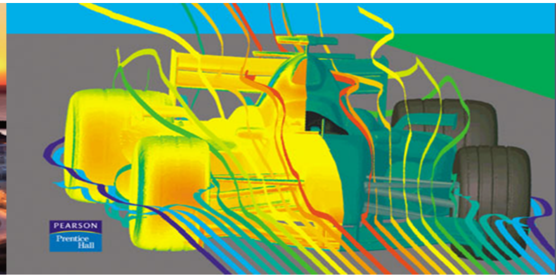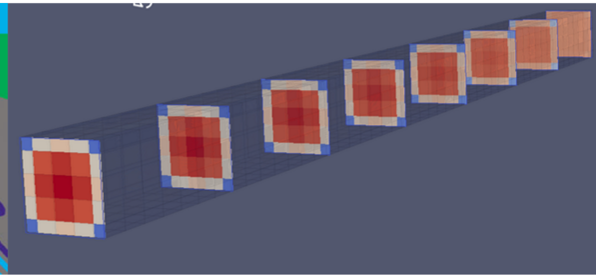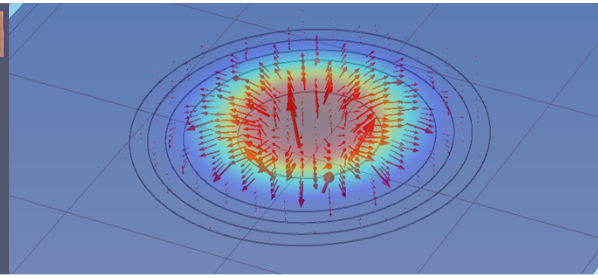

COMPUTATIONAL NUCLEAR THERMAL HYDRAULICS

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CHAPTER5.
THE FINITE VOLUME METHOD FOR CONVECTION-DIFFUSION PROBLEMS

Review

$$\frac{\partial(\rho\phi)}{\partial t} + \operatorname{div}(\rho\phi\mathbf{u}) = \operatorname{div}(\Gamma \operatorname{grad} \phi) + S_\phi \qquad \operatorname{div}(\Gamma \operatorname{grad} \phi) + S_\phi = 0$$

$$\int_{CV} \operatorname{div}(\Gamma \operatorname{grad} \phi)\mathrm{d}V + \int_{CV} S_\phi \mathrm{d}V = \int_A \mathbf{n} \,.\, (\Gamma \operatorname{grad} \phi)\mathrm{d}A + \int_{CV} S_\phi \mathrm{d}V = 0 \qquad \int_S f dS = \sum_k f_k S_k$$

$$\left(\frac{\Gamma_e}{\delta x_{PE}}A_e + \frac{\Gamma_w}{\delta x_{WP}}A_w - S_p\right)\phi_P = \left(\frac{\Gamma_w}{\delta x_{WP}}A_w\right)\phi_W + \left(\frac{\Gamma_e}{\delta x_{PE}}A_e\right)\phi_E + S_u$$

$$\boxed{a_P\phi_P = a_W\phi_W + a_E\phi_E + S_u}$$

a_W	a_E	a_P
$\frac{\Gamma_w}{\delta x_{WP}}A_w$	$\frac{\Gamma_e}{\delta x_{PE}}A_e$	$a_W + a_E - S_P$

Step 1: grid generation
Step 2: discretization
Step 3: Modification of the discretized equation
for the boundary cells
Step 4: Set-up systems of linear equations
Step 5: Linear system solver

Contents

Introduction

- Steady-state convection-diffusion equation

$$\frac{\partial(\rho\phi)}{\partial t} + \operatorname{div}(\rho\phi\mathbf{u}) = \operatorname{div}(\Gamma \operatorname{grad} \phi) + S_\phi$$

$$\boxed{\operatorname{div}(\rho\mathbf{u}\phi)} = \operatorname{div}(\Gamma \operatorname{grad} \phi) + S_\phi$$

- Integral type governing equation

$$\int_A \mathbf{n} \cdot (\rho\phi\mathbf{u})\mathrm{d}A = \int_A \mathbf{n} \cdot (\Gamma \operatorname{grad} \phi)\mathrm{d}A + \int_{CV} S_\phi \mathrm{d}V$$

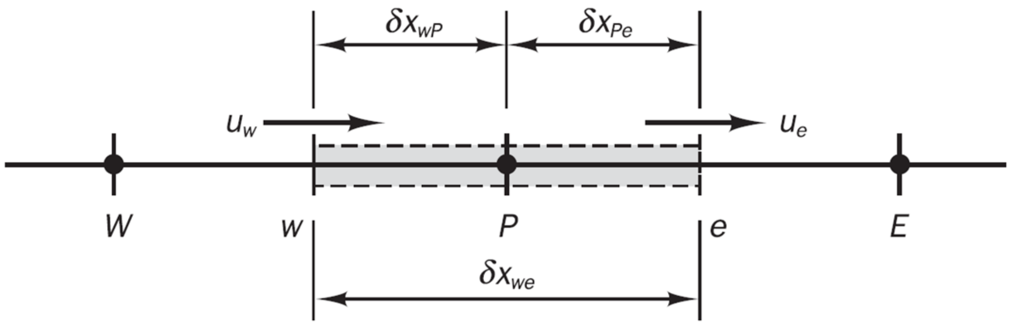
- The main problem in the discretization of the convective terms is the calculation of ϕ at CV faces and its convective flux across these boundaries.
- Diffusion process affects the distribution of ϕ in all directions.
- Convection spreads influence only in the flow direction.
- This sets a limit on the grid size for stable convection-diffusion calculations with central difference method.

