

## Ch.3 Finite Difference Methods

Steady :  $\frac{\partial}{\partial x_j} (\rho u_j \phi) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + g_\phi$  : convection-diffusion eq.

① Approximation of the 1st derivative

① Taylor series expansion

$$\phi(x) = \phi(x_i) + (x - x_i) \frac{\partial \phi}{\partial x} \Big|_i + \frac{(x - x_i)^2}{2!} \frac{\partial^2 \phi}{\partial x^2} \Big|_i + \frac{(x - x_i)^3}{3!} \frac{\partial^3 \phi}{\partial x^3} \Big|_i + \dots$$

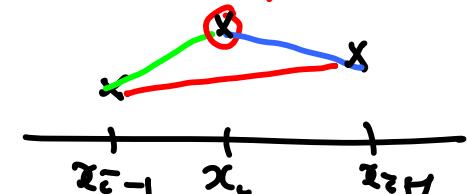
②  $x = x_{i+1}$

$$\rightarrow \frac{\partial \phi}{\partial x} \Big|_i = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \frac{x_{i+1} - x_i}{2} \frac{\partial^2 \phi}{\partial x^2} \Big|_i - \frac{(x_{i+1} - x_i)^2}{6} \frac{\partial^3 \phi}{\partial x^3} \Big|_i + \dots$$

forward difference (FD)

$\Theta(\Delta x)$

leading truncation error



②  $x = x_{i-1}$

$$\rightarrow \boxed{\frac{\partial \phi}{\partial x} \Big|_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}} + \underbrace{\frac{x_i - x_{i-1}}{2} \frac{\partial^2 \phi}{\partial x^2} \Big|_i}_{\text{backward difference (BD)}} - \frac{(x_i - x_{i-1})^2}{6} \frac{\partial^3 \phi}{\partial x^3} \Big|_i + \dots$$

backward difference (BD)  $\hookrightarrow$  leading truncation error  $O(\Delta x)$

③ forth

$$\boxed{\frac{\partial \phi}{\partial x} \Big|_i = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i}} - \underbrace{\frac{(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2}{2(x_{i+1} - x_{i-1})} \frac{\partial^2 \phi}{\partial x^2} \Big|_i}_{\text{central difference (CD)}} - \frac{(x_{i+1} - x_i)^3 + (x_i - x_{i-1})^3}{6(x_{i+1} - x_{i-1})} \frac{\partial^3 \phi}{\partial x^3} \Big|_i + \dots$$

central difference (CD) leading truncation error  $+ \dots$

$O(\Delta x)$

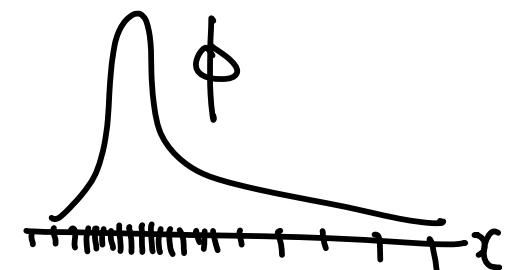
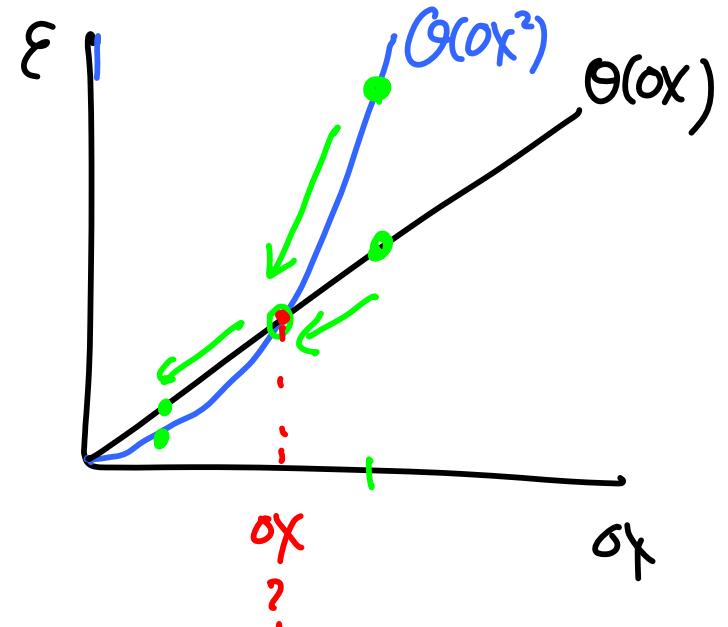
truncation error  $\epsilon_T$

$$\epsilon_T = \Delta x^m d_{mn} + (\Delta x)^{m+1} d_{m+2} + \dots ; \text{ accuracy } - m$$

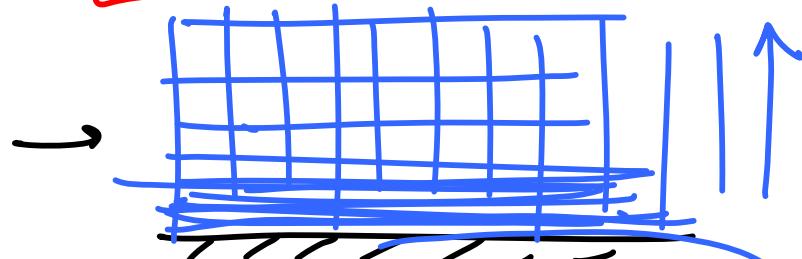
\* The order of an approx. indicates  
how fast the error is reduced  
when the grid is refined

It does not indicate the absolute magnitude of the error.

- \* When  $\Delta x_{i+1} = \Delta x_i$  ( $= x_i - x_{i-1}$ ),  
 FD becomes 2nd-order accurate.
- \* Why non-uniform mesh?  
 to resolve large gradients of  $\phi$



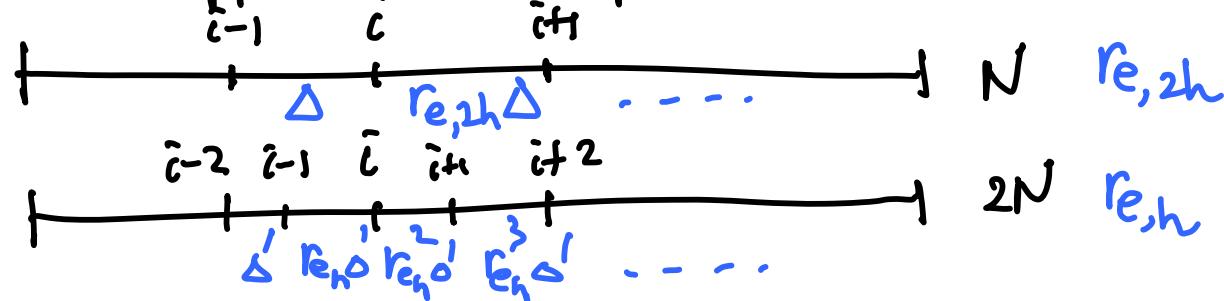
If  $\Delta x_{i+1} = r_e \Delta x_i$  (grids expand / contract at a constant factor,  $r_e$ ),



$$\hookrightarrow E_T = \left. \frac{1-r_e}{2} \Delta x_i \frac{\partial^2 \phi}{\partial x^2} \right|_i - \left. \frac{1-r_e+r_e^2}{6} \Delta x_i^2 \frac{\partial^3 \phi}{\partial x^3} \right|_i + \dots$$

(BD or FD :  $E_T = \left. \frac{\Delta x_i}{2} \frac{\partial^2 \phi}{\partial x^2} \right|_i + \dots$ )

Q : What happens when grid is refined in CD ?



$$\Delta = \Delta' + r_{e,h} \Delta' = (1+r_{e,h}) \Delta'$$

$$\Delta(1+r_{e,2h}) = \Delta'(1+r_{e,h} + r_{e,h}^2 + r_{e,h}^3)$$

$$= \frac{\Delta'(1+r_{e,h})(1+r_{e,h}^2)}{= \Delta} \Rightarrow r_{e,12h} = r_{e,h}^2$$

$$\text{or } r_{e,h} = \sqrt{r_{e,2h}}$$

$$(\Delta x_i)_{2h} = (\Delta x_i)_h + (\Delta x_{i-1})_h = (1+r_{e,h})(\Delta x_{i-1})_h$$

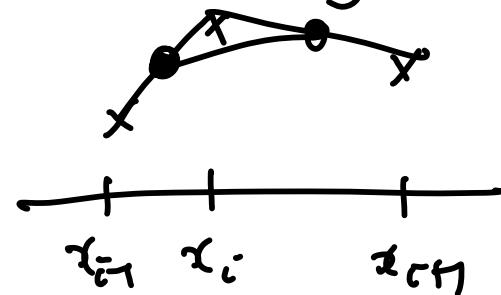
Then, the ratio of the leading truncation error is

$$r_T = \frac{(1-r_{e,2h}) \Delta x_{12h}}{(1-r_{e,h}) \Delta x_{1h}} = \frac{(1-r_{e,h})(1+r_{e,h})(\Delta x_{i-1})_h}{(1-r_{e,h}) r_{e,h} (\Delta x_{i-1})_h} = \frac{(1+r_{e,h})^2}{r_{e,h}} \geq 4$$

①  $r_e = 1$ ,  $r_T = 4$  second-order accurate.

$r_e \neq 1$ ,  $r_T > 4$  faster than 2nd-order accuracy  $\rightarrow$  good.

