Numerical Solution

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Numerical Solution

- Governing equations are partial differential equations
- Variables are fluid properties
- For numerical solution, equations must be transformed into algebraic form
- i.e. Equations must contain only numbers

Transformation

- Transformation of partial differential equations into algebraic form is called discretization
- Each term of equation must be transformed

Discretization

- Three major techniques:
- Finite volume
- Finite element
- Finite difference

- Flotherm uses finite volume method

Finite Volume

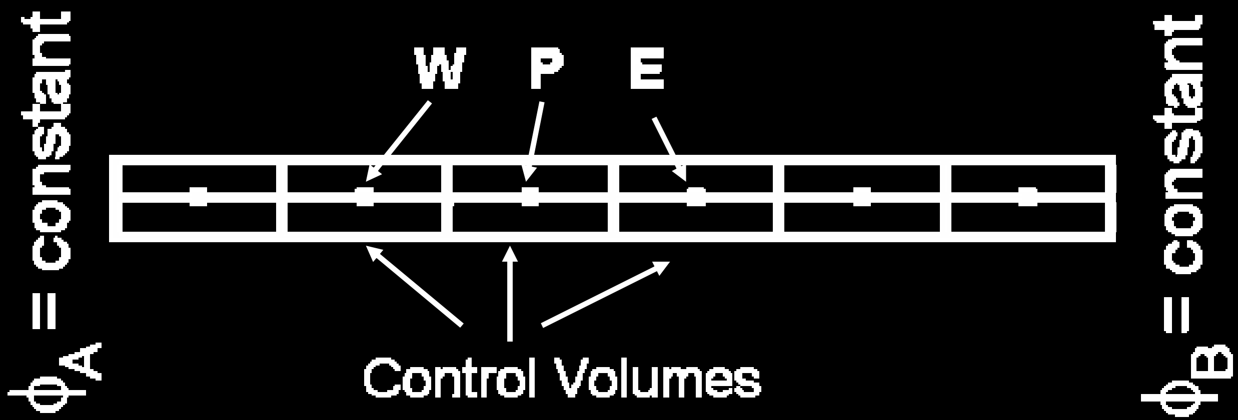
- Consider the simple case of steady-state 1-D diffusion
- Remove the convection and transient terms

$$\frac{\partial}{\partial t}(\rho\varphi)+div(\rho U\varphi-\Gamma grad\varphi)=S_\varphi$$

Finite Volume

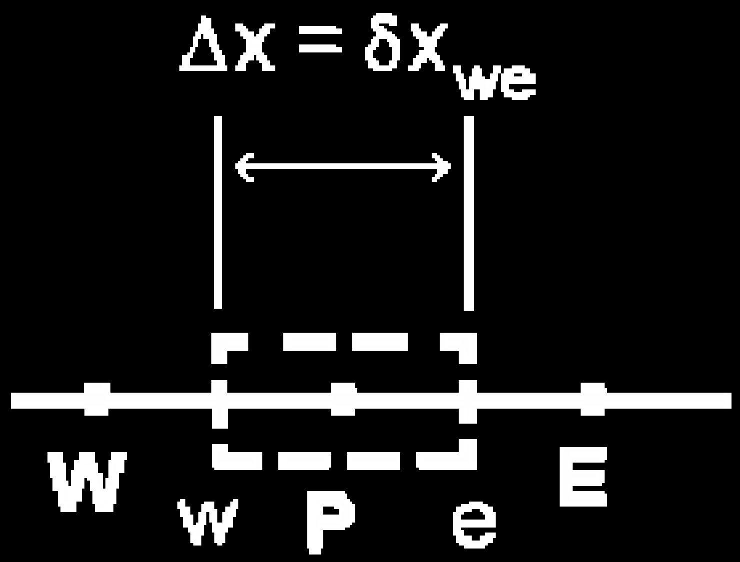
- In one dimension:

$$\frac{d}{dx}\Gamma\frac{d\varphi}{dx}+S_{\varphi}=0$$



Finite Volume

- W,E are adjacent cell centres, w,e are adjacent cell faces



Discretization

- Governing equation is integrated to give a discretized equation at the cell centre

$$\int_{CV} \frac{d}{dx}\left(\Gamma \frac{d\varphi}{dx}\right) dV + \int_{CV} S_{\varphi} dV = 0$$

$$\left(\Gamma A \frac{d\varphi}{dx}\right)_e - \left(\Gamma A \frac{d\varphi}{dx}\right)_w + \overline{S}\Delta V = 0$$

Discretization

- Need the diffusion coefficient and the gradient at each cell face
- Use harmonic average:

$$\Gamma_w^{-1} = \left(\frac{\Gamma_W}{2}\right)^{-1} + \left(\frac{\Gamma_P}{2}\right)^{-1}$$

$$\Gamma_e^{-1} = \left(\frac{\Gamma_P}{2}\right)^{-1} + \left(\frac{\Gamma_E}{2}\right)^{-1}$$