Contents

Steady 1D convection and diffusion

- Without source term

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



  - From the continuity,

$$\frac{\mathrm{d}(\rho u)}{\mathrm{d}x} = 0$$

- Integration and discretization

$$\int_V \frac{d}{dx}(\rho \phi \mathbf{u}) dV = \int_A \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA =$$

$$(\rho u A \phi)_e - (\rho u A \phi)_w = \left(\Gamma A \frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_e - \left(\Gamma A \frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_w \qquad (\rho u A)_e - (\rho u A)_w = 0$$

Steady 1D convection and diffusion

- Convective mass flux and diffusion conductance at cell faces

$$(\rho u A\phi)_e - (\rho u A\phi)_w = \left(\Gamma A\frac{d\phi}{dx}\right)_e - \left(\Gamma A\frac{d\phi}{dx}\right)_w \qquad (\rho u A)_e - (\rho u A)_w = 0$$

$$F = \rho u \qquad D = \frac{\Gamma}{\delta x}$$

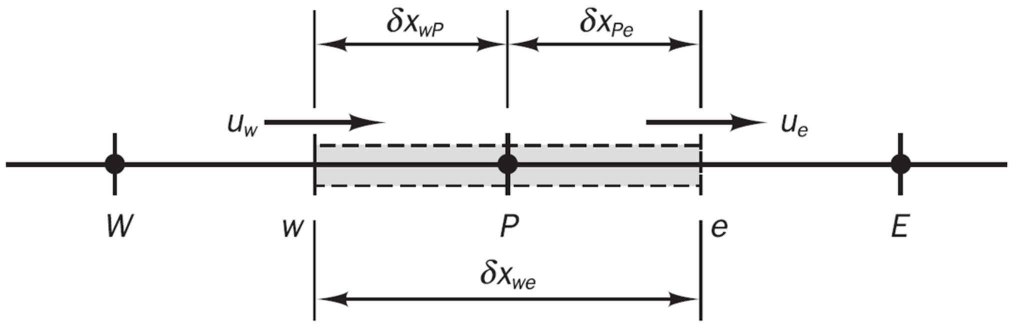
$$F_w = (\rho u)_w \qquad F_e = (\rho u)_e \qquad D_w = \frac{\Gamma_w}{\delta x_{WP}} \qquad D_e = \frac{\Gamma_e}{\delta x_{PE}}$$

- For 1D, equal cell face area

$$F_e\boxed{\phi_e} - F_w\boxed{\phi_w} = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

$$F_e - F_w = 0$$

Assume that the velocity field is 'somehow known'



Contents

CDS

- Central difference scheme
  - Works well for diffusion terms
  - For convective terms?

- For uniform grid,

$$\phi_e = (\phi_P + \phi_E)/2 \qquad \phi_w = (\phi_W + \phi_P)/2$$

$$F_e\phi_e - F_w\phi_w = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

$$\frac{F_e}{2}(\phi_P + \phi_E) - \frac{F_w}{2}(\phi_W + \phi_P) = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

$$\boxed{}\,\phi_P = \boxed{}\,\phi_W + \boxed{}\,\phi_E$$

CDS

- For uniform grid,

$$\left[\left(D_w - \frac{F_w}{2}\right) + \left(D_e + \frac{F_e}{2}\right)\right]\phi_P = \left(D_w + \frac{F_w}{2}\right)\phi_W + \left(D_e - \frac{F_e}{2}\right)\phi_E$$

$$\phi_P = \left(D_w + \frac{F_w}{2}\right)\phi_W + \left(D_e - \frac{F_e}{2}\right)\phi_E$$

$$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

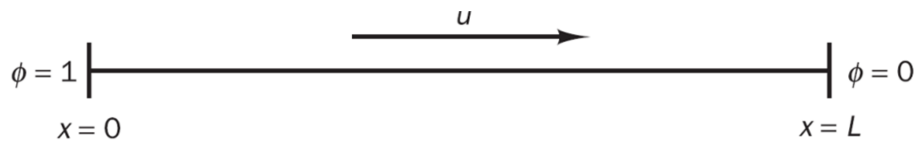
a_W	a_E	a_P

a_W	a_E	a_P
$\frac{\Gamma_w}{\delta x_{WP}}A_w$	$\frac{\Gamma_e}{\delta x_{PE}}A_e$	$a_W + a_E - S_P$

The same general form with the pure diffusion problem except the additional coefficients for convection