\* Absolutely 2nd-order formula



$$\frac{\partial \phi}{\partial x} \Big|_i = \frac{\phi_{i+1} \frac{\partial \phi}{\partial x} \Big|_{i-\frac{1}{2}} + \phi_i \frac{\partial \phi}{\partial x} \Big|_{i+\frac{1}{2}}}{\Delta x_i + \Delta x_{i+1}}$$

$$= \frac{\phi_{i+1} \Delta x_i^2 - \phi_{i-1} \Delta x_{i+1}^2 + \phi_i [\Delta x_{i+1}^2 - \Delta x_i^2]}{\Delta x_{i+1} \Delta x_i (\Delta x_i + \Delta x_{i+1})},$$

$$- \frac{\Delta x_{i+1} \Delta x_i}{6} \frac{\partial^3 \phi}{\partial x^3} \Big|_i + \dots$$

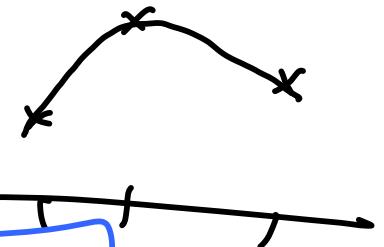
Leading truncation error  $\Theta(\Delta x^2)$

## ② Polynomial fitting

to fit the ft. to an interpolation curve  
and differentiate the resulting curve

e.g. parabola for  $x_{i-1}, x_i, x_{i+1}$

$$\rightarrow \left. \frac{d\phi}{dx} \right|_i = \frac{\phi_{i+1} \sigma x_i^2 - \phi_{i-1} \Delta x_{i+1}^2 + \phi_i [\Delta x_{i+1}^2 - \Delta x_i^2]}{\Delta x_{i+1} \Delta x_i (\sigma x_i + \sigma x_{i+1})}$$



Second-order accurate

other polynomials, splines, etc.

- \* in general, approximation of 1st derivative possesses a truncation error of the same order as the degree of the polynomial used to approximate the ft.

For example, 3rd-order polynomials (uniform mesh)

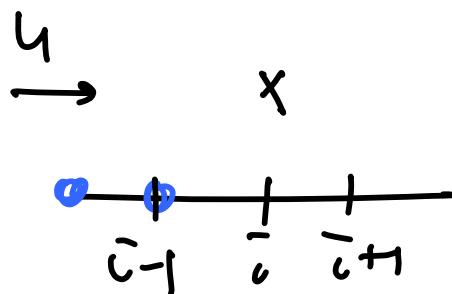
$$\frac{\partial \phi}{\partial x} \Big|_i = \frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6\Delta x} + O(\Delta x^3) \quad \text{BD}$$

$$= \frac{-\phi_{i+2} + 6\phi_{i+1} - 3\phi_i - 2\phi_{i-1}}{6\Delta x} + O(\Delta x^3) \quad \text{FD}$$

4th-order polynomial

$$\frac{\partial \phi}{\partial x} \Big|_i = \frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta x} + O(\Delta x^4) \quad \text{CF}$$

- N-S eqs  $\rightarrow \frac{\partial}{\partial x}(uu)$  or  $u \frac{\partial u}{\partial x}$ ,  $\frac{\partial}{\partial x}(u\phi)$  or  $u \frac{\partial \phi}{\partial x}$   
convection term



$u > 0 @ x_i \rightarrow BD$       } upwind scheme  
 $u < 0 @ x_i \rightarrow FD$

First-order upwind scheme (UD)

$$\boxed{\frac{\partial \phi}{\partial x} \Big|_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 \phi}{\partial x^2} \Big|_i + \dots}$$

$\uparrow O(\Delta x)$  inaccurate

$$\frac{\partial(\rho\phi)}{\partial t} + \underbrace{\frac{\partial}{\partial x}(\rho u\phi)}_{\rho u \frac{\partial \phi}{\partial x}} + \dots = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) + \dots$$

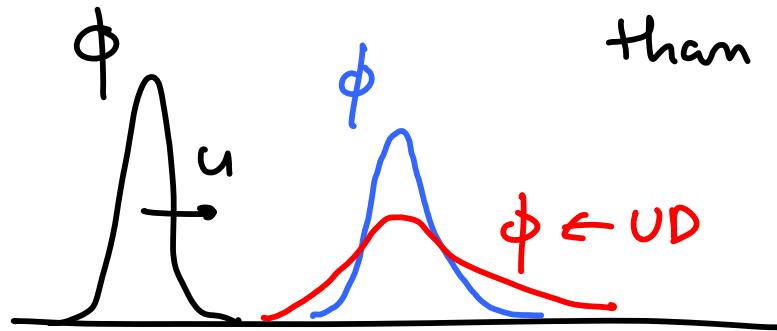
$$\rho u \frac{\partial \phi}{\partial x}$$

1st order UD =  $\frac{\phi_i - \phi_{i-1}}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 \phi}{\partial x^2} \Big|_i + \dots$

$$\rightarrow \rho \frac{\partial \phi}{\partial t} + \rho u \frac{\phi_i - \phi_{i-1}}{\Delta x} + \dots = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} + \underbrace{\frac{\rho u}{\Delta x^2} \frac{\partial^2 \phi}{\partial x^2}}_{\text{Truncation error}} \right) + \dots$$

$$= \frac{\partial}{\partial x} \left( \Gamma + \underbrace{\frac{\rho u}{\Delta x^2}}_{\text{Truncation error}} \right) \frac{\partial \phi}{\partial x} + \dots$$

Sometimes, truncation error can be bigger than actual diffusivity.



Higher-order upwind scheme  $\rightarrow$  e.g. QUICK scheme

$\Rightarrow$  In general, use CFD !

$\uparrow$  boundedness problem

$\hookrightarrow \epsilon_T = \alpha \Delta x \frac{\partial^3 \phi}{\partial x^3} + \dots$

$$\phi(x) \xrightarrow{FT} \hat{\phi}(k)$$

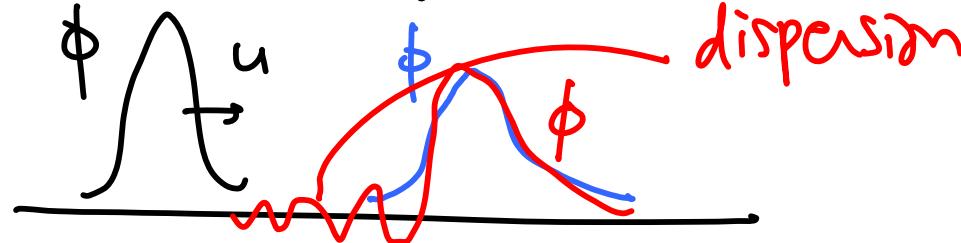
$$\frac{\partial^2 \phi}{\partial x^2}(x) \xrightarrow{FT} -k^2 \hat{\phi} : \text{diffusion}$$

$$\frac{\partial^3 \phi}{\partial x^3}(x) \xrightarrow{FT} -ik^3 \hat{\phi} : \text{dispersion}$$

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \xrightarrow{FT} \frac{d \hat{\phi}}{dt} = (-\alpha k^2) \hat{\phi}$$

$$\rightarrow \hat{\phi} = \hat{\phi}_0 e^{-\alpha k^2 t}$$

$$= \alpha \frac{\partial^3 \phi}{\partial x^3} \xrightarrow{FT} \frac{d \hat{\phi}}{dt} = (-i\alpha k^3) \hat{\phi} \rightarrow \text{sinusoidal ft.}$$

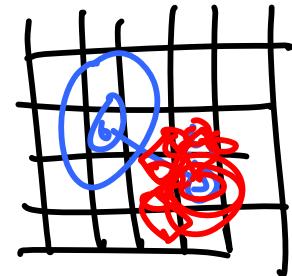


$$\phi(x) = \sum \hat{\phi}(k) e^{ikx}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \sum (-k^2 \hat{\phi}) e^{ikx}$$

$$\frac{\partial^3 \phi}{\partial x^3} = \sum (-ik^3 \hat{\phi}) e^{ikx}$$

wave component



### ③ Compact schemes

increase the accuracy with the same grids

⇒ Padé scheme : include the derivative @  $i-1$  &  $i+1$   
to determine the derivative @  $i$ .

$$a \left. \frac{\partial \phi}{\partial x} \right|_{i-1} + b \left. \frac{\partial \phi}{\partial x} \right|_i + c \left. \frac{\partial \phi}{\partial x} \right|_{i+1} + d \phi_{i-1} + e \phi_i + f \phi_{i+1} = 0$$

Using Taylor table

	$\phi_i$	$\frac{\partial \phi}{\partial x} _i$	$\frac{\partial^2 \phi}{\partial x^2} _i$	$\frac{\partial^3 \phi}{\partial x^3} _i$	...
$e \phi_i =$	$e$	$0$	$0$	$0$	$\dots$
$d \phi_{i-1} =$	$d$	$d(-\alpha x)$	$d\left(\frac{1}{2}\right)(-\alpha x)^2$	$d\left(\frac{1}{6}\right)(-\alpha x)^3$	$\dots$
$f \phi_{i+1} =$	$\dots$	$\dots$	$\dots$	$\dots$	
$b \left. \frac{\partial \phi}{\partial x} \right _{i-1} =$	$0$	$b$	$0$	$0$	
$a \left. \frac{\partial \phi}{\partial x} \right _i =$	$0$	$a$	$a(-\alpha x)$	$\dots$	

$$+ \left| c \frac{\partial \phi}{\partial x} \Big|_{i+h} \right| - \dots - \dots - \dots$$

$$\therefore = (\underbrace{e + d + f}_{O(1)} \phi_i + O(x) \underbrace{\phi}_{O(1)} + O(x^2) \underbrace{\phi}_{O(1)} + \dots)$$

determine a,b,c,d,e,f

$$\Rightarrow \frac{\partial \phi}{\partial x} \Big|_{i-1} + 4 \frac{\partial \phi}{\partial x} \Big|_i + \frac{\partial \phi}{\partial x} \Big|_{i+1} + \frac{3}{\partial x} \phi_{i-1} - \frac{3}{\partial x} \phi_{i+1} = O(\partial x^4)$$

$$\Rightarrow \boxed{\frac{\partial \phi}{\partial x} \Big|_{i-1} + 4 \frac{\partial \phi}{\partial x} \Big|_i + \frac{\partial \phi}{\partial x} \Big|_{i+1} = 3 \frac{\phi_{i+1} - \phi_{i-1}}{\partial x} + O(\partial x^4)}$$

4<sup>th</sup>-order accurate  
compact!

