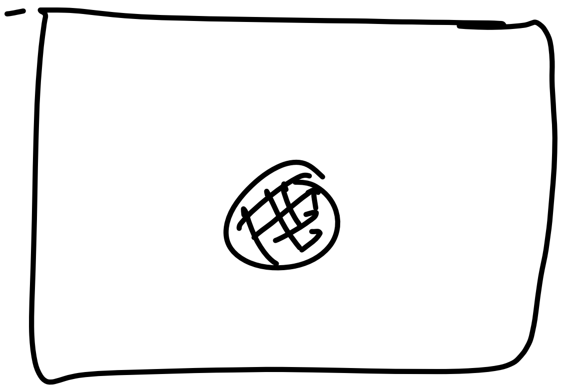
Ch.1 Basic Concepts of Fluid Flow

CFD – Computational Fluid Dynamics

~~(Colorful)~~

↳ $\underline{u}(\underline{x}, t),\ p \rightarrow \underline{\omega} = \nabla \times \underline{u},\ \cdots$

CV



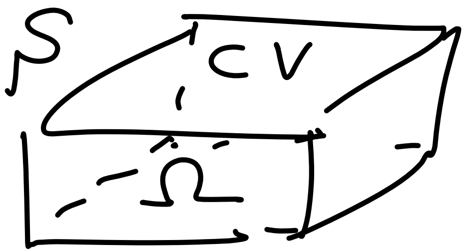
⊙ Conservation principles

→ Control volume approaches

Reynolds transport theorem

① mass conservation

out-normal unit vector



$$\frac{\partial}{\partial t}\int_{\Omega} \rho \, d\Omega + \int_{S} \rho \underline{u} \cdot \underline{n} \, dS = 0$$

density

velocity

$\cancel{\sum_{i=1}^{3}}$

$$\rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{u}) = 0 \,, \quad \boxed{\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0}$$

$$(i = 1, 2, 3) \quad \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_1}(\rho u_1) + \frac{\partial}{\partial x_2}(\rho u_2) + \frac{\partial}{\partial x_3}(\rho u_3) = 0$$

② momentum conservation

$$\frac{\partial}{\partial t}\int_{\Omega} \rho \underline{u} \, d\Omega + \int_{S} \rho \underline{u} (\underline{u} \cdot \underline{n}) \, dS = \Sigma \underline{f} = \int \frac{d}{dt}(\rho \underline{u})_{sys} \, d\Omega$$

pressure

$$\underset{\sim}{T} = -\left(p + \frac{2}{3}\mu \nabla\cdot\underline{u}\right)\underset{\sim}{1} + 2\mu \underset{\sim}{D}$$

viscosity

stress tensor $\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}$

surface forces
body forces

$$\underset{\sim}{D} = \frac{1}{2}\left(\nabla\underline{u} + (\nabla\underline{u})^T\right)$$: strain-rate tensor (deformation)

$$T_{ij} = -\left(p + \frac{2}{3}\underline{\mu}\frac{\partial u_k}{\partial x_k}\right)\delta_{ij} + 2\underline{\mu} D_{ij} \qquad \begin{pmatrix} i = 1,2,3 \\ j = 1,2,3 \end{pmatrix}$$

Kronecker delta
$\begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$

$$\underset{\sim}{1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$D_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$T_{ij} = -p\,\delta_{ij} + \tau_{ij}$$

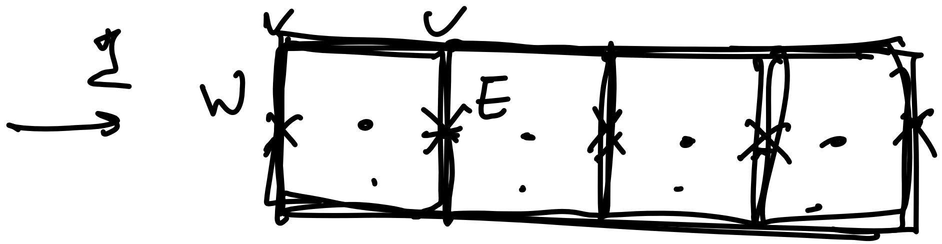
$$\tau_{ij} = 2\mu D_{ij} - \frac{2}{3}\mu\,\delta_{ij}\frac{\partial u_k}{\partial x_k}$$: viscous part of stress tensor

$$\rightarrow \frac{\partial}{\partial t}\int_\Omega \rho \underline{u}\, d\Omega + \int_S \rho \underline{u}(\underline{u}\cdot\underline{n})\, dS = \int_S \underset{\sim}{T}\cdot\underline{n}\, ds + \int_\Omega \rho \underline{b}\, d\Omega$$

$\underline{b}$: body force per unit mass

$$\rightarrow \frac{\partial}{\partial t}(\rho\underline{u}) + \nabla\cdot(\rho\underline{u}\,\underline{u}) = \nabla\cdot\underset{\sim}{T} + \rho\,\underline{b}$$

$$\boxed{\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = \frac{\partial T_{ij}}{\partial x_j} + \rho b_i}$$: <u>strong conservation form</u>



$$\int \frac{\partial}{\partial x_j}(\rho u_j u_i) \to \int \frac{\partial}{\partial x_1}(\rho u_1 u_i)\,dx_1 = \rho u_1 u_i\big|_E - \rho u_1 u_i\big|_W$$

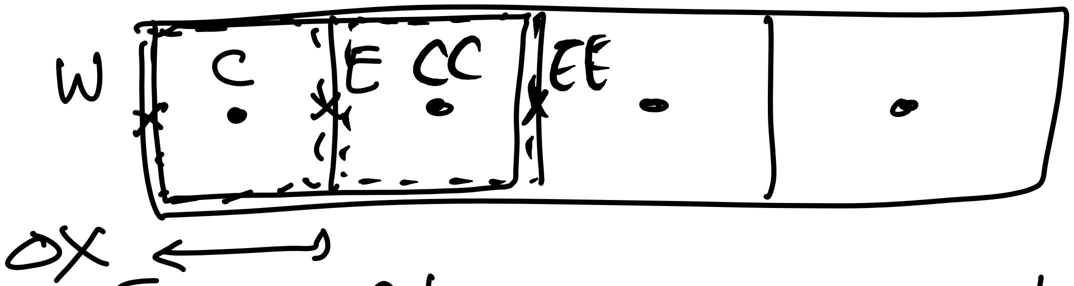
$$\frac{\partial}{\partial x_j}(\rho u_j u_i) = \rho u_j \frac{\partial u_i}{\partial x_j} + \boxed{u_i \frac{\partial}{\partial x_j}(\rho u_j)}$$

$$\frac{\partial}{\partial t}(\rho u_i) = \rho \frac{\partial u_i}{\partial t} + \boxed{u_i \frac{\partial \rho}{\partial t}}$$

$$= 0$$

$$\to \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} + \rho b_i$$

: weakly conservative form



$$\underline{\int \rho u_1 \frac{\partial u_i}{\partial x_1}\, dx_1} = \rho u_1\Big|_C \cdot \frac{\partial u_i}{\partial x_1}\Big|_C \Delta X$$

$$= \rho_C u_{1_C} \cdot \frac{u_{i_E} - u_{i_W}}{\Delta X} \cdot \Delta X$$

$$= \rho_C u_{1_C} \cdot \left(u_{i_E} - u_{i_W}\right)$$

$$+\Big| \quad \rho_{CC} u_{1CC} \cdot \left(u_{i_{EE}} - u_{i_E}\right)$$

$$\boxed{\rightarrow \frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho b_i}$$

$$(\rho b_i = \rho g_i)$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial T_{ij}}{\partial x_j} + \rho b_i \; : \; \text{non-conservative form}$$

③ conservation of scalar quantities

$$\frac{\partial}{\partial t}\int_\Omega \rho\phi \, d\Omega + \int_S \rho\phi(\underline{u}\cdot\underline{n})\, dS = \Sigma f_\phi$$

$$f_\phi^d = \int_S \Gamma \nabla\phi\cdot\underline{n}\, dS \; : \; \text{diffusion}$$

Γ : diffusivity

heat $\rightarrow$ Fourier law

mass diffusion $\rightarrow$ Fick's law

$$\rightarrow \frac{\partial}{\partial t}\int_{\Omega} \rho\phi \, d\Omega + \int_{S} \rho\phi(\underline{u}\cdot\underline{n})\, ds = \int_{S} \Gamma\nabla\phi\cdot\underline{n}\, ds + \int_{\Omega} q_{\phi}\, d\Omega$$

source/sink

$$\rightarrow \frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\phi\underline{u}) = \nabla\cdot(\Gamma\nabla\phi) + q_{\phi}$$

$$\boxed{\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x_j}(\rho\phi u_j) = \frac{\partial}{\partial x_j}\left(\Gamma\frac{\partial\phi}{\partial x_j}\right) + q_{\phi}}$$

energy eq. : $\frac{\partial}{\partial t}(\rho c_p T) + \frac{\partial}{\partial x_j}(\rho c_p T u_j) = \frac{\partial}{\partial x_j}\left(k\frac{\partial T}{\partial x_j}\right) + q_h$

temperature

① Dimensionless form of equations

$x_i^* = x_i / L_0$, $u_i^* = u_i / v_0$, $t^* = t / (L_0/v_0)$ $\cancel{t^* = t/t_0}$

$p^* = p / \rho v_0^2$, $T^* = \dfrac{T - T_0}{T_i - T_0}$

normalized gravitational acceleration vector

$$\rightarrow \begin{cases} \dfrac{\partial u_i^*}{\partial x_i^*} = 0 \\ \dfrac{\partial u_i^*}{\partial t^*} + \dfrac{\partial}{\partial x_j^*}(u_j^* u_i^*) = -\dfrac{\partial p^*}{\partial x_i} + \dfrac{1}{Re} \nabla^{*2} u_i^* + \dfrac{1}{F_r^2} \eta_i \\ \dfrac{\partial T^*}{\partial t^*} + \dfrac{\partial}{\partial x_j^*}(u_j^* T^*) = \dfrac{1}{RePr} \nabla^{*2} T^* \end{cases}$$

$$Re = \frac{\rho v_0 L_0}{\mu}, \quad Fr = \frac{v_0}{\sqrt{g L_0}}, \quad Pr = \mu c_p / k$$

⓪ Simplified mathematical models

continuity eq
N-S eq
> very difficult to solve.