CDS

- Example 5.1
  - A property ϕ is transported by convection and diffusion through the 1D domain.
  - Using CDS, find the distribution of ϕ for L =1, ρ = 1, Γ = 0.1.
  - Case 1: u = 0.1 m/s (use 5 CV's)
  - Case 2: u = 2.5 m/s (use 5 CV's)
  - Case 3: u = 2.5 m/s (20 CV's)
  - Analytical solution for this problem,



Problem description

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp(\rho u x/\Gamma) - 1}{\exp(\rho u L/\Gamma) - 1}$$

Derive by yourself!

$$\rho u \frac{d\phi}{dx} - \Gamma \frac{d^2\phi}{dx^2} = 0 \qquad \phi'' - \frac{\rho u}{\Gamma}\phi' = 0 \qquad \phi(0) = \phi_0 \ , \ \phi(L) = \phi_L$$

- Example 5.1
  - Five cells: $\delta x = 0.2 \text{ m}$

$$\frac{F_e}{2}(\phi_P + \phi_E) - \frac{F_w}{2}(\phi_W + \phi_P) = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

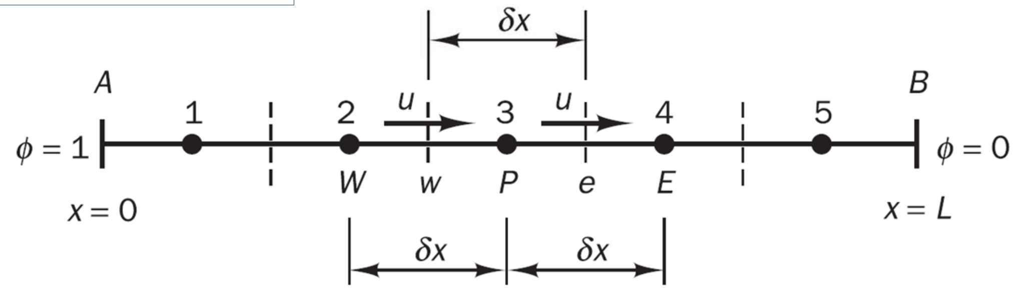
$$F = \rho u, \; D = \Gamma/\delta x \qquad F_e = F_w = F \text{ and } D_e = D_w = D$$

  - For cell 1

$$F_e\phi_e - F_w\phi_w = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) \qquad \phi_w = \phi_A \;, F_w = F_A = F$$

$$\boxed{\qquad\qquad} - F_A\phi_A = D_e(\phi_E - \phi_P) - \boxed{\qquad\qquad}$$

$$D_A = \frac{\Gamma}{0.5\delta x} = 2\frac{\Gamma}{\delta x} = 2D$$



- Example 5.1
  - For cell 1

$$\frac{F_e}{2}(\phi_P + \phi_E) - F_A\phi_A = D_e(\phi_E - \phi_P) - D_A(\phi_P - \phi_A)$$

$$F_w = F_A = F$$

$$\left(\frac{F_e}{2} + D_e + D_A\right)\phi_P = \left(D_e - \frac{F_e}{2}\right)\phi_E + 0\cdot\phi_W + \left(D_A + F_A\right)\phi_A$$

$$D_A = 2D$$

$$\left(\frac{F}{2} + 3D\right)\phi_P = \left(D - \frac{F}{2}\right)\phi_E + 0\cdot\phi_W + \left(2D + F\right)\phi_A$$

$$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + S_u$$

$$a_P = a_W + a_E + (F_e - F_w) - S_P$$

For internal cells

a_W	a_E	a_P
$D_w + \frac{F_w}{2}$	$D_e - \frac{F_e}{2}$	$a_W + a_E + (F_e - F_w)$

- Example 5.1
  - For cell 1

$$\left(\frac{F}{2}+3D\right)\phi_P=\left(D-\frac{F}{2}\right)\phi_E+0\cdot\phi_W+(2D+F)\phi_A$$

$$a_P\phi_P=a_W\phi_W+a_E\phi_E+S_u \qquad S_u=(2D+F)\phi_A$$

$$a_P=a_W+a_E+(F_e-F_w)-S_P \qquad S_P=-(2D+F)$$

Node	a_W	a_E	S_P	S_u
1	0	$D-F/2$	$-(2D+F)$	$(2D+F)\phi_A$
2, 3, 4	$D+F/2$	$D-F/2$	0	0
5	$D+F/2$	0	$-(2D-F)$	$(2D-F)\phi_B$

- Example 5.1
  - For cell 2~4

$$\frac{F_e}{2}(\phi_P + \phi_E) - \frac{F_w}{2}(\phi_W + \phi_P) = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

$$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

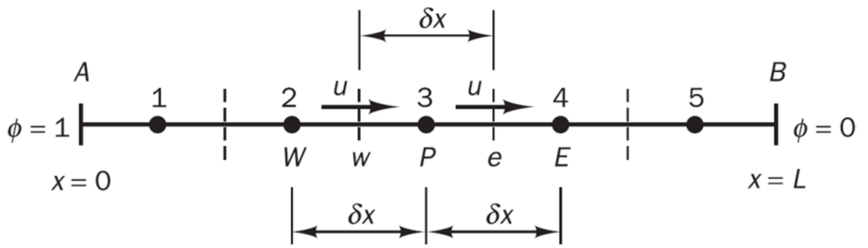
For internal cells

a_W	a_E	a_P
$D_w + \frac{F_w}{2}$	$D_e - \frac{F_e}{2}$	$a_W + a_E + (F_e - F_w)$