0 1 2 ... i-1 i i+1 ... N-1 N

$$\rightarrow \begin{bmatrix} 4 & 1 & & & & & \\ 1 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ & & & 1 & 4 & 1 & \\ & & & & 1 & 4 & \\ & & & & & 1 & \end{bmatrix} \begin{matrix} \phi \\ \vdots \\ \phi \\ \vdots \\ \phi \\ \vdots \\ \phi \end{matrix} \Big|_{i=1}^{i=N-1} =$$

tri-diagonal matrix system

$$\begin{bmatrix} 1 & & & & & \\ \vdots & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix} \begin{matrix} \frac{\partial \phi}{\partial x} \\ \vdots \\ \frac{\partial \phi}{\partial x} \\ \vdots \\ \frac{\partial \phi}{\partial x} \\ \vdots \\ \frac{\partial \phi}{\partial x} \end{matrix}$$

↑  
have to approximate these.

## 2. Approximation of 2nd derivative

① Taylor series expansion

② Use a formula for 1st derivative

$$\text{e.g. } \frac{\partial^2 \phi}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial \phi}{\partial x} \right) = \frac{\phi|_{i+\frac{1}{2}} - \phi|_{i-\frac{1}{2}}}{\frac{1}{2}(x_{i+1} - x_{i-1})} = \dots$$

③ Polynomial fitting

In general, the truncation error of the approx. to 2nd derivative is the degree of the interpolating polynomial minus one. One order is gained when the spacing is uniform and even-order polynomials are used.

\* One can use approx. of 2nd derivative to increase the accuracy  
to 1st derivative,

e.g.

$$\left. \frac{\partial \Phi}{\partial x} \right|_i = \frac{\Phi_{i+1} - \Phi_i}{x_{i+1} - x_i} - \frac{1}{2} \underbrace{\left( x_{i+1} - x_i \right)}_{\Theta(\Delta x)} \left. \frac{\partial^2 \Phi}{\partial x^2} \right|_i + \dots$$

$\uparrow$  C-D  $\rightarrow \Theta(\Delta x^2)$

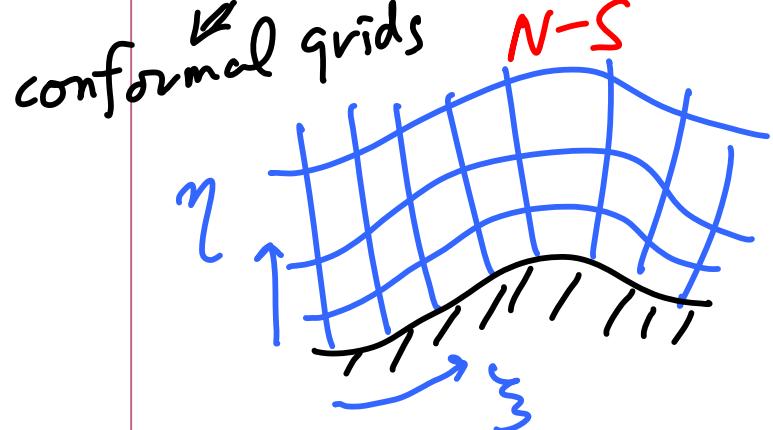
$\Theta(\Delta x^3)$

\* higher-order formula needs more pts.  
→ more complex to solve

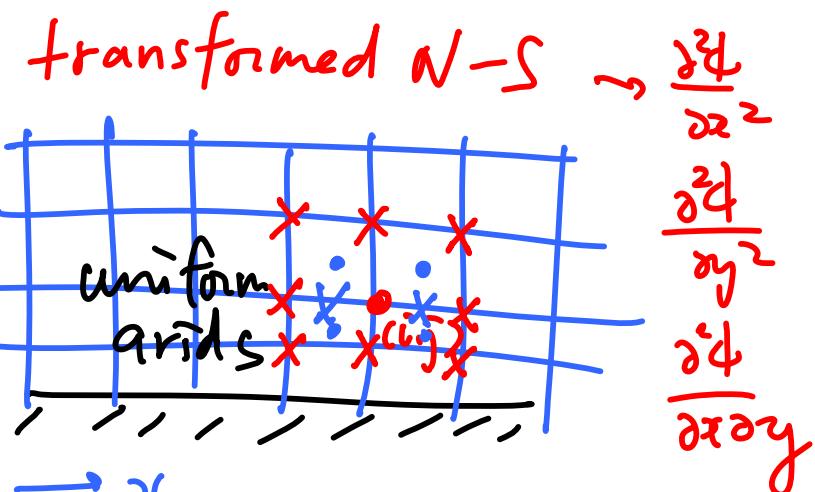
" " treatment of b.c.

\* Second-order accuracy is good for eng. applications

3. Mixed derivatives :  $\frac{\partial^2 \phi}{\partial x \partial y}$



coord.  
transf.



$$\begin{aligned} \text{transformed N-S} &\rightarrow \frac{\partial^2 \phi}{\partial x^2} \\ &\frac{\partial^2 \phi}{\partial y^2} \\ &\frac{\partial^2 \phi}{\partial x \partial y} \end{aligned}$$

$$\left. \frac{\partial^2 \phi}{\partial x \partial y} \right|_{i,j} = \frac{\partial}{\partial x} \left( \frac{\partial \phi}{\partial y} \right) = \frac{1}{\Delta x} \left[ \left. \frac{\partial \phi}{\partial y} \right|_{i+\frac{1}{2},j} - \left. \frac{\partial \phi}{\partial y} \right|_{i-\frac{1}{2},j} \right] \text{ CD2}$$

$$= \frac{1}{\Delta x} \left[ \frac{1}{\Delta y} \left( \phi_{i+\frac{1}{2},j+\frac{1}{2}} - \phi_{i+\frac{1}{2},j-\frac{1}{2}} \right) - \frac{1}{\Delta y} \left( \phi_{i-\frac{1}{2},j+\frac{1}{2}} - \phi_{i-\frac{1}{2},j-\frac{1}{2}} \right) \right] \text{ CD2}$$

9 grid pts.  $\rightarrow$  sparse matrix.

#### 4. Implementation of BC's

$$\text{Dirichlet BC. : } \phi_b = c$$

$$\text{Neumann BC : } \left. \frac{\partial \phi}{\partial x} \right|_b = c$$

When a high-order formula is used at interior pts., one can use a different scheme at  $j=2$ .

$\xrightarrow{\text{4-th order formula}}$

$$\left. \frac{\partial \phi}{\partial x} \right|_2 = \frac{-\phi_5 + 6\phi_4 + 18\phi_3 + 10\phi_2 - 33\phi_1}{60 \Delta x} + O(\Delta x^4)$$

for Dirichlet BC  $\phi_1$ .

$$\text{Neumann BC. } \left. \frac{\partial \phi}{\partial x} \right|_1 = 0 = \frac{\phi_2 - \phi_1}{\Delta x_1} + O(\Delta x)$$

Usually the approx. of the bdry value or near the bdry is of lower order than the approx. used deeper in the interior and may be one-sided difference.

⇒ global accuracy problem.

- Issues of global accuracy

Neumann b.c.  $\frac{\partial \phi}{\partial x} \Big|_{x=0} = cct$

GE :  $\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0 \quad \text{--- (1)}$

Implicit Euler + CD  $\Theta(\alpha t^2)$

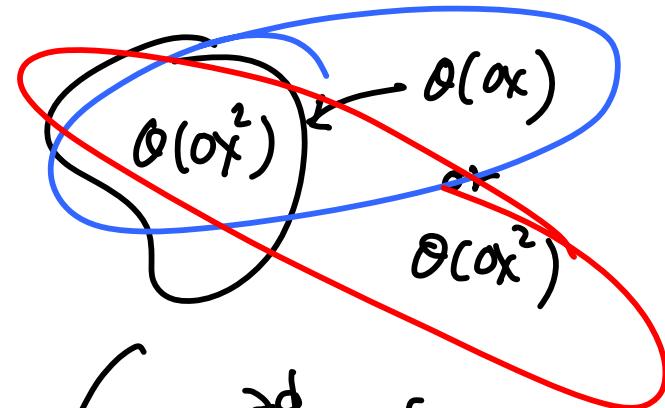
$$\frac{\phi_j^{n+1} - \phi_j^n}{\alpha t} - \alpha \frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\alpha x^2} = 0 \quad \text{--- (2)}$$

$j = 2, 3, 4, \dots$

Explicit Euler + CD  $\Theta(\alpha t^2)$

$$\frac{\phi_j^{n+1} - \phi_j^n}{\alpha t} - \alpha \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\alpha x^2} = 0 \quad \text{--- (2')}$$

