( \frac{T_n - T_p}{h_{pnw}} \right) - k_s A_s \left( \frac{T_p - T_s}{h_{ps}} \right) + S_u + S_p T_p = 0$$

$$\Rightarrow \alpha_c = \left( \frac{k_e A_c}{h_{pe}} \right) \quad \alpha_w = \left( \frac{k_w A_w}{h_{pw}} \right)$$

$$\Rightarrow \alpha_e = \left( \frac{1}{h_{pe}} \right) \quad \alpha_w = \left( \frac{1}{h_{pw}} \right)$$

$$\alpha_n = \left( \frac{k_n A_n}{h_{pn}} \right) \quad \alpha_{sp} = \left( \frac{k_s A_s}{h_{ps}} \right)$$

$$\alpha_p = \alpha_e + \alpha_w + \alpha_n + \alpha_{sp} - S_p$$

$$\boxed{\alpha_p T_p = \alpha_e T_e + \alpha_w T_w + \alpha_n T_N + \alpha_{sp} T_s - S_p}$$

Final Governing equation

$$\boxed{S = h q \times A} \rightarrow \begin{aligned} q &\rightarrow \text{Heat source per unit volume} \\ A &\rightarrow \text{Area} \\ h &\rightarrow \text{Spacing} \end{aligned}$$

We are considering here

constant source term.

## 1D Convection [with Pecllet number]

$$\alpha_p T_p = \alpha_e T_e + \alpha_w T_w$$

$$\alpha_p / \rho = \gamma c / h$$

$$\alpha_c = \frac{\gamma}{h} + \frac{\rho u}{2} = \alpha_w$$

[Taking  $\gamma$ ,  $h$ ,  $\rho$  and  $u$  as constant]

$\gamma \rightarrow$  diffusivity

$h \rightarrow$  grid spacing

$\rho \rightarrow$  density

$u \rightarrow$  velocity

Peclet number needs to be  
remain below 2

$$Pe = \frac{\rho * u * h}{\gamma}$$

## Upwind Scheme

Steady equation,

$$\frac{d}{dx} (\rho u \phi) = \frac{d}{dx} \left( \Gamma \frac{\partial \phi}{\partial x} \right)$$

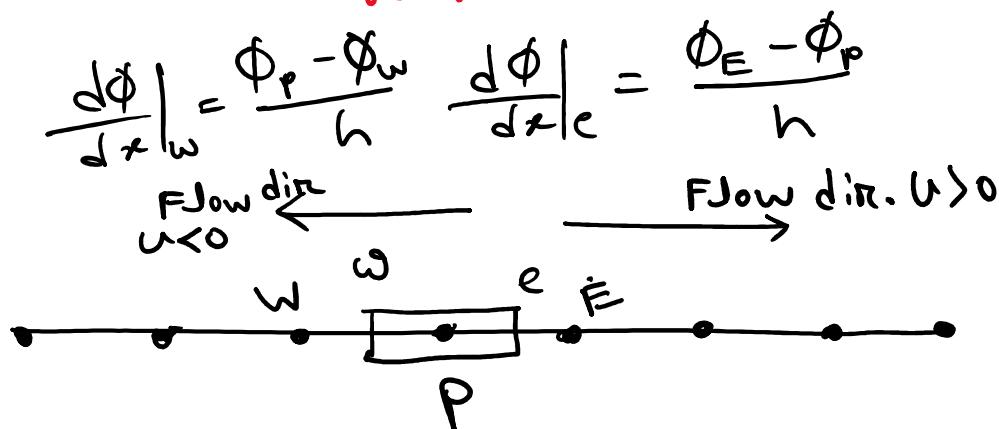
$$\left. \frac{d\phi}{dx} \right|_e - \left. \frac{d\phi}{dx} \right|_w = (\rho u \phi)_e - (\rho u \phi)_w$$

using gauss divergence theorem

$$\Gamma \left. \frac{d\phi}{dx} \right|_e - \Gamma \left. \frac{d\phi}{dx} \right|_w = (\rho u \phi)_e - (\rho u \phi)_w$$

For pure conduction  $\rightarrow$  Central

differential scheme



The upwind scheme says,

$$\phi_c = \begin{cases} \phi_p, & u > 0 \text{ [Flow is from } P \text{ to } E] \\ \phi_e, & u < 0 \text{ [Flow is from } E \text{ to } P] \end{cases}$$

Again,

$$\alpha_w = \begin{cases} \alpha_w & , u > 0 \\ \alpha_p & , u < 0 \end{cases}$$

We have equation,

We have equation,

$$(\rho u \phi A)_e - (\rho u \phi A)_w = \Gamma A \frac{d\phi}{dx} \Big|_e - \Gamma A \frac{d\phi}{dx} \Big|_w$$

Taking  $A$  as constant  
And  $F = \rho u$  Strength of convection

Case-1  $\rightarrow u > 0$

$$F_e \phi_p - F_w \phi_w = D_c (\phi_E - \phi_p) - D_w (\phi_p - \phi_w)$$

$$\Rightarrow \phi_p = \frac{(D_w + F_w) \phi_w + D_c \phi_E}{D_w + D_c + F_c}$$

Case -2  $\rightarrow u < 0$

$$F_e \phi_E - F_w \phi_p = D_c (\phi_E - \phi_p) - D_w (\phi_p - \phi_w)$$

$$\Rightarrow D_c \phi_p + D_w \phi_p - F_w \phi_p = D_c \phi_E + F_w \phi_E$$

$$\Rightarrow \phi_p = \frac{(D_c - F_c) \phi_E + D_w \phi_w}{D_c + D_w - F_w}$$

$$- \gamma P = D_E + D_W - F_W$$

For upwind scheme general equation can be written as,

$$\alpha_W = P_W + \max(F_W, 0)$$

$$\alpha_E = D_E + \max(F_E, 0)$$