Node	$\boldsymbol{a_W}$	$\boldsymbol{a_E}$	$\boldsymbol{S_P}$	$\boldsymbol{S_u}$
1	0	$D - F/2$	$-(2D + F)$	$(2D + F)\phi_A$
2, 3, 4	$D + F/2$	$D - F/2$	0	0
5	$D + F/2$	0	$-(2D - F)$	$(2D - F)\phi_B$

CDS

- Example 5.1
  - For cell 5



$$F_e\phi_e - F_w\phi_w = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

$$F_B\phi_B - \frac{F_w}{2}(\phi_P + \phi_W) = D_B(\phi_B - \phi_P) - D_w(\phi_P - \phi_W)$$

$$\left(-\frac{F}{2} + 3D\right)\phi_P = 0 \cdot \phi_E + \left(D + \frac{F}{2}\right)\phi_W + (2D - F)\phi_B$$

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + S_u \qquad S_u = (2D - F)\phi_B$$

$$a_P = a_W + a_E + (F_e - F_w) - S_P \qquad S_P = -(2D - F)$$

Node	a_W	a_E	S_P	S_u
1	0	$D - F/2$	$-(2D + F)$	$(2D + F)\phi_A$
2, 3, 4	$D + F/2$	$D - F/2$	0	0
5	$D + F/2$	0	$-(2D - F)$	$(2D - F)\phi_B$

- Example 5.1
  - Case-1
    - Matrix form of the linear equations

$$u = 0.1\ \mathrm{m/s} \qquad F = \rho u = 0.1 \qquad D = \Gamma/\delta x = 0.1/0.2 = 0.5$$

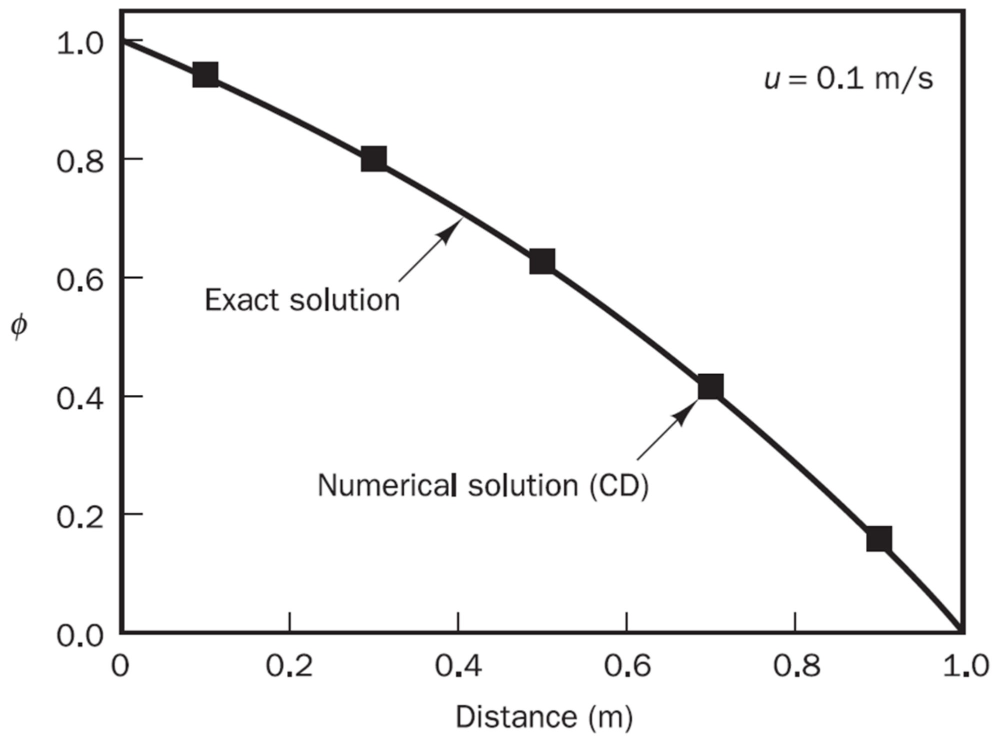
$$\phi_A = 1 \text{ and } \phi_B = 0$$

$$\begin{bmatrix} 1.55 & -0.45 & 0 & 0 & 0 \\ -0.55 & 1.0 & -0.45 & 0 & 0 \\ 0 & -0.55 & 1.0 & -0.45 & 0 \\ 0 & 0 & -0.55 & 1.0 & -0.45 \\ 0 & 0 & 0 & -0.55 & 1.45 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 1.1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 0.9421 \\ 0.8006 \\ 0.6276 \\ 0.4163 \\ 0.1579 \end{bmatrix}$$

CDS

- Example 5.1
  - Case-1
    - Comparison with the analytical solution
    - Error max.: ~ 5 %

Good enough !