$j = 2, 3, 4, \dots$



$$\frac{\partial \phi}{\partial t} = f(\phi)$$

$$IE: \frac{\phi^{n+1} - \phi^n}{\alpha t} = f(\phi_j^n) + \Theta(\alpha t)$$

$$EE: \frac{\phi_j^{n+1} - \phi_j^n}{\alpha t} = f(\phi_j^n) + \Theta(\alpha t)$$

$$\frac{\partial \phi}{\partial x} \Big|_{x=0} = c(t)$$

1st-order b.c.:

$$\left[ \begin{array}{c} 1 + 0 \cdot \delta \\ - \\ \vdots \\ \vdots \end{array} \right] \left[ \begin{array}{c} \phi_1^n \\ \phi_2^n \\ \vdots \\ \vdots \end{array} \right] \quad O(\delta x)$$

2nd-order b.c.:

$$\frac{\phi_2^{n+1} - \phi_1^{n+1}}{\delta x} = c^{n+1} \rightarrow \phi_1^{n+1} = \phi_2^{n+1} - c^{n+1} \delta x$$

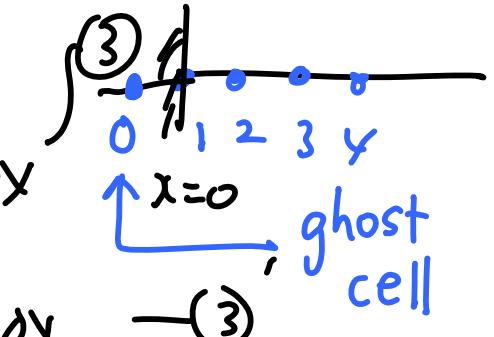
$$\frac{\phi_2^n - \phi_1^n}{\delta x} = c^n \rightarrow \phi_1^n = \phi_2^n - c^n \delta x \quad - (3)$$

$$\frac{\phi_2^{n+1} - \phi_0^n}{2\delta x} = c^{n+1} \rightarrow \phi_0^n = \phi_2^{n+1} - 2c^{n+1} \delta x \quad - (4)$$

$$\frac{\phi_2^n - \phi_0^n}{2\delta x} = c^n \rightarrow \phi_0^n = \phi_2^n - 2c^n \delta x \quad - (4)'$$

Apply ② at  $j=1$  and use  $\phi_0^{n+1}$  from ④:

$$\rightarrow \left( 1 + 2 \frac{\alpha \sigma t}{\delta x^2} \right) \phi_1^{n+1} - 2 \frac{\alpha \sigma t}{\delta x^2} \phi_2^{n+1} = \phi_1^n - 2 \frac{\alpha \sigma t}{\delta x^2} \delta x c^{n+1} \quad - (5)$$



$$\begin{bmatrix} \left(1 + 2\frac{\alpha \Delta t}{\Delta x^2}\right) & -2\frac{\alpha \Delta t}{\Delta x^2} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 \end{bmatrix} \begin{bmatrix} \phi_1^{n+1} \\ \phi_2^{n+1} \\ \phi_3^{n+1} \\ \vdots \\ \phi_N^{n+1} \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \quad \leftarrow \text{use ghost cell } O(\Delta x^2)$$

or, ② & ④'  $\rightarrow \phi_1^{n+1} = -2\frac{\alpha \Delta t}{\Delta x^2} \phi_0^n + \left(1 - 2\frac{\alpha \Delta t}{\Delta x^2}\right) \phi_1^n + 2\frac{\alpha \Delta t}{\Delta x^2} \phi_2^n \quad \text{--- } ⑤'$

ex)  $\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0 \quad 0.1 \leq x \leq 1.5$

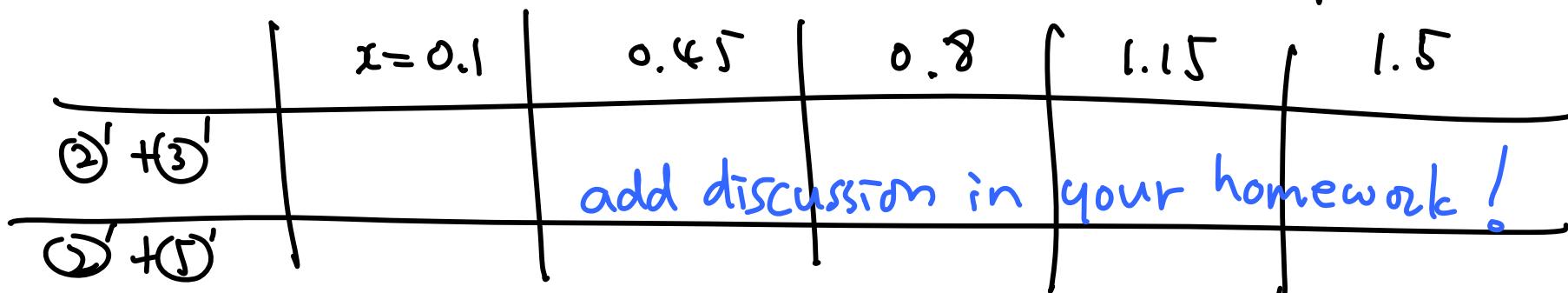
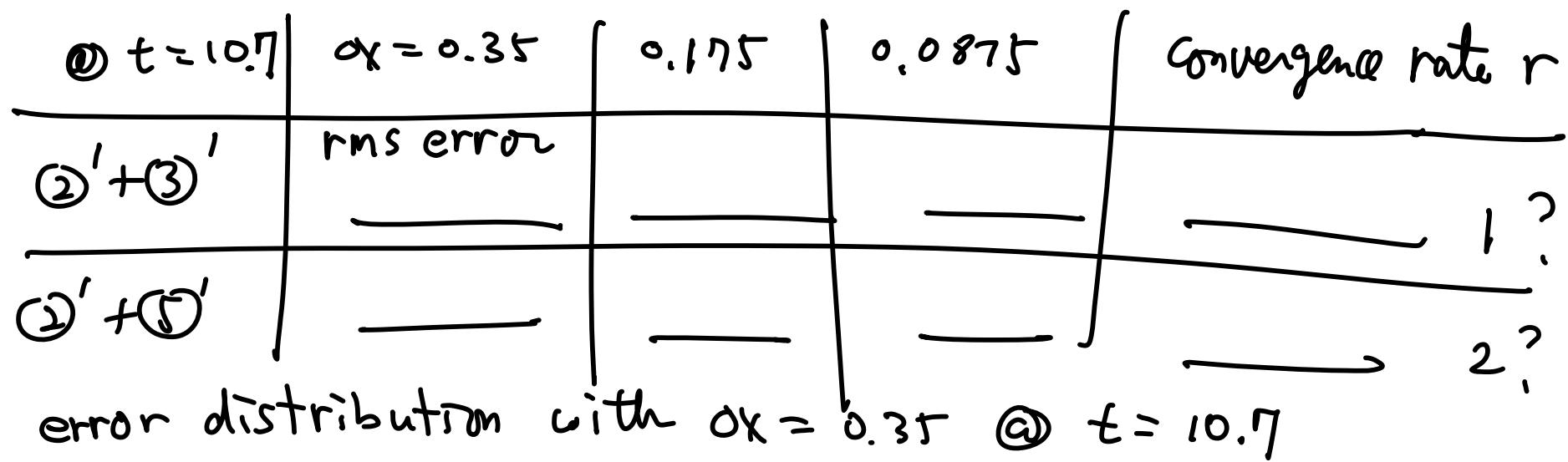
b.c.  $\left\{ \begin{array}{l} \frac{\partial \phi}{\partial x} = C = 2 - \pi \sin\left(\frac{\pi}{30}\right) e^{-\alpha\left(\frac{\pi}{3}\right)^2 t} \\ \phi = 3 \quad @ x=1.5 \end{array} \right. \quad @ t=0.1$

i.c.  $\phi = 2x + 3 \cos\left(\frac{\pi}{3}x\right) e^{-\alpha\left(\frac{\pi}{3}\right)^2 \cdot 0.9} \quad @ t=0.9$   
 $\rightarrow \phi_{\text{exact}} = 2x + 3 \cos\left(\frac{\pi}{3}x\right) e^{-\alpha\left(\frac{\pi}{3}\right)^2 t}$

HW2 due: April 3

$$\alpha = 0.25, \quad S = \frac{\partial^2 t}{\partial x^2} = 0.2$$

rms  $\rightarrow$  root-mean-square

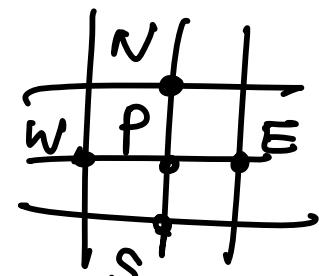
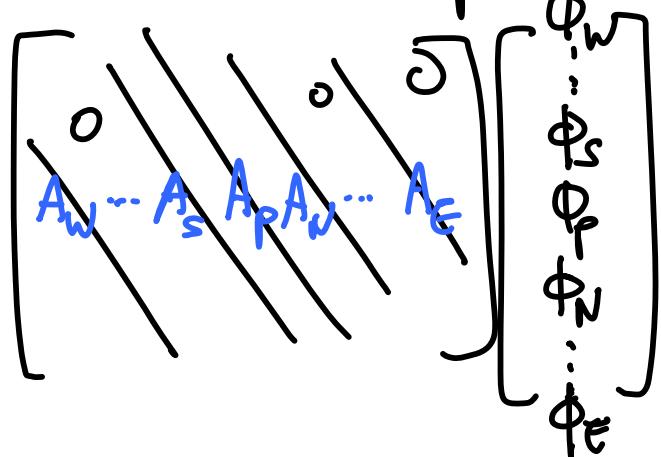


→ In conclusion, 1st-order b.c. approximation in general deteriorates numerical sol.