Discretization

- For the gradients:

$$\left(\Gamma A \frac{d\varphi}{dx}\right)_e = \Gamma_e A_e \left(\frac{\varphi_E - \varphi_P}{\delta x_{PE}}\right)$$

$$\left(\Gamma A \frac{d\varphi}{dx}\right)_w = \Gamma_w A_w \left(\frac{\varphi_P - \varphi_W}{\delta x_{WP}}\right)$$

Discretization

- The source term may be a function of ϕ
- In this case, a linear function is used:

$$\overline{S}\Delta V = \left(S_u + S_p \varphi_P\right)$$

Discretization

- The discretized equation may be written:

$$\Gamma_e A_e \left(\frac{\varphi_E - \varphi_P}{\delta x_{PE}} \right) - \Gamma_w A_w \left(\frac{\varphi_P - \varphi_W}{\delta x_{WP}} \right) + \left(S_u + S_p \varphi_P \right) = 0$$

Discretization

- Rearrange:

$$\left(\frac{\Gamma_e}{\delta x_{PE}}A_e+\frac{\Gamma_w}{\delta x_{WP}}A_w-S_p\right)\varphi_P=\left(\frac{\Gamma_w}{\delta x_{WP}}A_w\right)\varphi_W+\left(\frac{\Gamma_e}{\delta x_{PE}}A_e\right)\varphi_E+S_u$$

Discretization

- Now, we have an algebraic equation relating field values at P with values at W and E

$$a_P \varphi_P = a_W \varphi_W + a_E \varphi_E + S_u$$

Discretization

- Need to set up equations at each point in the domain
- At domain boundaries, use boundary conditions

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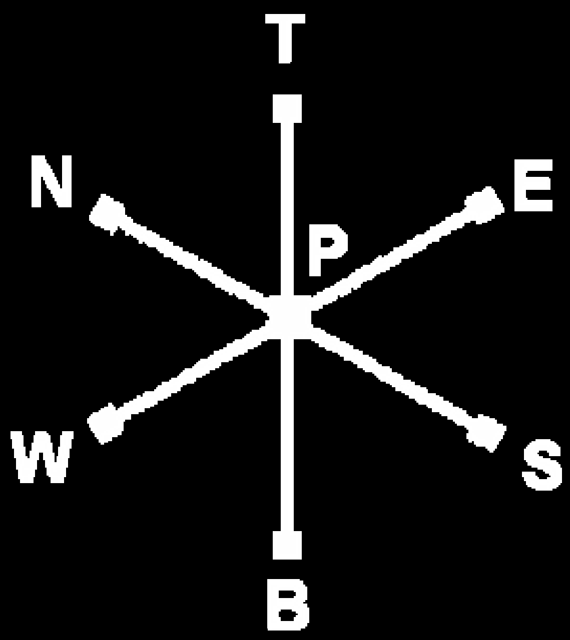
Discretization

- In 3-D:
- P has 6 neighbours
- North, South
- East, West
- Top, Bottom



Discretization

- Full equation in 3-D

$$a_P \varphi_P = a_W \varphi_W + a_E \varphi_E + a_N \varphi_N +$$

$$a_S \varphi_S + a_T \varphi_T + a_B \varphi_B + S_u$$

Discretization

- Convection

$$div\left(\rho U\varphi - \Gamma grad\varphi\right) = S_{\varphi}$$

Discretization

- Steady, 1-D convection and diffusion:

$$\frac{d}{dx}\left(\rho U \varphi\right) = \frac{d}{dx}\left(\Gamma \frac{d\varphi}{dx}\right)$$

- Continuity:

$$\frac{d}{dx}\left(\rho U\right) = 0$$

Discretization

- Integrating over a control volume:

$$\left(\rho UA\varphi\right)_e - \left(\rho UA\varphi\right)_w = \left(\Gamma A \frac{d\varphi}{dx}\right)_e - \left(\Gamma A \frac{d\varphi}{dx}\right)_w$$

$$\left(\rho UA\right)_e - \left(\rho UA\right)_w = 0$$

Discretization

- Now, define:

$$F = \rho U$$

$$D = \frac{\Gamma}{\delta x}$$

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Discretization

- Substituting:

$$F_e \varphi_e - F_w \varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$F_e - F_w = 0$$

Discretization

- So far, we have used central differencing
- This scheme can be unstable if the Peclet number for a cell is greater than 2

$$Pe = \frac{F}{D}$$

Discretization

- Upwind differencing
- The convected value of ϕ at the cell face depends on the direction of flow

$$\varphi_w = \varphi_W \quad and \quad \varphi_e = \varphi_P$$

Discretization

- Upwind discretization is used by FLOTHERM

Discretization

- Non-uniform grid leads to large range of matrix terms in solution
- But, need fine grid to resolve boundary layers

Discretization

- False diffusion is consequence of upwind scheme of discretization