CDS

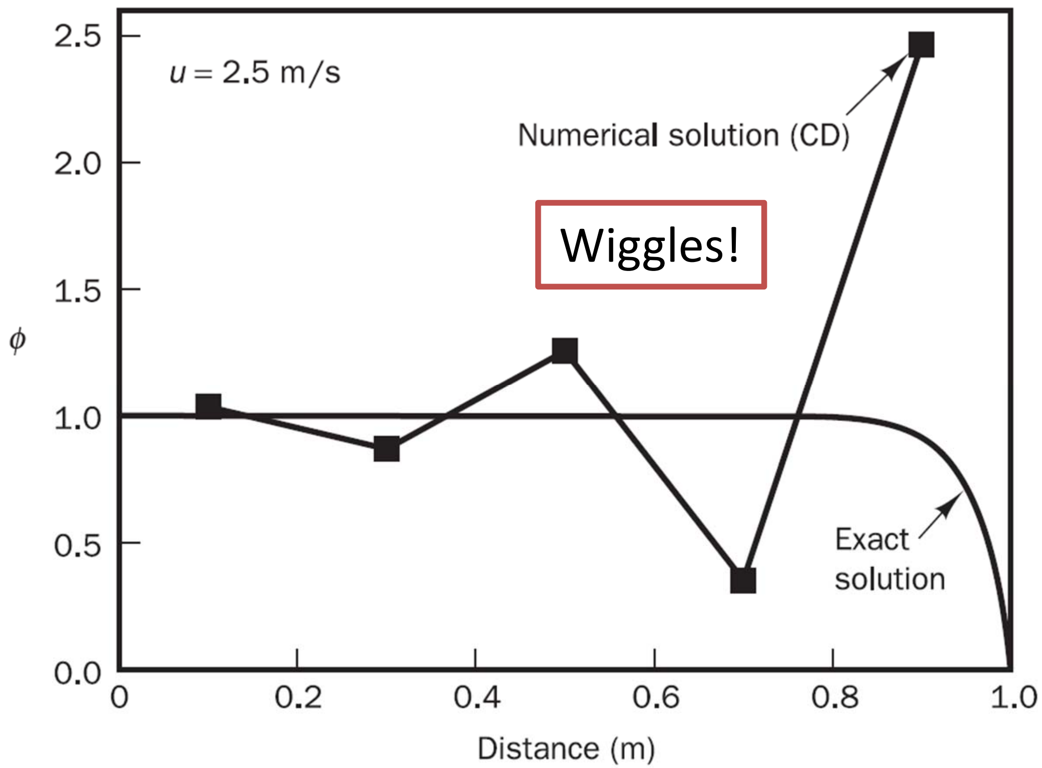
- Example 5.1
  - Case-2
    - Matrix form of the linear equations

25 times faster flow than case-1

$$u = 2.5 \text{ m/s} \qquad F = \rho u = 2.5 \qquad D = \Gamma/\delta x = 0.1/0.2 = 0.5$$

$$\phi_A = 1 \text{ and } \phi_B = 0$$

Unstable !



Max. error≈170%

CDS

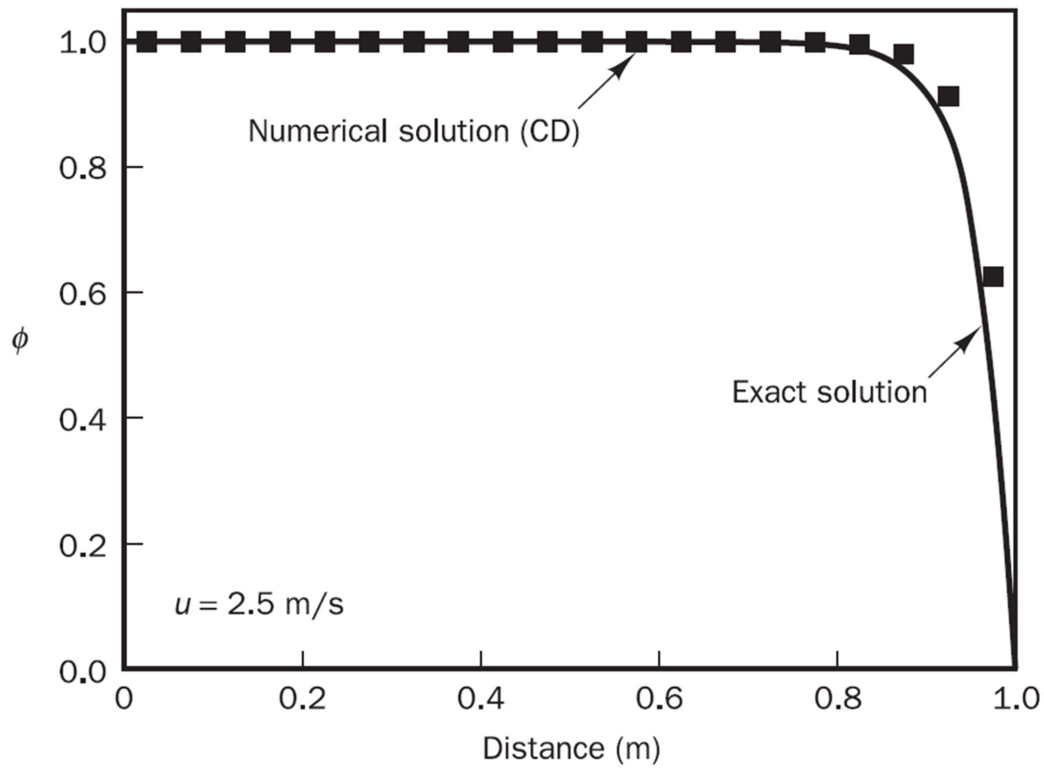
- Example 5.1
  - Case-3
    - Matrix form of the linear equations