## 5. Algebraic eqs and discretization error

- FDM  $\rightarrow A_p \phi_p + \sum_l A_l \phi_l = Q_p$

$$A_w \phi_w + A_s \phi_s + A_p \phi_p + A_n \phi_N + A_e \phi_e = Q_p \leftarrow \text{from 2nd-order FDM.}$$



- Truncation error (Taylor series truncation)

$$L(\bar{\phi}) = L_h(\bar{\phi}) + \tau_h = 0$$

↑                   ↑                   ↑  
 diff'l operator   difference      truncation  
 operator                               error  
 h: grid size

$$L_h(\phi_h) = (A\phi - Q)_h = 0 \quad \phi_h: \text{exact sol. of } L_h(\bar{\phi})$$

then, discretization error  $\varepsilon_h^\phi \equiv \bar{\phi} - \phi_h$

$$L_h(\phi_h) = L_h(\bar{\phi} - \varepsilon_h^\phi) = L_h(\bar{\phi}) - L_h(\varepsilon_h^\phi) = -\tau_h - L_h(\varepsilon_h^\phi) = 0$$

$\rightarrow L_h(\varepsilon_h^\phi) = -\tau_h \leftarrow \text{truncation error is a source of discretization error}$

Since we don't know the magnitude of  $\tilde{\epsilon}_h$ ,  
we have to do grid refinement test.

$$\alpha x^2 \frac{d^3\phi}{dx^3}$$

For sufficiently fine grids,

$$\epsilon_h^\phi = \alpha h^P + \text{HOT} \quad P: \text{order of scheme}$$

$$\hat{\phi} = \phi_h + \epsilon_h^\phi = \phi_{2h} + \epsilon_{2h}^\phi$$

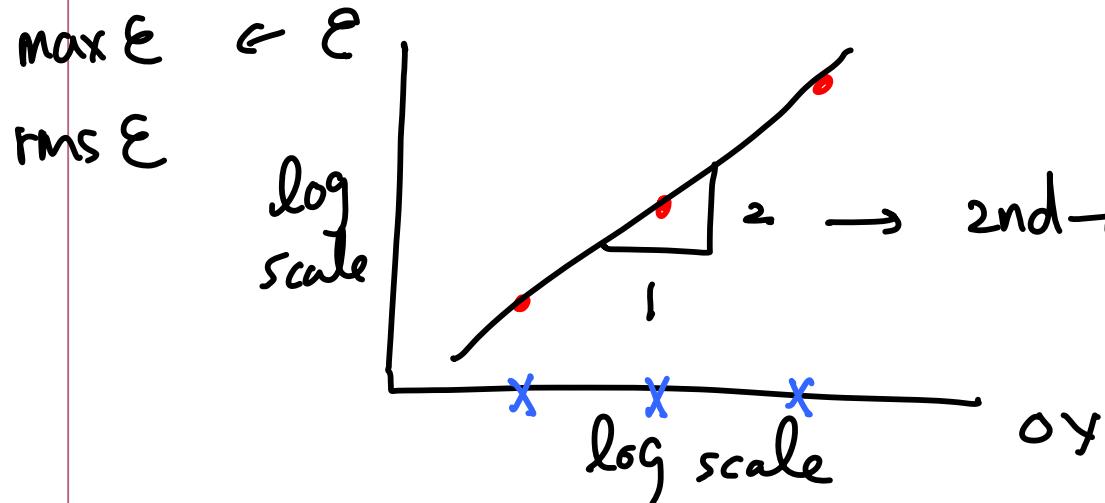
$$\phi_h + \alpha h^P + \text{HOT} = \phi_{2h} + \alpha (2h)^P + \text{HOT}$$

$$\rightarrow (\phi_h - \phi_{2h}) \approx \alpha h^P (2^P - 1)$$

$$(\phi_{2h} - \phi_{4h}) = \alpha h^P 2^P (2^P - 1)$$

$$\rightarrow P = \log \left( \frac{\phi_{2h} - \phi_{4h}}{\phi_h - \phi_{2h}} \right) / \log 2 \leftarrow$$

useful tool to check  
the order of accuracy



in practice,  
when  $h$  is fine enough,  
convergence is monotonic.

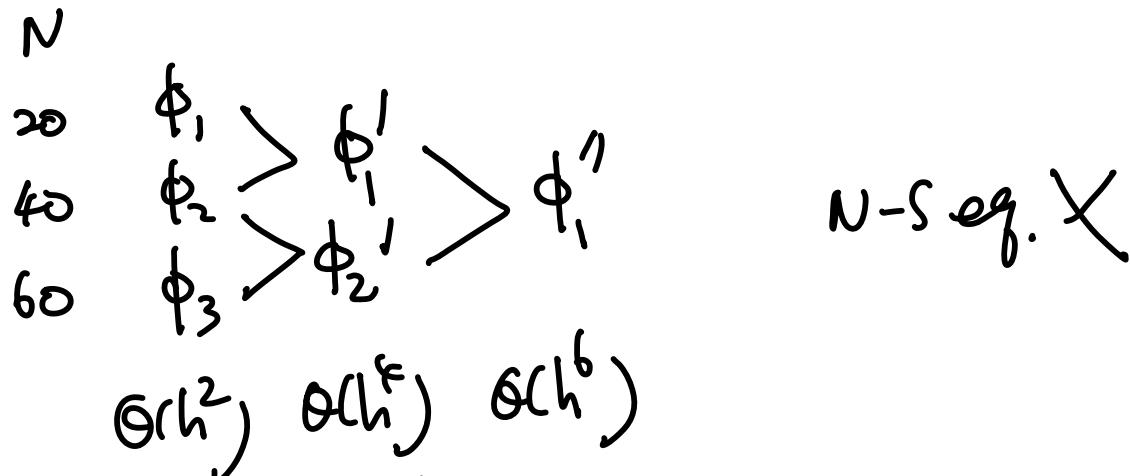
$$\text{Also, } \varepsilon_h^\phi = \alpha h^p + \text{HOT} = \bar{\phi} - \phi_h$$

$$\vdash \varepsilon_{2h}^\phi = \alpha 2^p h^p + \text{HOT} = \bar{\phi} - \phi_{2h}$$

$$\alpha h^p (2^p - 1) \approx \phi_h - \phi_{2h}$$

$$\therefore \varepsilon_h^\phi = (\phi_h - \phi_{2h}) / (2^p - 1)$$

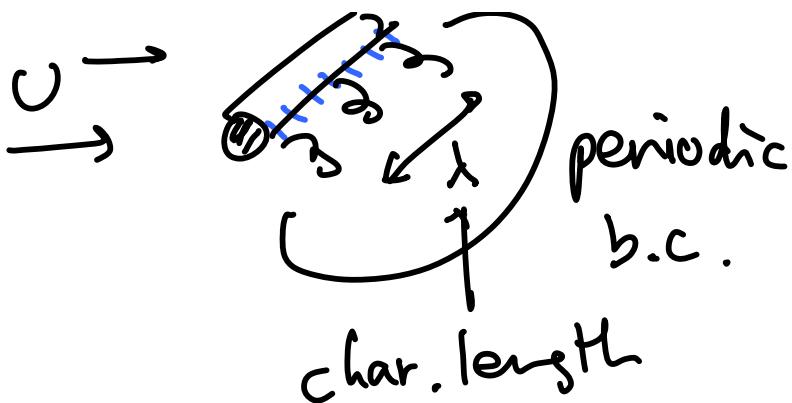
If we have sols. of  $\phi_h, \phi_{2h}, \phi_{4h}, \dots$ , we could get better sol. of  $\phi$  than  $\phi_h$  by using  $\mathcal{E}_h^\phi$ .  $\rightarrow$  Richardson extrapolation.



## 6. Introduction to spectral method

### (1) Fourier transform

- uniformly spaced set of grid pts.
- periodic b.c.



- discrete Fourier series

$$\left\{ \begin{array}{l} f(x_i) = \sum_{g=-N/2}^{N/2} \hat{f}(kg) e^{ikg x_i} \\ \hat{f}(kg) = \frac{1}{N} \sum_{c=1}^N f(x_c) e^{-ikg x_c} \end{array} \right.$$

↑ Fourier coeff.