Sol. unique? exist? ⇐ Navier-Stokes eqs. by Roger Temam

① Incompressible flow : $\rho \equiv$ const. ($Ma < 0.3$)

$$\rightarrow \begin{cases} \dfrac{\partial u_i}{\partial x_i} = 0 \\ \dfrac{\partial u_i}{\partial t} + \dfrac{\partial}{\partial x_j}(u_i u_j) = -\dfrac{1}{\rho}\dfrac{\partial p}{\partial x_i} + \dfrac{1}{\rho}\dfrac{\partial}{\partial x_j}\left(\mu \dfrac{\partial u_i}{\partial x_j}\right) + b_i \end{cases}$$

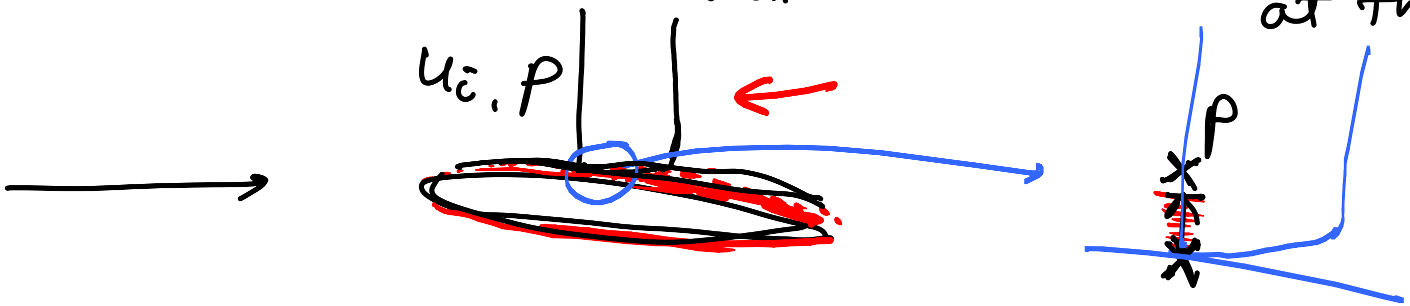
still very difficult to solve.

② Inviscid (Euler) Flow : $\nu \equiv 0$, $\underset{\sim}{T} = -p \underset{\sim}{I}$

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x_i}(\rho u_i) = 0 \\ \dfrac{\partial}{\partial t}(\rho u_i) + \dfrac{\partial}{\partial x_j}(\rho u_i u_j) = -\dfrac{\partial p}{\partial x_i} + \rho b_i \end{cases}$$

Euler eq.

At high Re, viscous effect } are important only
turbulence " } at the near-wall region



Euler eq. → there is no need to put dense grid near the wall

③ Potential flow (inviscid irrotational flow)

$\nu \equiv 0$ $\quad\quad$ $\underline{\omega} = \nabla \times \underline{u} \equiv 0$

ϕ : velocity potential $\quad\quad$ $\underline{u} = \nabla \phi$ $\quad$ $\frac{\partial \phi}{\partial x}$ $\frac{\partial \phi}{\partial y}$

$\underline{u} = \nabla \phi$, $\quad \nabla \cdot \underline{u} = 0 \rightarrow \boxed{\nabla^2 \phi = 0}$ $\quad$ u, v

u
v $\quad \boxed{\phi(x, y, z)}$:

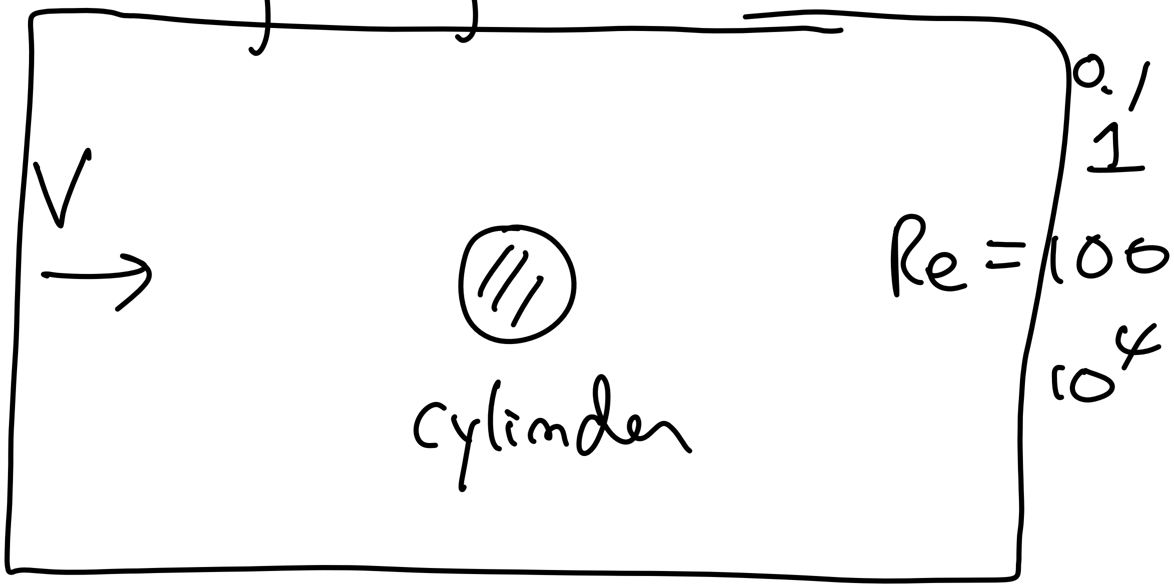
Bernoulli eq. $\frac{p}{\rho} + \frac{v^2}{2} + gz = C$

④ Creeping (Stokes) flow

viscous term
pressure "
body-force " $\gg$ inertia term (nonlinear) $\rightarrow$ Stokes eq. (linear eq.

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j}\right) - \frac{\partial p}{\partial x_i} + \rho b_i = 0$$



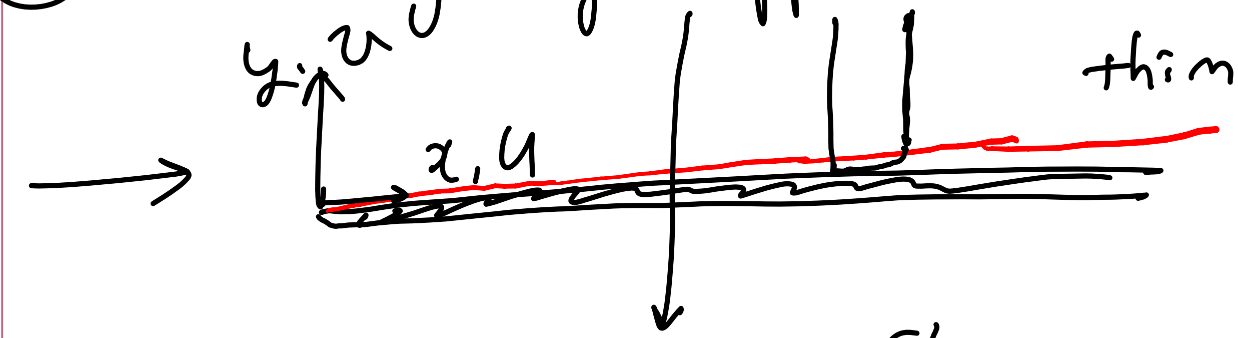
coeff. of volumetric expansion

(5) Boussinesq approximation: $(\rho - \rho_0) g_i = -\rho_0 g_i \beta (T - T_0)$

if density variation is not large, treat ρ as constant in unsteady and convection terms and treat ρ