4 times more cells than case-2

$$u = 2.5\ \mathrm{m/s} \quad \delta x = 0.05,\ F = \rho u = 2.5 \quad D = \Gamma/\delta x = 0.1/0.05 = 2.0$$

$$\phi_A = 1 \text{ and } \phi_B = 0$$

Good enough ?



- Example 5.1
  - Discussion
    - Case-1, stable, $F=0.1, D=0.5, F/D=0.2$
    - Case-2, unstable $F=2.5, D=0.5, F/D=5$
    - Case-3, stable $F=2.5, D=2, F/D=1.25$
  - CDS
    - Seems to yield accurate results when the F/D ratio is low!
    - Large F: highly convective
    - Small F: diffusive

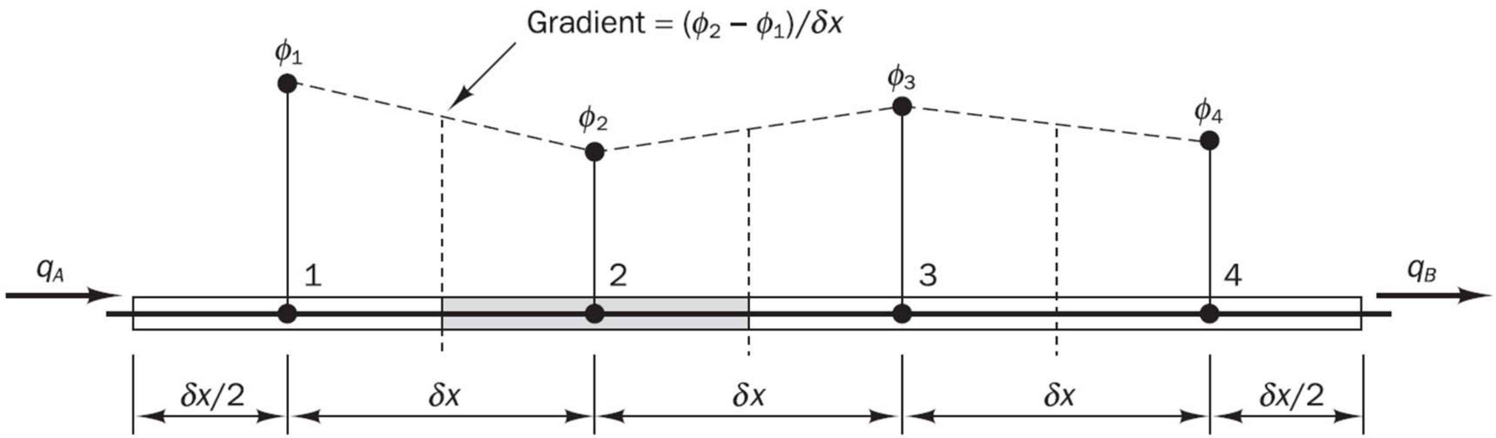
Contents

Properties of discretization schemes

- Limitation of the computational meshes
  - Numerical results may be obtained that are indistinguishable from the 'exact' solution of the transport equation when the number of computational cells is infinitely large, irrespective of the differencing method used.
  - However, in practical calculations we can only use a finite number of cells.
  - Our numerical results will only be physically realistic when the discretization scheme has certain fundamental properties.