$$\frac{df}{dx} = \sum \hat{f} \cdot ikg e^{ikg x_i}$$

$$L_z = \lambda ?$$

$$= 2\lambda ?$$

$$= 4\lambda ?$$

|||

|||



$$x_i = i \Delta x$$

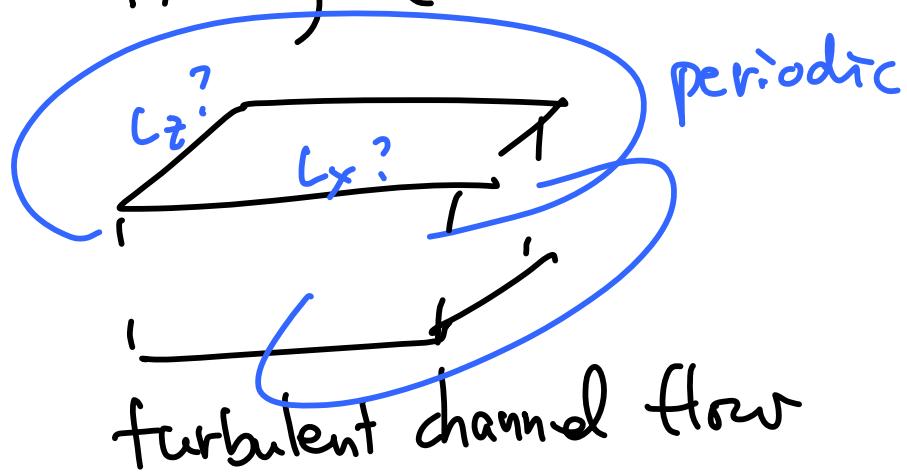
$$kg = 2\pi g / (N \Delta x)$$

↑ wave number

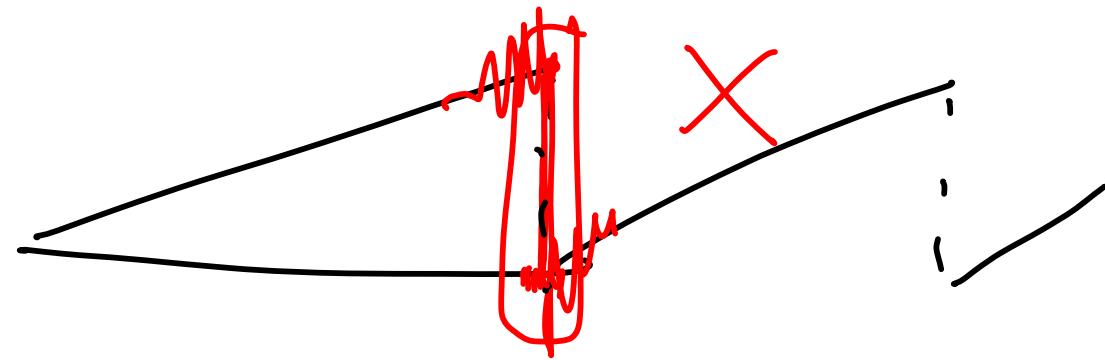
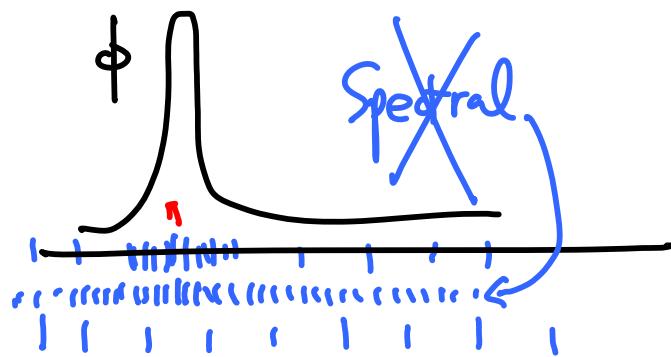
$$f(x) \xrightarrow{\text{FT}} \hat{f} \rightarrow ikg \hat{f} \xrightarrow{\text{IFT}} \frac{df}{dx}$$

$$\frac{d^2 f}{dx^2} = \sum \hat{f}(-k_g^2) e^{ik_g x_i} \quad f(x) \xrightarrow{\text{FT}} \hat{f} \rightarrow (-k_g^2) \hat{f} \xrightarrow{\text{IFT}} \frac{d^2 f}{dx^2}$$

- Error decreases exponentially with  $N$ , when  $N$  is large enough.  
→ much more accurate than FD, FV, FE.  
but it may be worse when  $N$  is small.



- Cost of FT needs  $\Theta(N^2)$  operations. ← expensive!  
FFT →  $\Theta(N \log_2 N)$  ← cheap!



## (2) Modified wavenumber

$$\phi \sim \hat{\phi} e^{ikx}$$

$$\frac{d\phi}{dx} \sim \hat{\phi} ik e^{ikx}$$

CD2:  $\phi = e^{ikx}$

$$\left. \frac{d\phi}{dx} \right|_0 = \frac{\phi_{+1} - \phi_{-1}}{2\Delta x} = \frac{e^{ik(x+\Delta x)} - e^{ik(x-\Delta x)}}{2\Delta x}$$

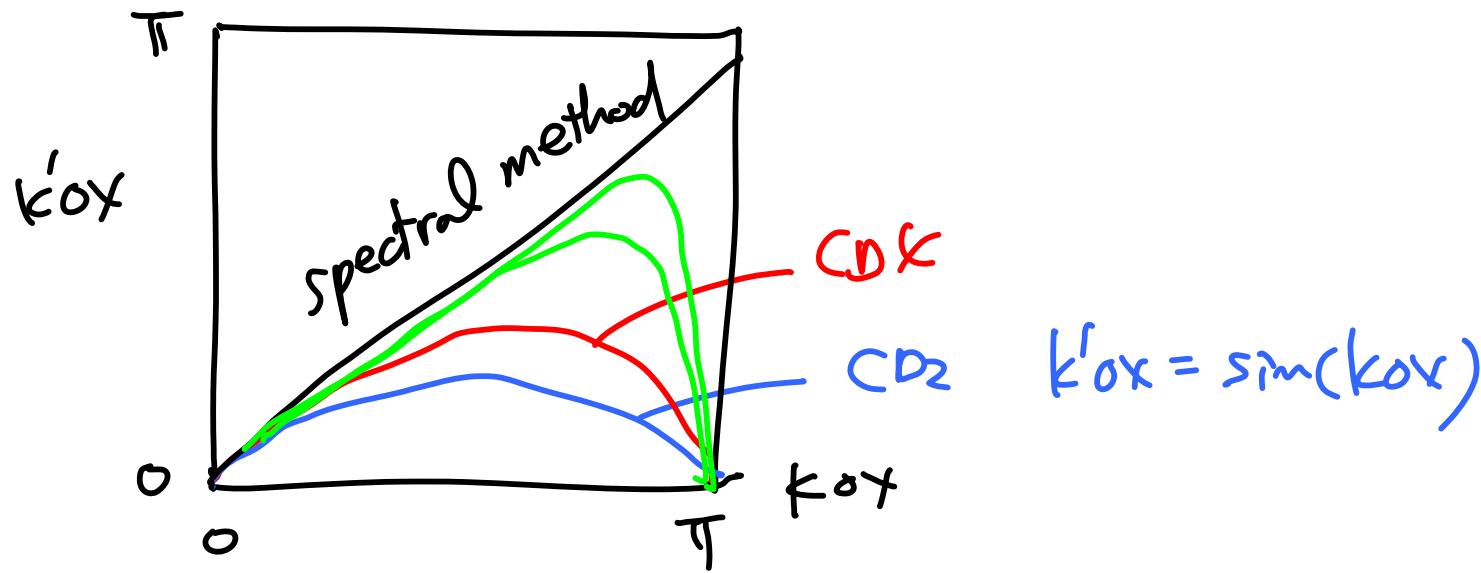
$$\phi = e^{ikx}$$

$$\frac{d\phi}{dx} = ik e^{ikx}$$

$k'$ : modified wavenumber

$$k' = \frac{\sin(k\Delta x)}{\Delta x} (4 - \cos(k\Delta x))$$

CD4:  $k' = \frac{\sin(k\Delta x)}{3\Delta x} (4 - \cos(k\Delta x))$



upwind schen :

$$\text{UD} \quad \left. \frac{d\phi}{dx} \right|_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} = \frac{e^{ikx} - e^{ik(x-\Delta x)}}{\Delta x} = i \left( -\frac{i(1-e^{-ik\Delta x})}{\Delta x} \right) e^{ikx}$$

$$\rightarrow k' = -\frac{i(1-e^{-ik\Delta x})}{\Delta x} : \text{complex number}$$

$$= \frac{1}{\Delta x} (\sin k\Delta x - i(1 - \cos k\Delta x))$$

$$\rightarrow ik'e^{ikx} = \underbrace{i \frac{\sin kox}{ox} e^{ikx}}_{\frac{d\phi}{dx}|_{UD1}} + \underbrace{\frac{-\cos kox}{ox} e^{ikx}}_{-\frac{d^2\phi}{dx^2}|_{CP2}}$$

$$GE : u \frac{\partial \phi}{\partial x} = v \frac{\partial^2 \phi}{\partial x^2}$$

$\uparrow$        $\uparrow$   
 $UD1$      $CP2$

$$v \frac{\partial \phi}{\partial x} = u \frac{\partial \phi}{\partial x} - u \frac{\partial^2 \phi}{\partial x^2}$$

$\uparrow$        $\uparrow$   
 $UD1$      $CP2$

$$\Rightarrow u \frac{\partial \phi}{\partial x} \Big|_{CP2} = (v + \cancel{u}) \frac{\partial^2 \phi}{\partial x^2} \Big|_{CP2}$$

## 7. Example

노트 제목

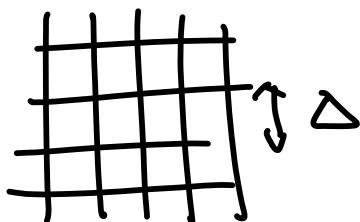
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1-D convection/diffusion eq.

$$\left\{ \begin{array}{l} \frac{\partial}{\partial x} (\rho u \phi) = \frac{\partial}{\partial x} (\Gamma \frac{\partial \phi}{\partial x}) \\ \phi = \phi_0 \text{ @ } x=0 \\ \phi = \phi_L \text{ @ } x=L \end{array} \right. \quad \rho, u, \Gamma \text{ constant}$$

$$\rightarrow \text{Exact sol. } \phi = \phi_0 + \frac{e^{x \text{Pe}/L} - 1}{e^{\text{Pe}} - 1} (\phi_L - \phi_0)$$

where  $\text{Pe} = \rho u L / \Gamma$  (Peclet number)



$\rho u \Delta / \Gamma$  : cell Peclet number

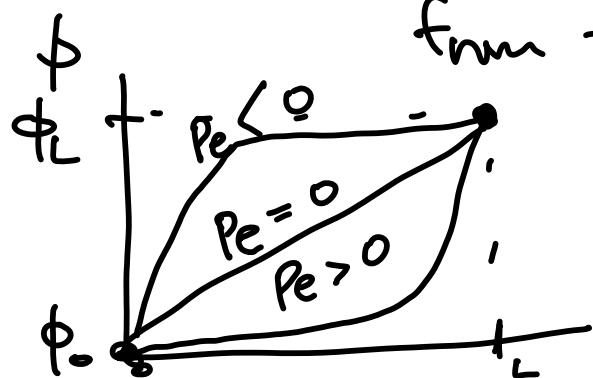
Physics : convection is balanced by diffusion.