as variable only in the gravitational form

⑥ Boundary layer approximation



thin shear layer

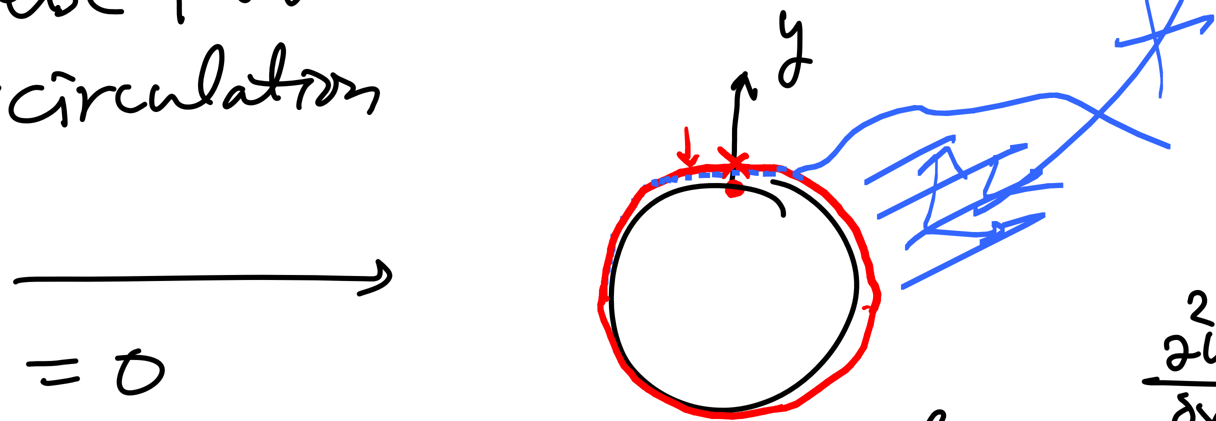
$\frac{\partial u}{\partial y} \neq 0$

$\frac{\partial}{\partial x} \ll \frac{\partial}{\partial y}$

$v \ll u$

no reverse flow

no recirculation

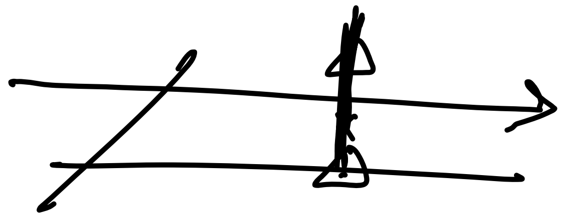


$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

$\frac{\partial^2 u}{\partial x^2}$

2D: $$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) + \frac{\partial}{\partial y}(\rho u v) = -\frac{\partial p}{\partial x} + \mu \frac{\partial^2 u}{\partial y^2}$$

$$\cancel{\frac{\partial}{\partial t}(\rho v)} = -\frac{\partial p}{\partial y}$$



x

$$\frac{\partial p}{\partial y} = 0$$

⊙ Mathematical Classification of Flows

$$a u_{xx} - 2b u_{xy} + u_{yy} = f$$

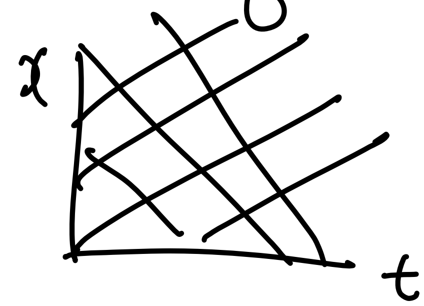
$b^2 - ac > 0 \rightarrow$ hyperbolic $\rightarrow$ two real eigenvalues

$= 0 \rightarrow$ parabolic $\rightarrow$ one " eigenvalue

$< 0 \rightarrow$ elliptic $\rightarrow$ imaginary or complex eigenvalues

Numerical method should respect the properties of the eqs.

① Hyperbolic flows



unsteady inviscid compress. flow

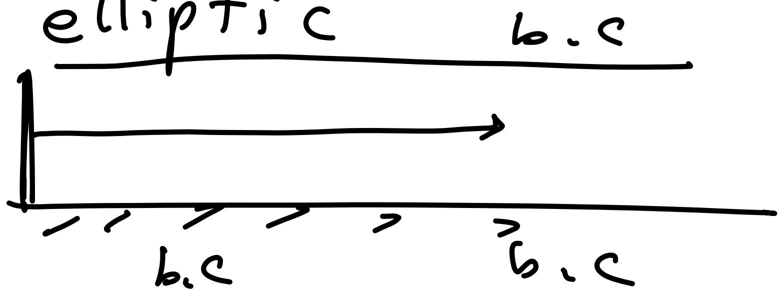
Steady comp. supersonic flow

② parabolic flows

boundary layer approx. → parabolic char.

but pressure should be obtained by potential flow approach → elliptic

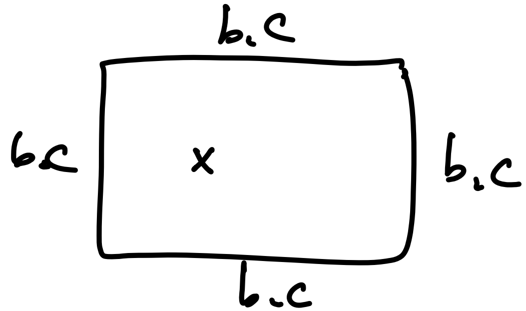
→ mixed type

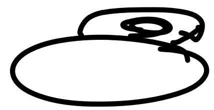


③ elliptic flows

recirculating flow

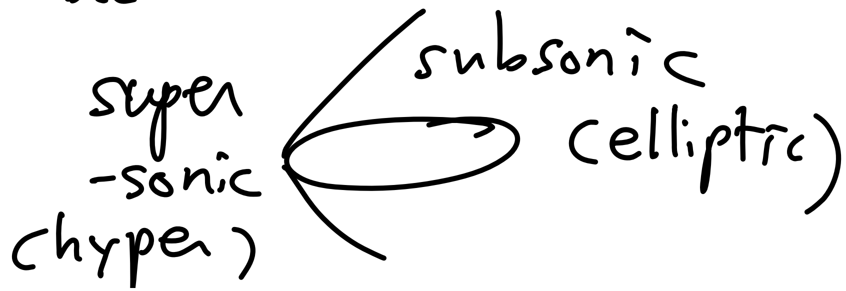
unsteady incomp. flow (mixed)





④ mixed flow types

steady transonic flow



CFD → { Fluid mechanics, Numerical analysis } ⇒ J. Comput. Phys.

Ch. 2 Introduction to Numerical Methods

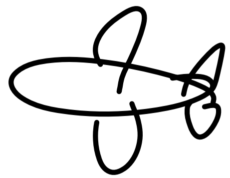
1. Approaches to fluid dynamical problems

- Dimensional analysis & experiments

$$F_D = \underbrace{C_D} \cdot A \cdot \frac{1}{2} \rho U^2$$

$\underline{C_D \text{ vs. } Re}$

$$Re = \frac{U_\infty d}{\nu}$$



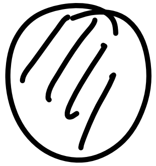
$Ma = 0.9$

WT

$1/10$

$U \uparrow 10 \rightarrow Ma = 9$

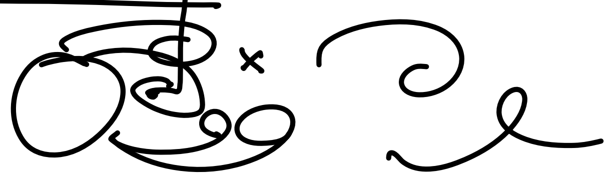
Re & Ma , Re & Fr , Re & We

→  experiment : efficient means to measure global parameters like drag, lift, heat transfer rate, etc.

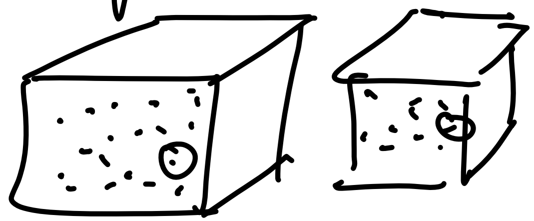
→ most of time, no detailed measurement.

i.e. some important phenomena are missing like flow separation

~~not true~~ from PIV people.



$\Delta s / \Delta t$



t $\quad$ t_{tot}

⇒ use CFD

but errors in CFD ... turbulence → constants

CFD requires "good" experiments ...

2. Components of a numerical sol. method

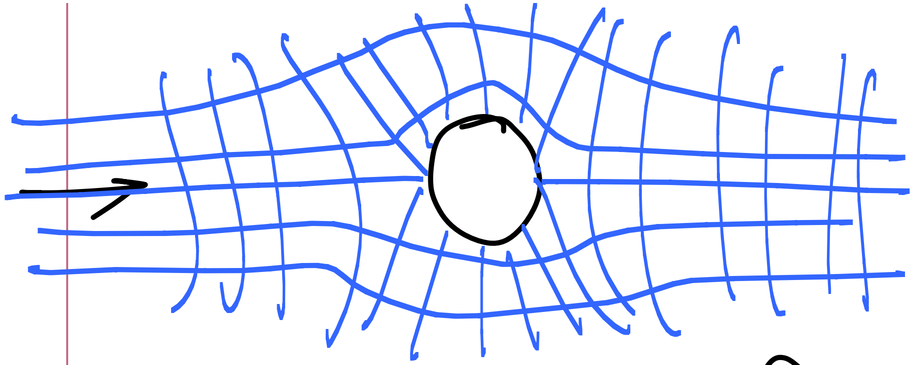
① mathematical model

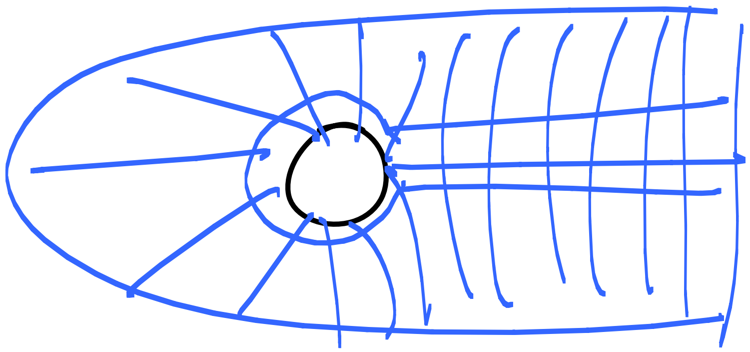
Governing eqs., b.c's, i.c's.