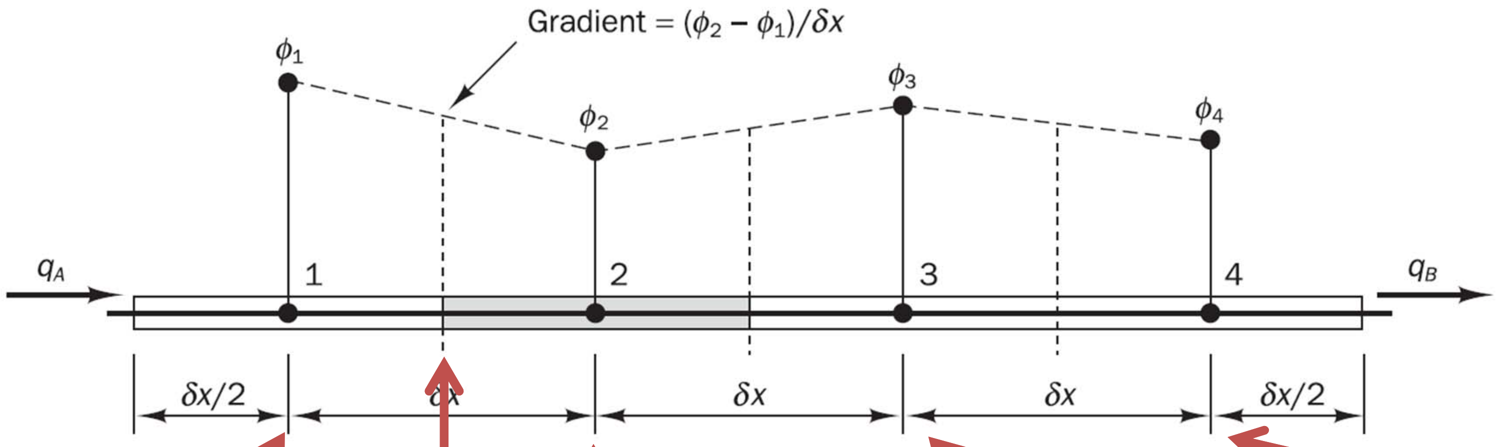
Properties of discretization schemes

- Conservativeness
  - To ensure conservation of ϕ for the whole solution domain
    - The flux of ϕ leaving a CV across a certain face must be equal to the flux of ϕ entering the adjacent CV through the same face.
  - To achieve this
    - The flux through a common face must be represented in a consistent manner