Almost no flow in this kind of balance.

Convection is balanced by press. gradient  
or diffusion in the direction  
normal to the flow.

$$\underline{\frac{\partial}{\partial x}(\rho u u) + \dots} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) + \dots$$

Thus, it is very misleading to conclude anything  
from this 1D conv.-diff. eq.



(Let  $u \geq 0, \phi_0 < \phi_L$ )

Let's apply UDS and CDS for convection term

& CDS for diffusion term

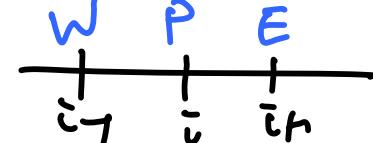
$$+ \underset{i-1}{\overset{i}{\underset{i+1}{\text{---}}}} \quad \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right)_i = \frac{\frac{\partial \phi}{\partial x} \Big|_{i+\frac{1}{2}} - \frac{\partial \phi}{\partial x} \Big|_{i-\frac{1}{2}}}{\frac{1}{2}(x_{i+1} - x_{i-1})} + O(\Delta x)$$

Conv. term

$$\text{UDS} \quad \frac{\partial}{\partial x} (\rho u \phi)_i = \begin{cases} \rho u \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} & \text{if } u > 0 \quad O(\Delta x) \\ \rho u \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} & \text{if } u < 0 \quad O(\Delta x) \end{cases}$$

$$\text{CDS} \quad \frac{\partial}{\partial x} (\rho u \phi)_i = \rho u \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}} \quad O(\Delta x^2)$$

$$\Rightarrow \text{construct } A_w \phi_w + A_p \phi_p + A_E \phi_E = Q_p$$



$$\begin{bmatrix} 0 & \diagup & 0 \\ & \diagdown & \\ 0 & & \end{bmatrix} \phi = Q \quad \text{TDMA} \rightarrow \text{obtain } \phi.$$

Numerical simulation:  $L=1, \rho=1, u=1, \Gamma=0.02$

$$\phi_0=0, \phi_L=1, Pe = \frac{\rho u L}{\Gamma} = 50.$$

① # of grid pts.  $N=11$  including bdry pts.

$$N=11 \rightarrow \Delta x = L/10 = 0.1, \text{ uniform grids}$$

$$\text{cell Peclet number } Pe_\Delta = \rho u \Delta x / \Gamma = 0.1 / 0.02 = 5$$

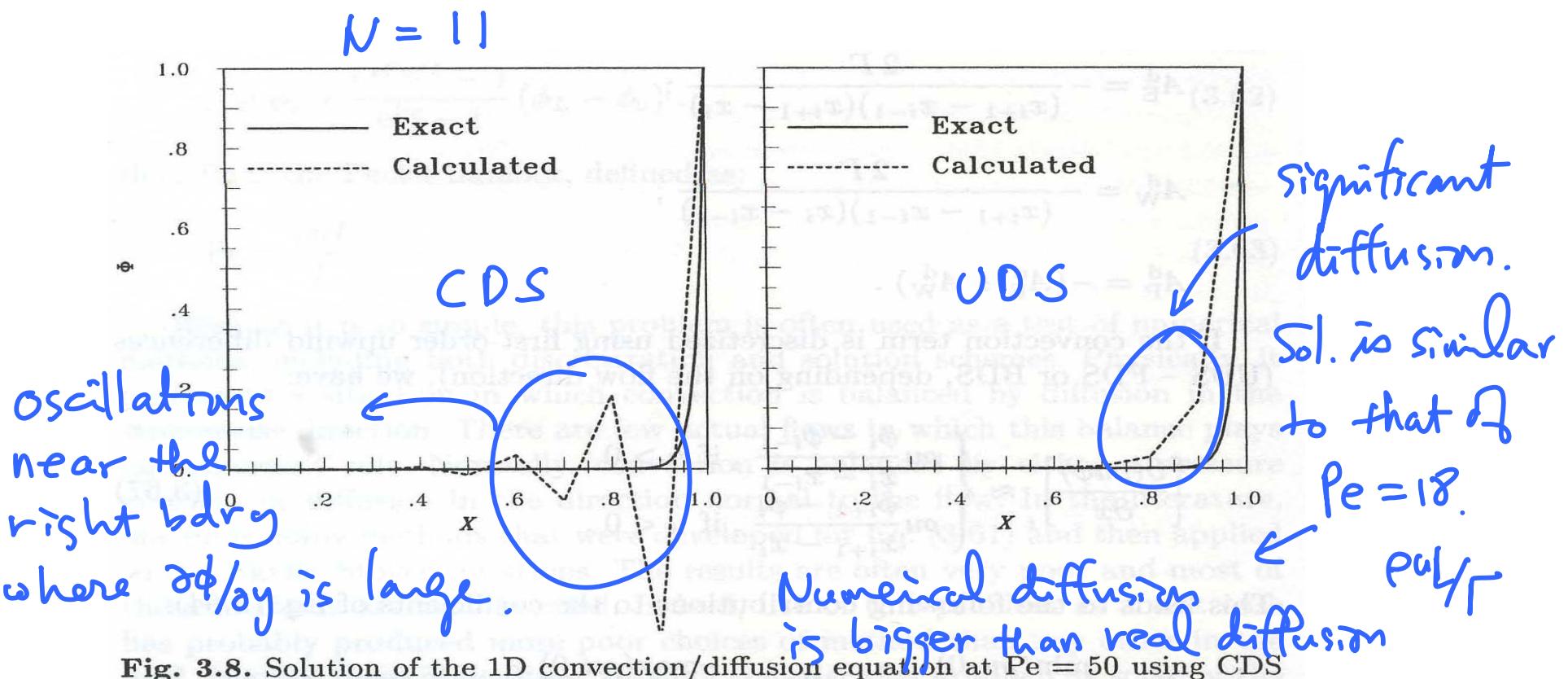
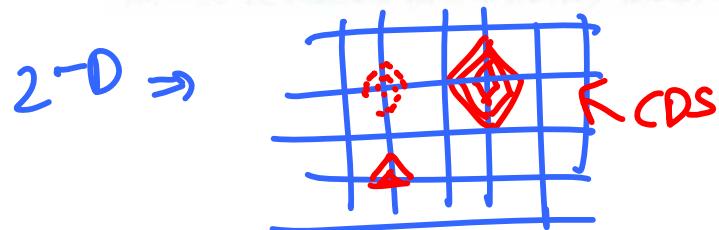
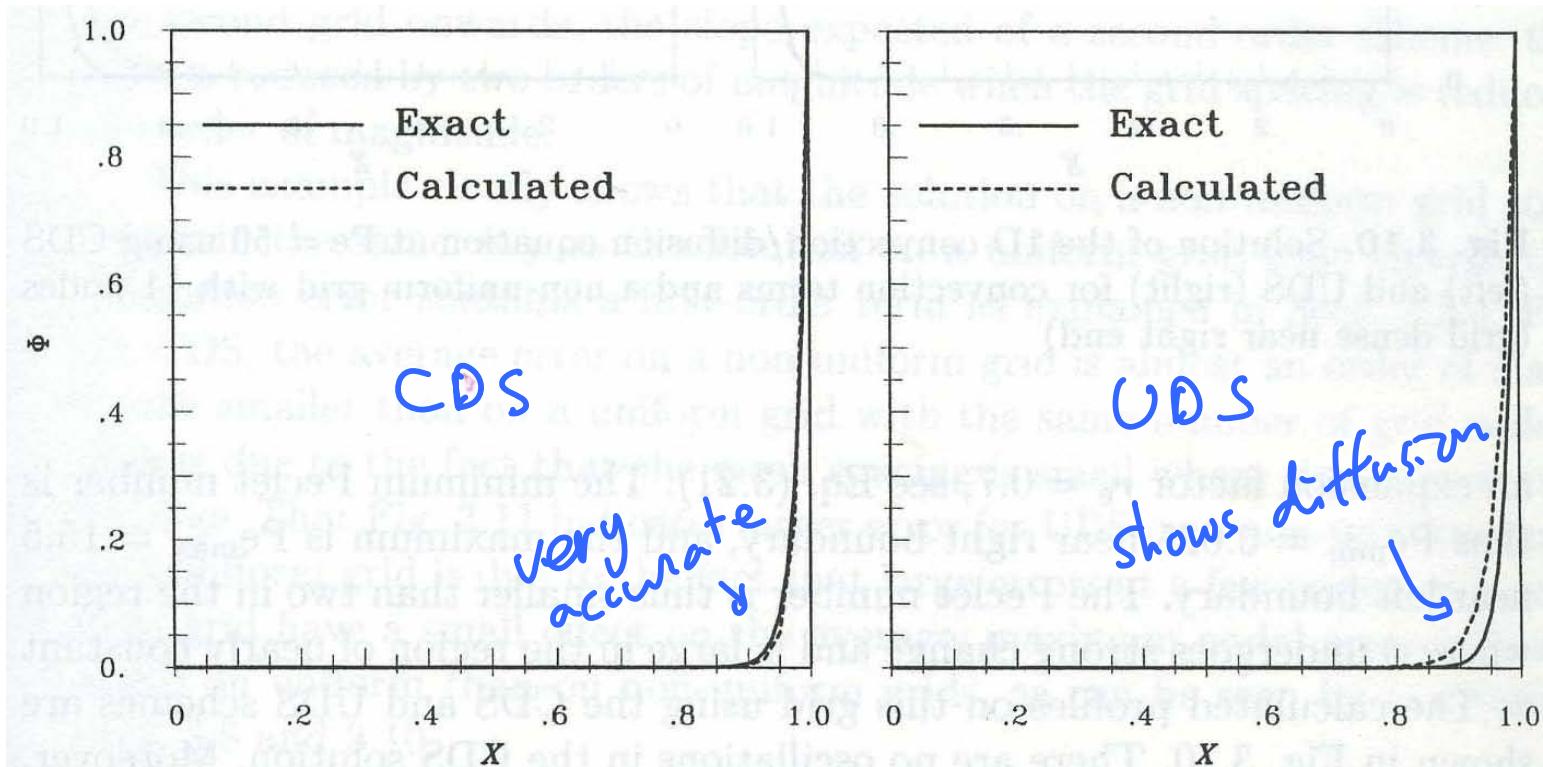