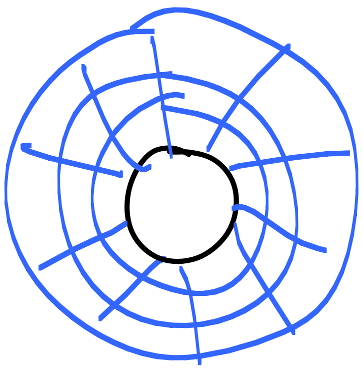
② discretization method

FDM, FVM, FEM, etc.

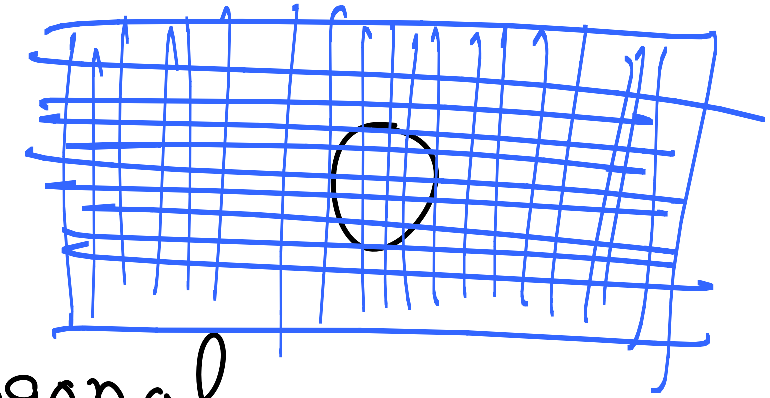
③ coordinates and basis vector systems







Cartesian
cylindrical
spherical
curvilinear orthogonal
" non-orthogonal
covariant or contra-variant



④ Grid

- Structured grid

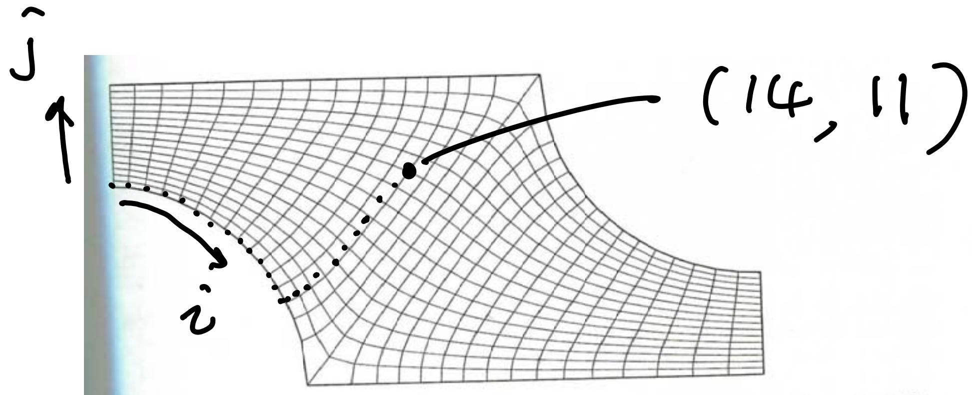


Fig. 2.1. Example of a 2D, structured, non-orthogonal grid, designed for calculation of flow in a symmetry segment of a staggered tube bank

- Block-structured grid with matching interface

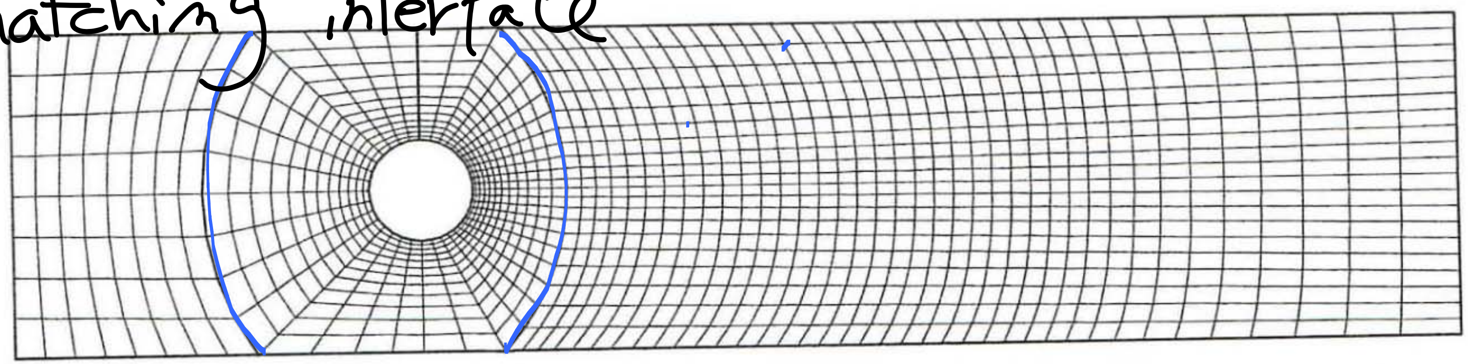


Fig. 2.2. Example of a 2D block-structured grid which matches at interfaces, used to calculate flow around a cylinder in a channel

can be treated in a fully conservative manner without " "

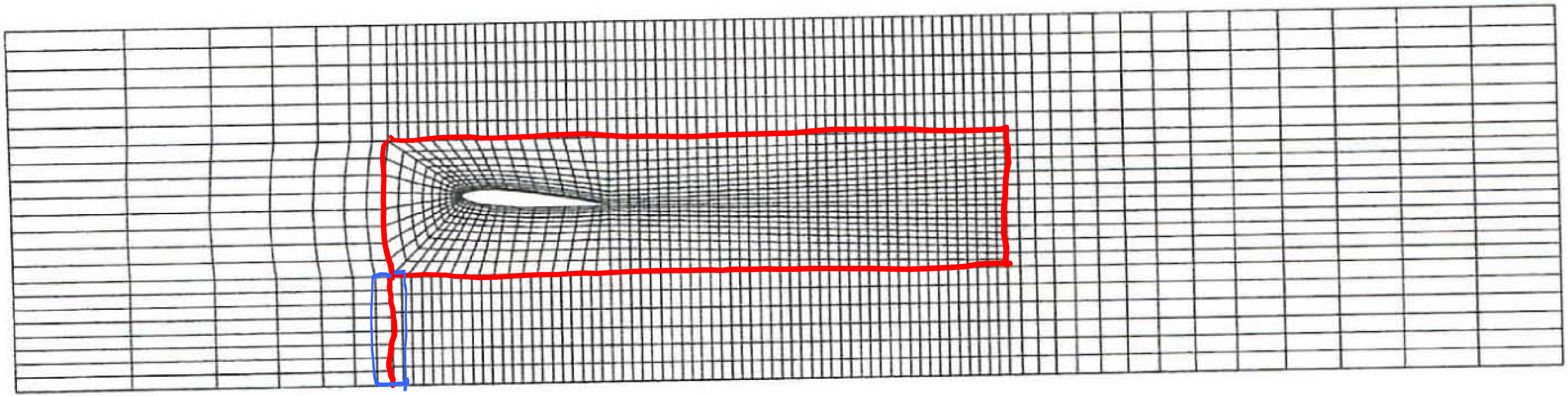


Fig. 2.3. Example of a 2D block-structured grid which does not match at interfaces, designed for calculation of flow around a hydrofoil under a water surface

with overlapping blocks
(composite grid, chimera grid) → difficulty in conserving properties
good for complex domain.