Properties of discretization schemes

- Conservativeness

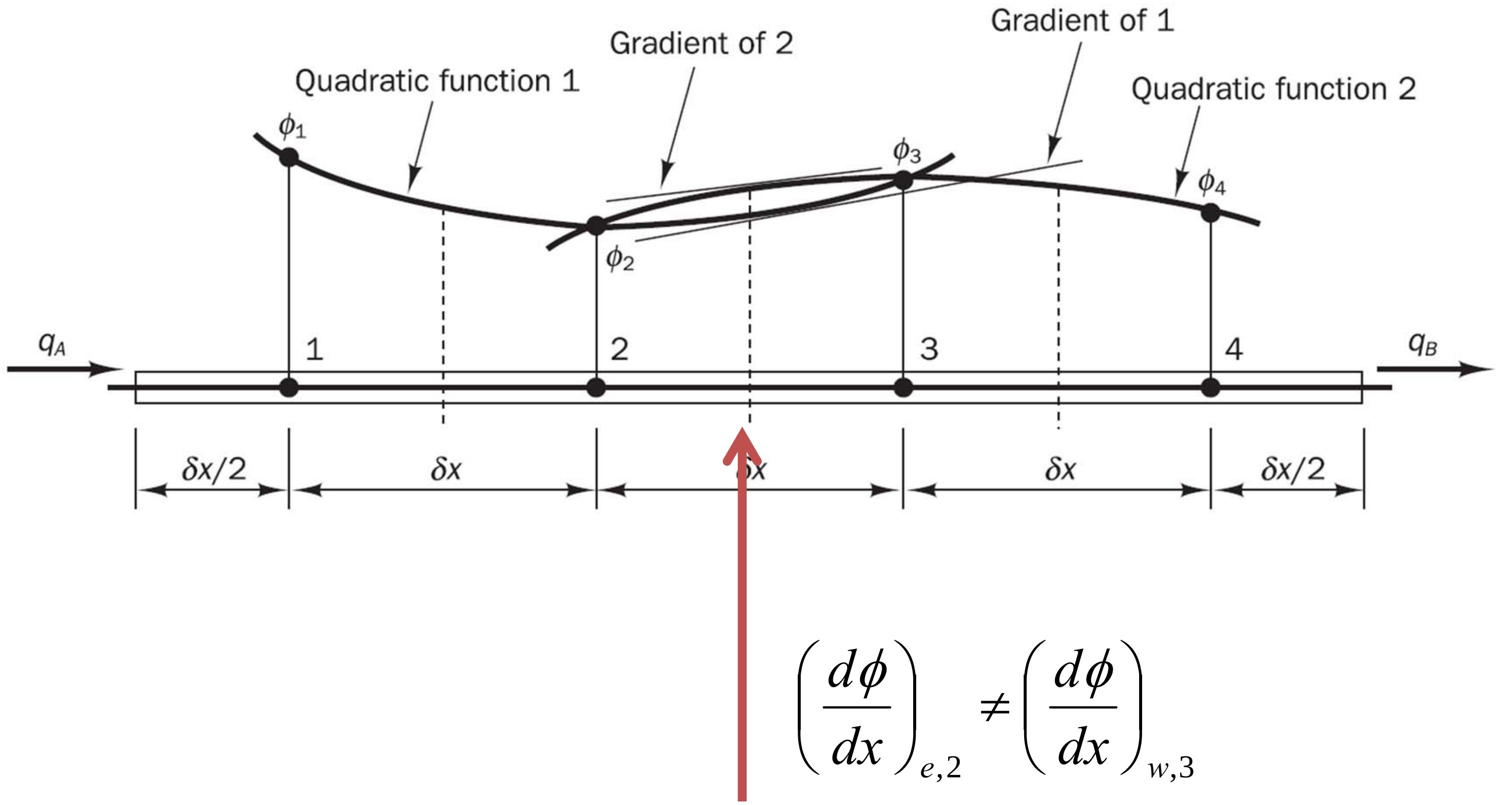


$$\left[\Gamma_{e_1}\frac{(\phi_2-\phi_1)}{\delta x} - q_A\right] \quad \left[\Gamma_{e_2}\frac{(\phi_3-\phi_2)}{\delta x} - \Gamma_{w_2}\frac{(\phi_2-\phi_1)}{\delta x}\right] \quad \left[\Gamma_{e_3}\frac{(\phi_4-\phi_3)}{\delta x} - \Gamma_{w_3}\frac{(\phi_3-\phi_2)}{\delta x}\right] \quad \left[q_B - \Gamma_{w_4}\frac{(\phi_4-\phi_3)}{\delta x}\right]$$

$$\Gamma_{e_1}\frac{(\phi_2-\phi_1)}{\delta x} \qquad \Gamma_{w_2}\frac{(\phi_2-\phi_1)}{\delta x}$$

Properties of discretization schemes

- Conservativeness
  - Inconsistent use of a quadratic interpolation formula
    - East face of CV2: CVs 1,2,3
    - West face of CV3: CVs 2,3,4
  - Overall conservation is not satisfied.



$$\left(\frac{d\phi}{dx}\right)_{e,2} \neq \left(\frac{d\phi}{dx}\right)_{w,3}$$

Properties of discretization schemes

- Boundedeness
  - Sufficient condition for a convergent iterative method

$$a_p' = a_p - S_p = a_W + a_E + (F_e - F_w) - S_p$$

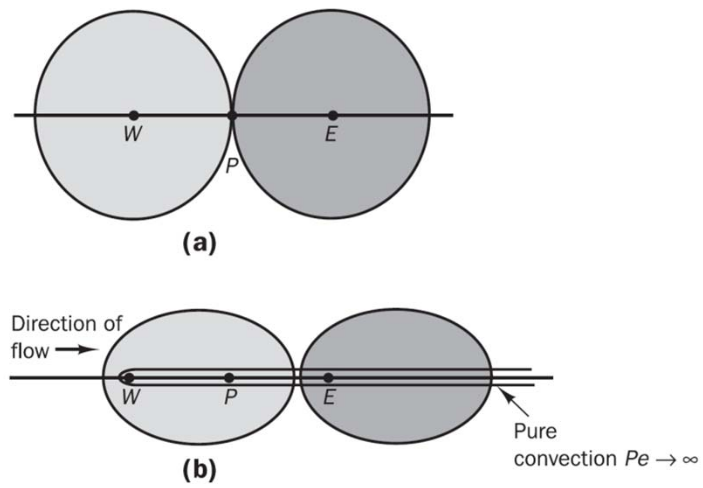
    - Diagonally dominant

  - For diagonal dominance, $S_p < 0$
    - Diagonal dominance is a desirable feature for satisfying the boundedness criterion.
    - All coefficients of the discretized equations should have the same sign.
      - Usually positive
      - Increase in the variable ϕ at one should result in an increase in ϕ at neighboring cells.

Node	a_W	a_E	S_P	S_u
1	0	$D - F/2$	$-(2D + F)$	$(2D + F)\phi_A$
2, 3, 4	$D + F/2$	$D - F/2$	0	0
5	$D + F/2$	0	$-(2D - F)$	$(2D - F)\phi_B$

Properties of discretization schemes

- Transportiveness
  - The transportiveness property of a fluid flow can be illustrated by considering two constant sources of ϕ at point W and E



  - Two extreme cases
    - No convection and pure diffusion ($Pe \rightarrow 0$)
    - No diffusion and pure convection ($Pe \rightarrow \infty$)
      - All of property ϕ emanating from the sources at W and E is immediately transported downstream.
      - Thus, conditions at P are now unaffected by the downstream source at E and completely dictated by the upstream source at W.
      - No diffusion,

$$\phi_P = \phi_W$$

Contents

Assessment of CDS for C-D problems

- Conservativeness
  - Consistent evaluation of cell faces $\Rightarrow$ conservative

- Boundedness
  - Internal coefficients
    - Satisfied?
  - Sign of the coefficients

a_W	a_E	a_P
$D_w + \frac{F_w}{2}$	$D_e - \frac{F_e}{2}$	$a_W + a_E + (F_e - F_w)$

$$\frac{\sum |a_{nb}|}{|a'_P|} \begin{cases} \leq 1 \text{ at all nodes} \\ < 1 \text{ at one node at least} \end{cases}$$

$$Pe = \frac{F}{D} = \frac{\rho u}{\Gamma / \delta x}$$

$$D_e - \frac{F_e}{2} > 0$$

$$\frac{F_e}{D_e} = Pe_e < 2$$

- Otherwise, the requirements for boundedness will be violated and this may lead to physically impossible solutions.
- Case-1, stable, $F = 0.1, D = 0.5, F/D = 0.2$
- Case-2, unstable $F = 2.5, D = 0.5, F/D = 5$
- Case-3, stable $F = 2.5, D = 2, F/D = 1.25$