Fig. 3.8. Solution of the 1D convection/diffusion equation at  $Pe = 50$  using CDS (left) and UDS (right) for convection terms and a uniform grid with 11 nodes



$$\textcircled{2} \quad N = 41 \quad \alpha_x = L/\ell_{\text{ref}} = 1/\ell_{\text{ref}} \quad \text{uniform grids}$$

$$\text{cell } Pe_\Delta = \rho u \Delta / \Gamma = 1/0.8 \approx 1$$



**Fig. 3.9.** Solution of the 1D convection/diffusion equation at  $Pe = 50$  using CDS (left) and UDS (right) for convection terms and a uniform grid with 41 nodes

$\Rightarrow$  CDS oscillation depends on local (cell) Pe.

Patanjali (1980) showed no oscillation if cell Pe  $\leq 2$ .

Hybrid scheme (Spalding 1972)

Switch from CDS to UDS when cell Pe  $\geq 2$

together with  $\Gamma \equiv 0$ .

$\rightarrow$  too restrictive

reduce accuracy

oscillation occurs only when sol. changes rapidly  
in a region of high cell Pe.

③ Non-uniform grids with  $N=11$  ( $\Delta x_i = r_e \Delta x_{i-1}$ ,  $r_e = 0.75$ )

$$\Delta x_{\max} = 0.31 \rightarrow Pe_\delta = 15.5$$

$$\Delta x_{\min} = 0.0125 \rightarrow Pe_\delta = 0.625$$

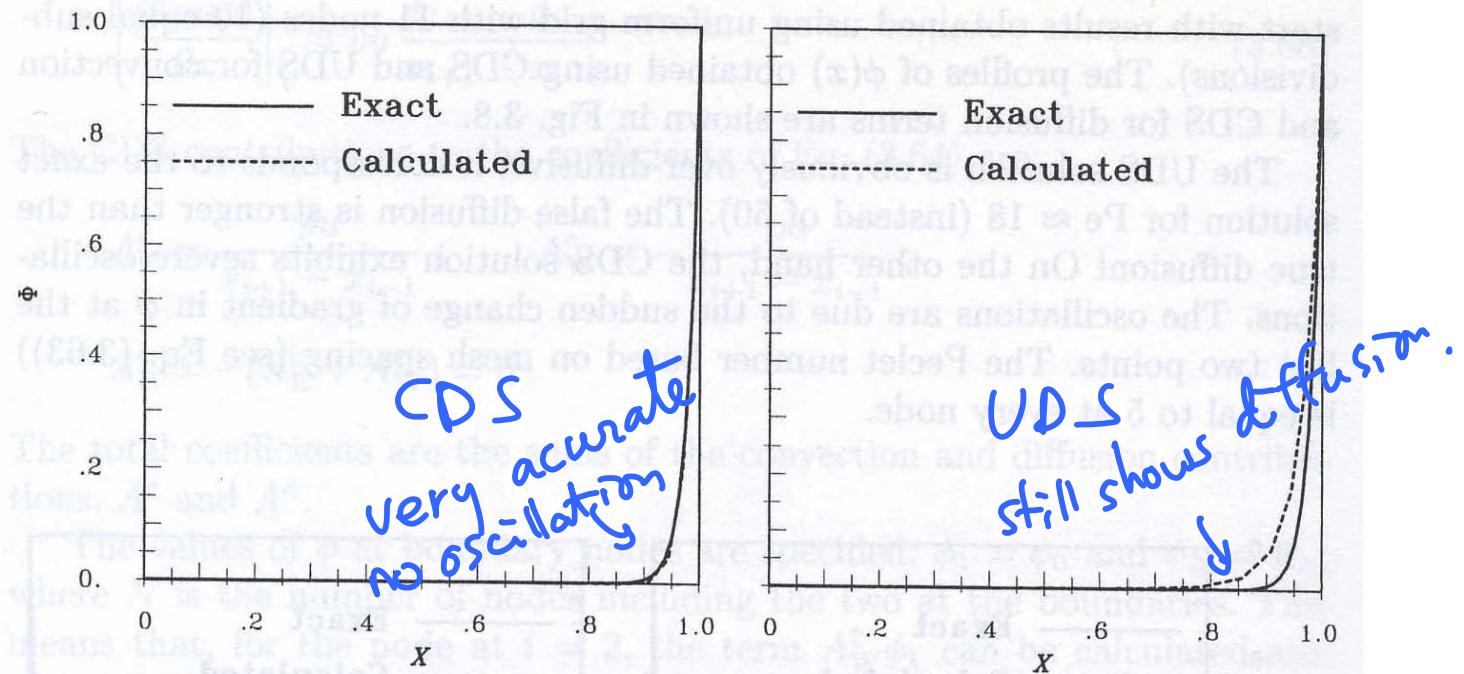


Fig. 3.10. Solution of the 1D convection/diffusion equation at  $Pe = 50$  using CDS (left) and UDS (right) for convection terms and a non-uniform grid with 11 nodes (grid dense near right end)

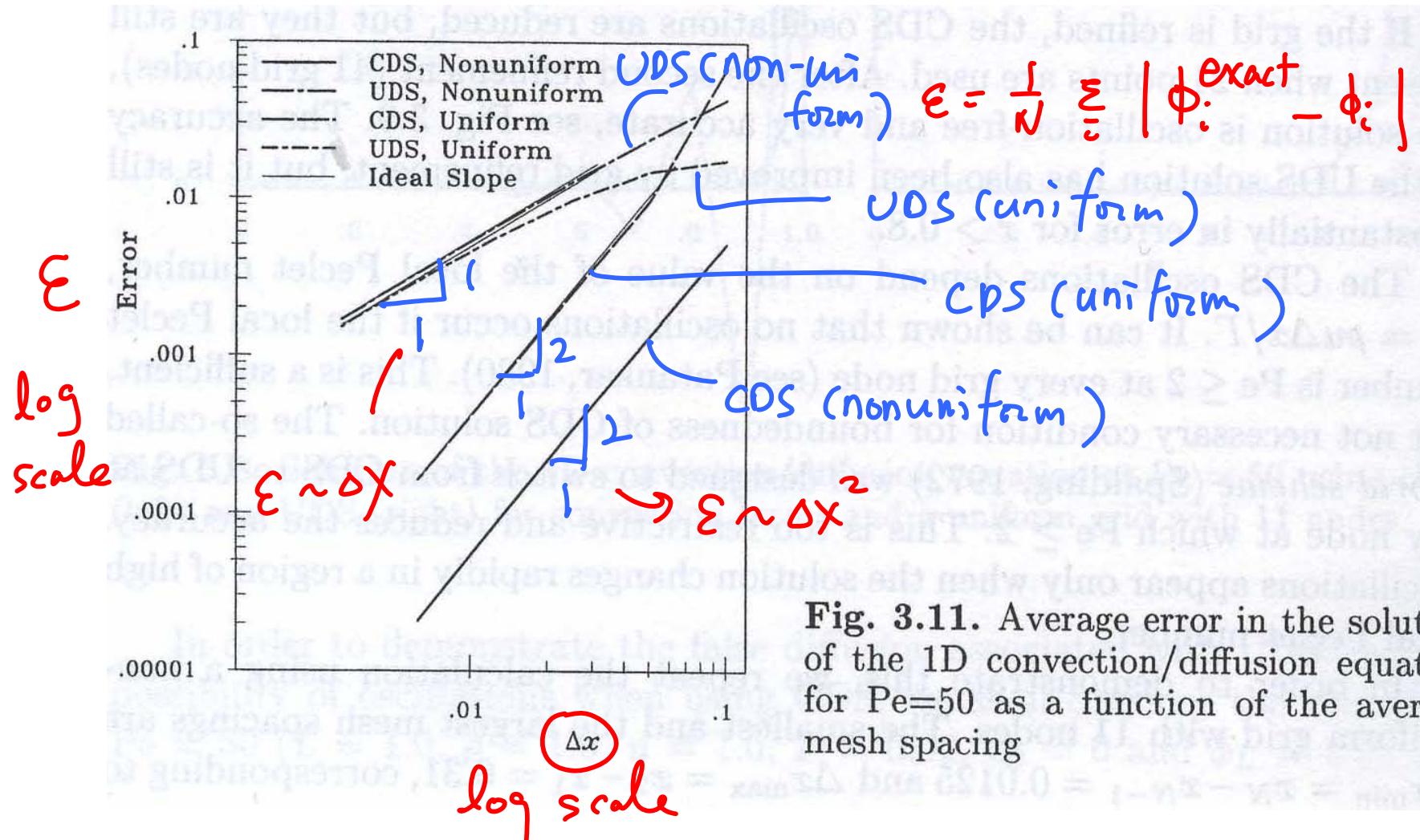


Fig. 3.11. Average error in the solution of the 1D convection/diffusion equation for  $\text{Pe}=50$  as a function of the average mesh spacing