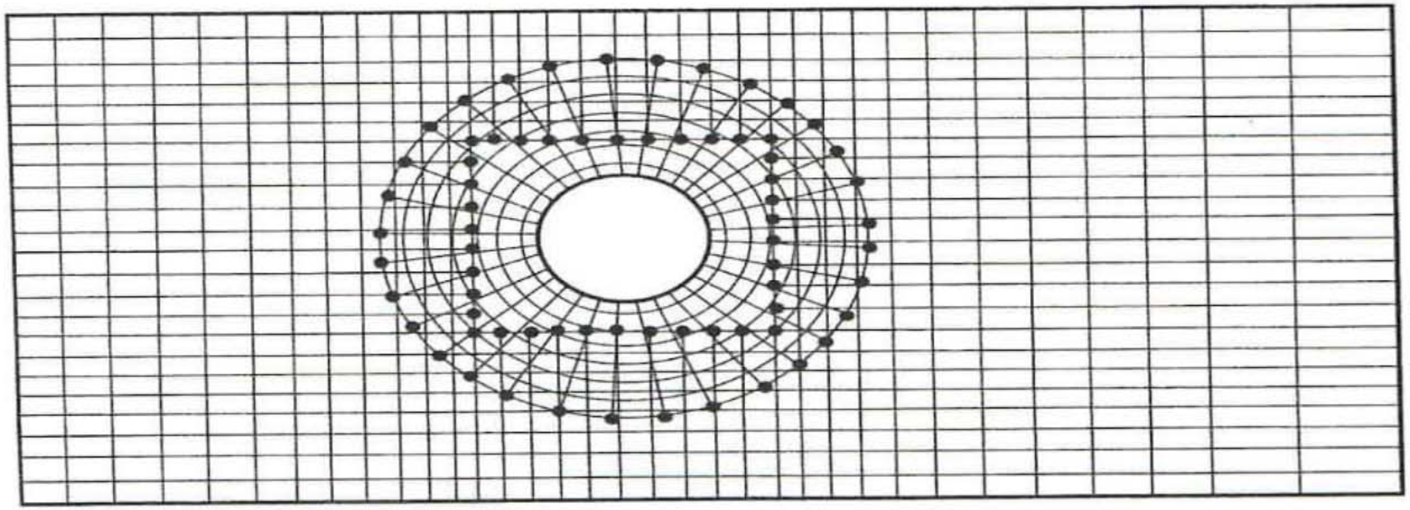


Fig. 2.4. A composite 2D grid, used to calculate flow around a cylinder in a channel

- Unstructured grid
  - very complex geometries
  - good for FVM, FEM
  - irregularity of the data structure
    $\longrightarrow$ sparse matrix

$$\underline{A}u = \phi$$

$$u \downarrow \quad \begin{matrix} u_1 \\ u_2 \\ \vdots \\ u_{100} \end{matrix}$$

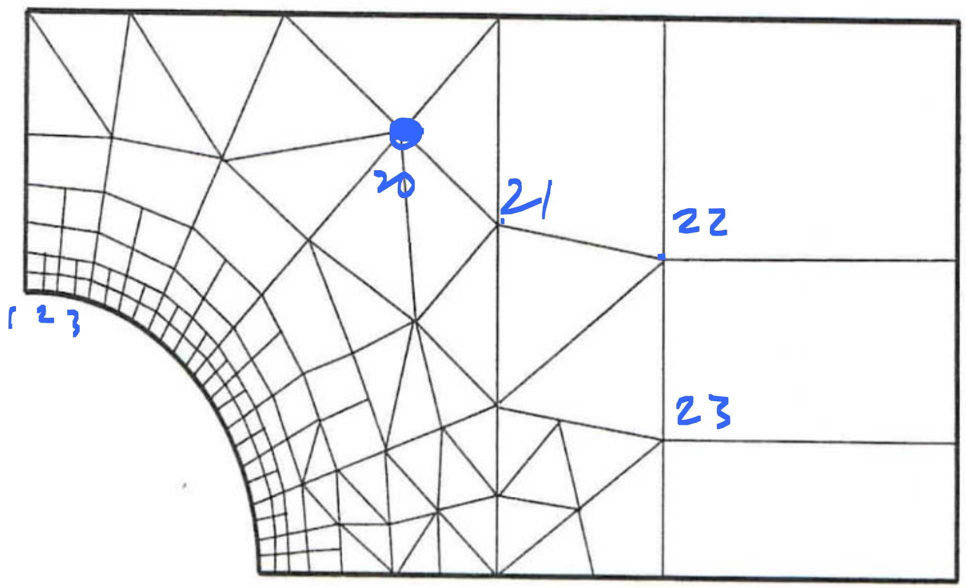


Fig. 2.5. Example of a 2D unstructured grid

grid generation is difficult.

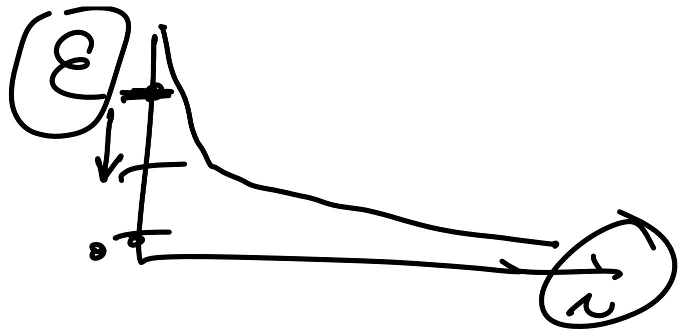
Book : Numerical grid generation by Thompson et al. (1985)

⑤ Finite approximations … accuracy, memory

⑥ Solution method for nonlinear algebraic eqs.

⑦ convergence criteria

⑧ "good" physics



3. Properties of numerical sol. methods

① consistency : modified PDE → truncation error

→ should go to zero when $\Delta x \to 0$ & $\Delta t \to 0$

② stability : von Neumann stability analysis

modified wavenumber analysis

→ absolutey stable

conditionally stable

unstable

③ convergence : resolution test
(only by numerical experiments)

$100 \times 100 \rightarrow 200 \times 200$

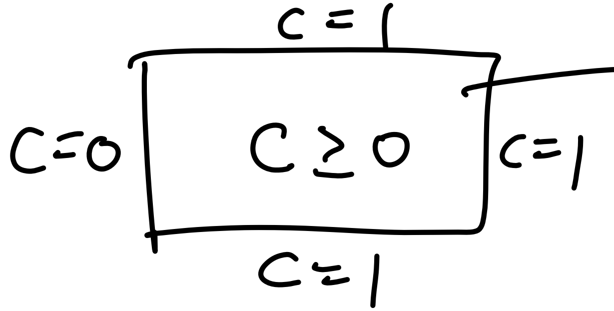
$1000 \times 1000 \times 1000 \rightarrow \cancel{2000 \times 2000 \times 2000}$ $\quad 1500 \times 1000 \times 1000$

$1 \; : \; \cancel{16}$ $\quad 1000 \times 1500 \times 1000$

④ conservation : strong conservative form of G.E.
+ FVM → conservative

non-conservative scheme → artificial source/sink
→ goes to zero as $\Delta x \to 0$

⑤ boundedness : difficult to guarantee



→ $c < 0$ or $c > 1$

some 1st-order schemes guarantees this property.

but higher-order schemes can produce unbounded sols.

⑥ realizibility : models of phenomena should be correct.

turbulence, combustion, multi-phase flow

⑦ accuracy

i) modeling error : actual flow vs. exact sol. of math. model

N-S eq. (N-S eq + TM)

ii) discretization error : exact sol. of GE vs. exact sol. of algebraic eqs.

iii) iteration error : iterative vs. exact sols. of algebraic eqs.

4. Discretization approaches

① FDM : oldest method

PDE ⟶ algebraic eq.

simple & effective

easy to obtain higher-order scheme on regular grids

conservation is not enforced
restricted to simple geometries

② FVM : integral eq. → algebraic eq.
suitable for complex geometries
higher order schemes are difficult
most popular in engineering

③ FEM : eqs. are multiplied by a weighting fct
in a way that guarantees continuity of the
sol. across element boundaries
arbitrary geometries

sparse matrix.

Ch.3 Finite Difference Methods (FDM)

$$\frac{\partial(\rho\phi)}{\partial t} + \underbrace{\frac{\partial}{\partial x_j}(\rho u_j \phi)}_{\text{convection}} = \underbrace{\frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right)}_{\text{diffusion}} + S_\phi$$

$$\xrightarrow{\text{steady}} \quad \frac{\partial}{\partial x_j}(\rho u_j \phi) = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S_\phi$$

1. Approximation of the 1st derivative

(1) Taylor series expansion

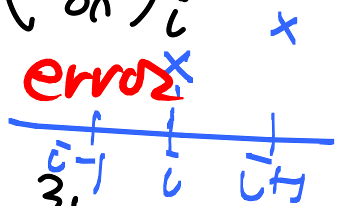
$$\phi(x) = \phi(x_i) + (x-x_i)\left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(x-x_i)^2}{2!}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i$$

$$+ \frac{(x-x_i)^3}{3!}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + \cdots + \frac{(x-x_i)^n}{n!}\left(\frac{\partial^n\phi}{\partial x^n}\right)_i + HOT$$

@ $x = x_{i+1}$,

$$\boxed{\left(\frac{\partial\phi}{\partial x}\right)_i = \frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}} \underbrace{- \frac{x_{i+1}-x_i}{2}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i}_{\text{leading truncation error}} - \frac{(x_{i+1}-x_i)^2}{6}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + HOT$$

forward difference (FD)



@ $x = x_{i-1}$

$$\boxed{\left(\frac{\partial\phi}{\partial x}\right)_i = \frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}} \underline{+ \frac{x_i-x_{i-1}}{2}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i} - \frac{(x_i-x_{i-1})^2}{6}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + HOT$$

backward difference (BD)

@ both

$$\boxed{\left(\frac{\partial\phi}{\partial x}\right)_i = \frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}}} \underline{- \frac{(x_{i+1}-x_i)^2-(x_i-x_{i-1})^2}{2(x_{i+1}-x_{i-1})}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i}$$

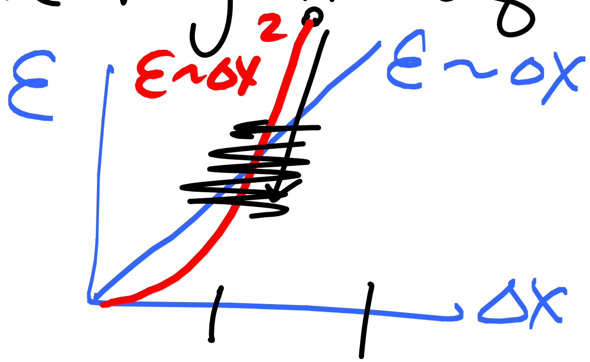
central difference (CD)

$$-\frac{(x_{i+1}-x_i)^3+(x_i-x_{i-1})^3}{6(x_{i+1}-x_{i-1})}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + HOT$$

truncation error $\epsilon_T = (\Delta x)^n \alpha_{n+1} + (\Delta x)^{n+1}\alpha_{n+2} + \cdots$

- The order of an approximation indicates how fast the errors is reduced when the grid is refined.

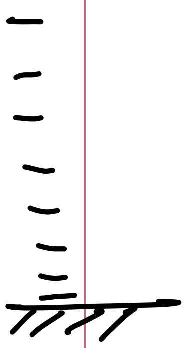
It does not indicate the absolute magnitude of the error.

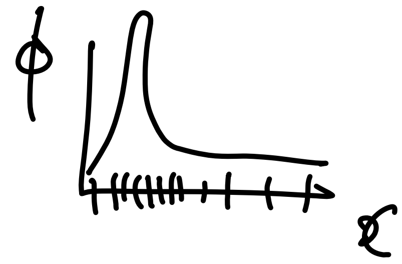


- When $\Delta x_{i+1} (= x_{i+1} - x_i) = \Delta x_i (= x_i - x_{i-1})$, CD becomes 2nd-order accurate.

- ϵ_T for CD :

$$\epsilon_T = -\underbrace{\frac{(\Delta x_{i+1})^2 - (\Delta x_i)^2}{2(\Delta x_{i+1} + \Delta x_i)}}_{O(\Delta x)} \left(\frac{\partial^2 \phi}{\partial x^2}\right)_i - \frac{(\Delta x_{i+1})^3 + (\Delta x_i)^3}{6(\Delta x_{i+1} + \Delta x_i)} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + HOT$$





why use non-uniform grid?

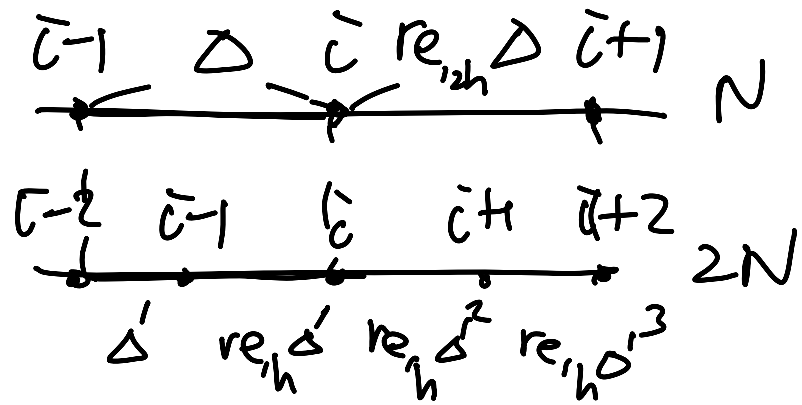
$\rightarrow$ to resolve large gradients of ϕ

If $\boxed{\Delta x_{i+1} = \underline{r_e} \Delta x_i}$, then

$$\epsilon_T = \frac{1-r_e}{2}\,\delta x_i\left(\frac{\partial^2\phi}{\partial x^2}\right)_i - \frac{1-r_e+r_e^2}{6}\,\delta x_i^2\left(\frac{\partial^3\phi}{\partial x^3}\right)_i + HOT$$

As $r_e \to 1$, $\frac{1-r_e}{2} \to 0$

What happens when grid is refined in CD?



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

$$\Delta(1+r_{e,2h})$$

$$= \Delta'(1+r_{e_h}+r_{e_h}^2+r_{e_h}^3)$$

✓ $r_{e,h} = \sqrt{r_{e,2h}}$

✓ $(\delta x_i)_{2h} = (\delta x_i)_h + (\delta x_{i-1})_h = (1+r_{e_h})(\delta x_{i-1})_h$

the ratio of the leading truncation errors $= \underbrace{\dfrac{(1-re_{,2h})\,\Delta x_{i,2h}}{(1-re_{,h})\,\Delta x_{i,h}}}$ $= \dfrac{(1+re_{,h})^2}{re_{,h}} \geq 4$

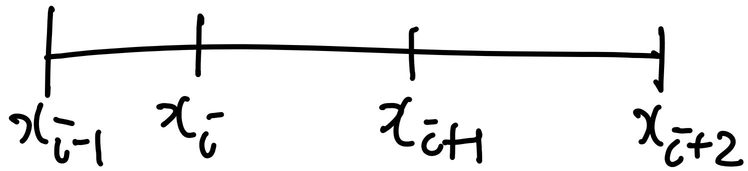
when $re=1 \rightarrow 4$ (second order)

$re \neq 1$ (ie. $re>1$, $re<1$) $\rightarrow\ >4$ (faster than 2nd-order)

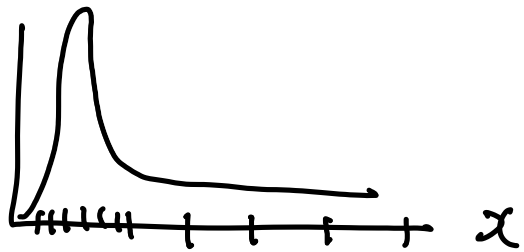
good !

Even when the grid is properly non-uniform, the truncation error is reduced as in a second-order scheme when the grid is refined !

non-uniform grids



CD $\longrightarrow$ $\underline{O(\Delta x)}$

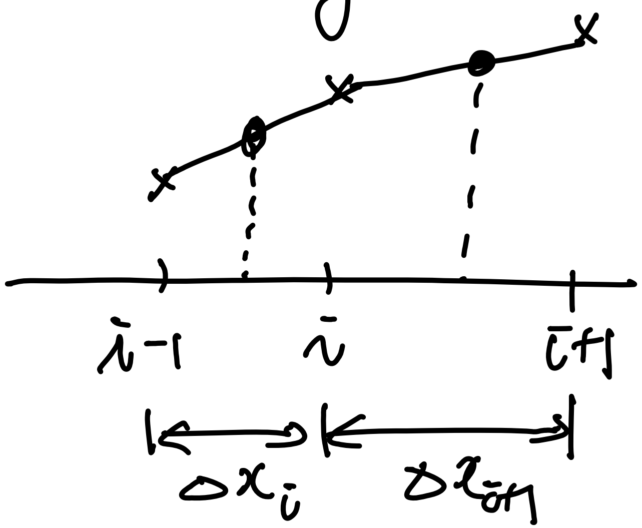


$\rightarrow$ $\underline{\Delta x_{i+1} = r_e \Delta x_i}$

the ratio of the leading truncation errors

$$r_T = \frac{\varepsilon_{Th}}{\varepsilon_{T2h}} = \frac{(1+r_{eh})^2}{r_{eh}} \geq 4 \rightarrow \text{at least second order!}$$

- Absolutely second order



$$\left.\frac{\partial \phi}{\partial x}\right|_i = \frac{\Delta x_{i+1} \left.\frac{\partial \phi}{\partial x}\right|_{i-\frac{1}{2}} + \Delta x_i \left.\frac{\partial \phi}{\partial x}\right|_{i+\frac{1}{2}}}{\Delta x_i + \Delta x_{i+1}}$$

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

$$\underbrace{- \frac{\Delta x_{i+1}\Delta x_i}{6} \left.\frac{\partial^3 \phi}{\partial x^3}\right|_i}_{\hookrightarrow\ \theta(\Delta x^2)} + HOT$$

(2) Polynomial fitting

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

ex) parabola for x_{i-1}, x_i, x_{i+1}

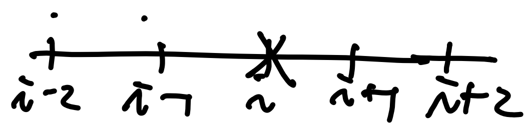
$$\rightarrow \left.\frac{\partial \phi}{\partial x}\right|_i = \frac{\phi_{i+1}(\Delta x_i)^2 - \phi_{i-1}(\Delta x_{i+1})^2 + \phi_i\left[(\Delta x_{i+1})^2 - (\Delta x_i)^2\right]}{\Delta x_{i+1}\,\Delta x_i\,(\Delta x_i + \Delta x_{i+1})}$$

second order

other polynomials, splines etc.

In general, approximation of the 1st derivative possesses a truncation error of the same order as the degree of the polynomial used to approximate the function.

3rd-order polynomials



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

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

4th-order polynomials

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

For convection terms, $u\frac{\partial\phi}{\partial x}$

$u>0 \rightarrow$ BD
$u<0 \rightarrow$ FD

} upwind schemes

$$u\frac{\partial \phi}{\partial x}\Big|_i = \begin{cases} u_i \cdot \dfrac{\phi_i - \phi_{i-1}}{\Delta x} & \text{BD} \quad \text{if } u_i > 0 \\ u_i \dfrac{\phi_{i+1} - \phi_i}{\Delta x} & \text{FD} \quad \text{if } u_i < 0 \end{cases}$$

$$\frac{\partial \phi}{\partial x}\Big|_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} - \underbrace{\boxed{\frac{\Delta x}{2}\frac{\partial^2 \phi}{\partial x^2}\Big|_i}}_{O(\Delta x)} + \cdots$$

First-order upwind scheme

→ very inaccurate

truncation error sometimes bigger than actual diffusivity.

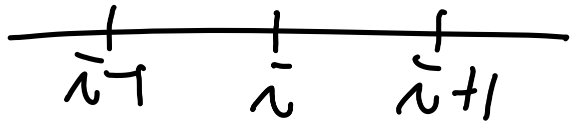
$$u\boxed{\frac{\partial \phi}{\partial x}} + v\frac{\partial \phi}{\partial y} = \boxed{\Gamma}\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) + \boxed{\frac{\Delta x}{2}}\frac{\partial^2 \phi}{\partial x^2}$$

← false diffusion.

Higher-order upwind scheme is costive.

$\longrightarrow$ use CD.

(3) compact schemes



$\rightarrow$ 2nd order accuracy

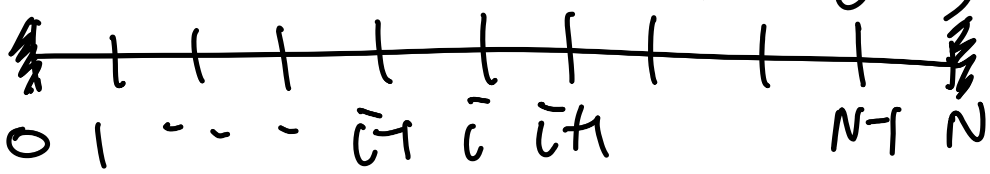
$\rightarrow$ increase the accuracy w/ the same grids but by including derivatives at $i-1$ and $i+1$.

(Padé scheme)

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

$$\rightarrow \left.\frac{\partial\phi}{\partial x}\right|_{i-1} + 4\left.\frac{\partial\phi}{\partial x}\right|_{i} + \left.\frac{\partial\phi}{\partial x}\right|_{i+1} = 3\,\frac{\phi_{i+1}-\phi_{i-1}}{\Delta x} + O(\Delta x^4)$$

TDMA → $O(N)$



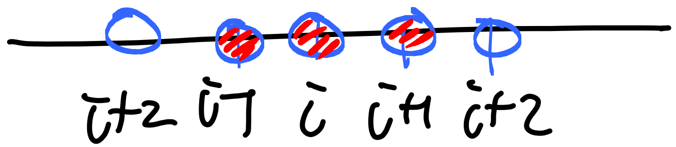
$\underline{i = 1, \cdots, N-1}$ **compact**

* A family of compact centered approximations of up to sixth order can be written as

$$\Rightarrow \alpha \left.\frac{\partial \phi}{\partial x}\right|_{i+1} + \left.\frac{\partial \phi}{\partial x}\right|_{i} + \alpha \left.\frac{\partial \phi}{\partial x}\right|_{i-1} = \beta \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + \gamma \frac{\phi_{i+2} - \phi_{i-2}}{4\Delta x}$$

$A\phi = b$ → 5 pts

3pts → TDMA



Scheme	Truncation error	α	β	γ

CDS-2	$\frac{(\Delta x)^2}{3!}\frac{\partial^3\phi}{\partial x^3}$	0	1	0
CDS-4	$-\frac{13(\Delta x)^4}{3\cdot 3!}\frac{\partial^5\phi}{\partial x^5}$	0	$\frac{4}{3}$	$-\frac{1}{3}$
Padé-4	$\frac{(\Delta x)^4}{5!}\frac{\partial^5\phi}{\partial x^5}$	$\frac{1}{4}$	$\frac{3}{2}$	0
Padé-6	$\frac{4(\Delta x)^6}{7!}\frac{\partial^7\phi}{\partial x^7}$	$\frac{1}{3}$	$\frac{14}{9}$	$\frac{1}{9}$

2. Approximation of the 2nd derivative

(1) Taylor series expansion

(2) Use a formula for 1st derivative

ex) $$\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial x}\right) = \frac{\left.\frac{\partial \phi}{\partial x}\right|_{i+\frac{1}{2}} - \left.\frac{\partial \phi}{\partial x}\right|_{i-\frac{1}{2}}}{\frac{1}{2}(x_{i+1} - x_{i-1})} + \cdots$$

(3) Polynomial fitting

In general, the truncation error of the approx. to the 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 the 2nd derivative to increase the accuracy of approx. to the 1st derivative.

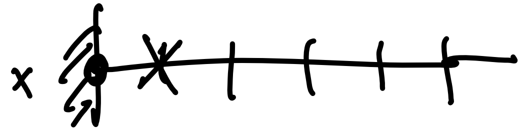
$$\left.\frac{\partial \phi}{\partial x}\right|_i = \underbrace{\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}}_{\text{FD}} - \frac{1}{2}\underbrace{(x_{i+1}-x_i)}_{O(\Delta x)}\underbrace{\left.\frac{\partial^2 \phi}{\partial x^2}\right|_i}_{\Uparrow\ \text{CD} + O(\Delta x)} + \cdots$$

$O(\Delta x^2)$

$\rightarrow$ 2nd-order accurate

* higher order schemes need <u>more</u> grid points

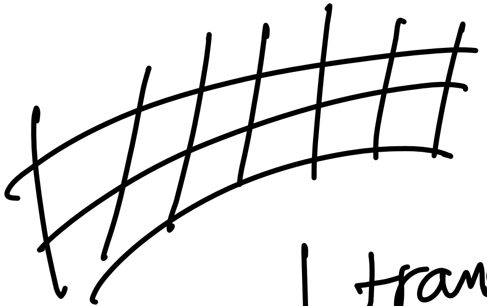
  $\rightarrow$ more complex eqs to solve
  more complex to treat b.c.



* second-order accuracy is good enough for engineering applications.

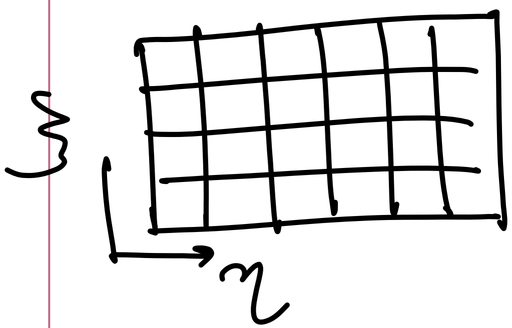
$$\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right) = \frac{1}{\frac{1}{2}(x_{i+1}-x_{i-1})}\left[\left(\Gamma\frac{\partial \phi}{\partial x}\right)_{i+\frac{1}{2}} - \left(\Gamma\frac{\partial \phi}{\partial x}\right)_{i-\frac{1}{2}}\right]$$

3. Mixed derivatives $\dfrac{\partial^2 \phi}{\partial x \partial y}$ occurs when non-orthogonal grids are used.



$\nabla^2 \phi$

$\downarrow$ transf.



$\dfrac{\partial^2 \phi}{\partial \eta^2}$ $\quad \underline{\dfrac{\partial^2 \phi}{\partial \eta \partial \xi}}$ $\quad \dfrac{\partial^2 \phi}{\partial \xi^2}$

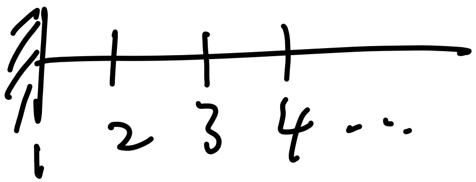
$$\frac{\partial^2 \phi}{\partial \eta \partial \xi} = \frac{\partial}{\partial \eta}\left(\frac{\partial \phi}{\partial \xi}\right)$$

4. Implementation of boundary conditions

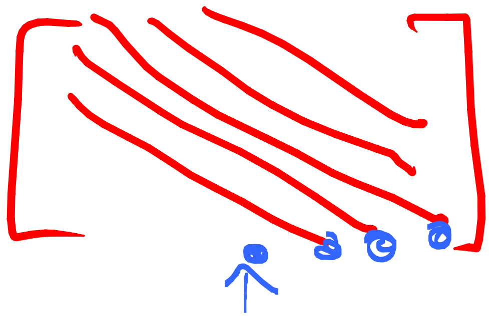
Dirichlet b.c. : $\phi_1 = c$

Neumann b.c. : $\left.\frac{\partial \phi}{\partial x}\right|_1 = 0$

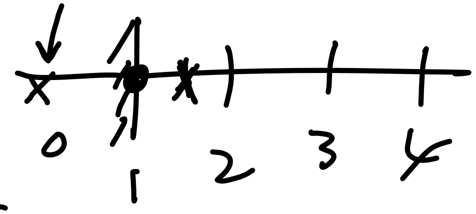
$\longrightarrow$ when high order scheme is used at interior pt., one may use a different scheme at $j=2$: eg.,



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



Neumann b.c. : $\left.\frac{\partial\phi}{\partial x}\right|_1 = 0 = \underline{\frac{\phi_2-\phi_1}{x_2-x_1}}$

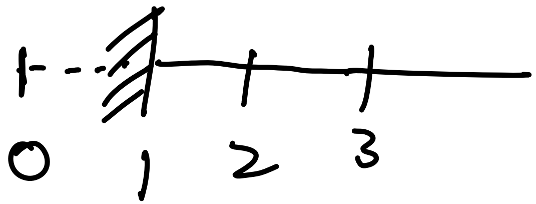


Usually the approx. of the b.d. value or near the b.d. is of lower order than the approx. used deeper in the interior and may be one-sided difference.

* <u>Issues of global accuracy</u> (Fletcher's book)

Dirichlet b.c. $\rightarrow$ no prob.

Neumann b.c. $\rightarrow$ $\boxed{\left.\frac{\partial\phi}{\partial x}\right|_1 = c(t)}$



$$\frac{\partial\phi}{\partial t} - \alpha\frac{\partial^2\phi}{\partial x^2} = 0 \qquad (1)$$

CD2 + "Implicit" Euler (IE) $\quad \frac{\partial y}{\partial t} = f(y) \rightarrow \frac{y^{n+1} - y^n}{\Delta t} = f(y^{n+1}) + O(\Delta t)$

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

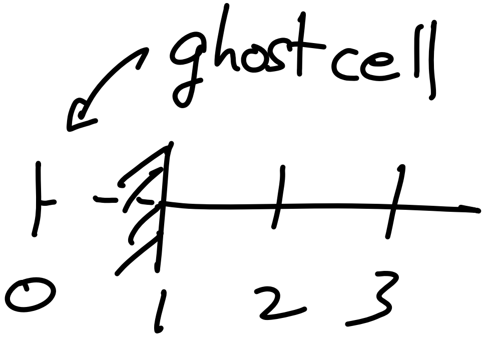
$O(\Delta t, \Delta x^2)$

CD2 + "Explicit" Euler (EE) $\quad \frac{y^{n+1} - y^n}{\Delta t} = f(y^n) + O(\Delta t)$

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

$O(\Delta t, \Delta x^2)$

1st order b.c. $\quad \frac{\phi_2^{n+1} - \phi_1^{n+1}}{\Delta x} = c^{n+1}$



$$\rightarrow \phi_1^{n+1} = \phi_2^{n+1} - c^{n+1}\Delta x \quad \text{— ③}$$

or $\quad \phi_1^{n} = \phi_2^{n} - c^{n}\Delta x \quad \text{— ③}'$

2nd order b.c. $\dfrac{\phi_2^{n+1}-\phi_0^{n+1}}{2\Delta x} = c^{n+1} \rightarrow \phi_0^{n+1} = \phi_2^{n+1} - 2c^{n+1}\Delta x$ — ④

or $\phi_0^{n} = \phi_2^{n} - 2c^{n}\Delta x$ — ④'

Apply ② (or ②') at $j=1$ and use ϕ_0^{n+1} from ④ (or ④').

$$\longrightarrow \left(1+2\boxed{\frac{\alpha\Delta t}{\Delta x^2}}\right)\phi_1^{n+1} - 2\boxed{\frac{\alpha\Delta t}{\Delta x^2}}\,\phi_2^{n+1} = \phi_1^{n} - 2\boxed{\frac{\alpha\Delta t}{\Delta x^2}}\cdot\underline{\Delta x}\cdot c^{n+1} \quad \text{— ⑤}$$

or (②' & ④')

$$\phi_1^{n+1} = -2\frac{\alpha\Delta t}{\Delta x^2}\cdot\Delta x\cdot c^{n} + \left(1-2\frac{\alpha\Delta t}{\Delta x^2}\right)\phi_1^{n} + 2\frac{\alpha\Delta t}{\Delta x^2}\phi_2^{n} \quad \text{— ⑤'}$$

Ex) $\dfrac{\partial\phi}{\partial t} - \alpha\dfrac{\partial^2\phi}{\partial x^2} = 0 \qquad 0.1 \le x \le 1 \longleftarrow$ HW1 (1 week)

b.c. $\dfrac{\partial\phi}{\partial x} = 2 - 2\pi\sin 0.5\pi\cdot e^{-\alpha\left(\frac{\pi}{2}\right)^2 t}$ @ $x = 0.1$

$\phi = 2$ @ $x = 1$

i.c. $\phi = 2x + 4\cos 0.5\pi x \cdot e^{-\alpha\left(\frac{\pi}{2}\right)^2 \cdot 0.8}$ @ $t = 0.8$

$\rightarrow \phi_{exact} = 2x + 4\cos 0.5\pi x \, e^{-\alpha\left(\frac{\pi}{2}\right)^2 t}$

$\left(S \equiv \frac{\alpha \Delta t}{\Delta x^2} = 0.3 \right)$

@ $t = 9$

	Δx	0.225	0.1125	0.05625	convergence rate, r
②' + ③'	rms error	0.1958	0.09978	0.03538	1.2
②' + ⑤'	//	0.1753×10^{-2}	0.4235×10^{-3}	0.1064×10^{-3}	2.0

(error distribution) $\Delta x = 0.225$

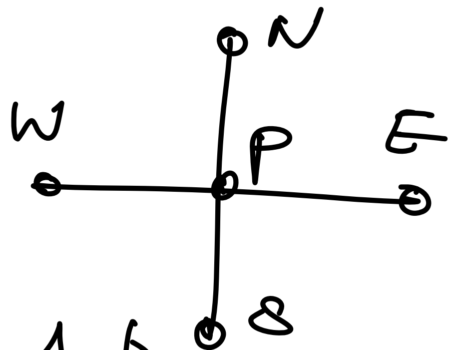
x	0.1	0.325	0.550	0.775	1
②′ + ③′	-0.3799	-0.1989	-0.08366	-0.02610	0
②′ + ⑤′	0.332×10^{-3}	-0.224×10^{-2}	-0.272×10^{-2}	-0.173×10^{-2}	0

biggest error due to 1st-order b.c. approx.

$\boxed{\text{HW 1 : do it for max. error !}}$ (due: Mar. 28)

In conclusion, 1st order b.c. approx. deteriorates numerical sol.

5. Algebraic eqs.



FDM $\longrightarrow A_P \phi_P + \sum_l A_l \phi_l = Q_P$

2nd order $\rightarrow A_W \phi_W + A_S \phi_S + A_P \phi_P + A_N \phi_N + A_E \phi_E = Q_P$

$$\begin{bmatrix} \ddots & \ddots & \ddots & & \ddots & 0 \\ 0 & \ddots & \ddots & 0 & & \ddots \\ A_W & A_S & A_P & A_N & & A_E \\ & \ddots & \ddots & \ddots & & 0 \\ 0 & 0 & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ \phi_W \\ \vdots \\ \phi_S \\ \phi_P \\ \phi_N \\ \vdots \\ \phi_E \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

6. Discretization errors

* truncation error (Taylor series truncation)

$$\mathcal{L}(\Phi) = L_h(\Phi) + \tau_h = 0 \qquad \Phi : \text{exact sol.}$$

diff'l operator   difference operator   truncation error

h : grid size

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

Then, discretization error ε_h^d

$$\varepsilon_h^d = \Phi - \phi_h$$

$$L_h(\phi_h) = L_h(\Phi - \varepsilon_h^d) = -\tau_h - L_h(\varepsilon_h^d) = 0$$

$$\rightarrow \quad \underline{L_h(\varepsilon_h^d) = -\tau_h} \quad \Leftarrow$$ truncation error is a source of the discretization error.

Since we don't know the mag. of τ_h, we have to do grid refinement test.

For sufficiently fine grids,

$$\varepsilon_h^d \simeq \alpha h^p + HOT \qquad p: \text{order of scheme.}$$

$$\Phi = \phi_h + \varepsilon_h^d = \phi_{2h} + \varepsilon_{2h}^d$$

$$\rightarrow \quad \phi_h + \alpha h^p + \cancel{HOT} = \phi_{2h} + \alpha(2h)^p + \cancel{HOT}$$

$$\rightarrow \begin{cases} \phi_h - \phi_{2h} = \alpha h^p (2^p - 1) \\ \phi_{2h} - \phi_{4h} = \alpha h^p 2^p (2^p - 1) \end{cases}$$

$$\rightarrow \quad p = \log\left(\frac{\phi_{2h} - \phi_{4h}}{\phi_h - \phi_{2h}}\right) \Big/ \log 2$$

useful tool to check the order of accuracy in practice when h is fine enough and convergence is monotonic.

Also,

$$\varepsilon_h^d = \alpha h^p = \Phi - \phi_h$$

$$\varepsilon_{2h}^d = 2^p \alpha h^p = \Phi - \phi_{2h}$$

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

$$\rightarrow \varepsilon_h^d = \frac{\phi_h - \phi_{2h}}{2^p - 1}$$

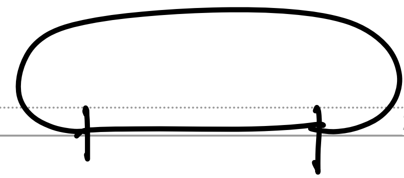
↗ to get p

If we have sols. of ϕ_h, ϕ_{2h} (and ϕ_{4h}), we could get better sol. of Φ than ϕ_h by using ε_h^d

$$\rightarrow \Phi \doteq \phi_h + \varepsilon_h^d$$

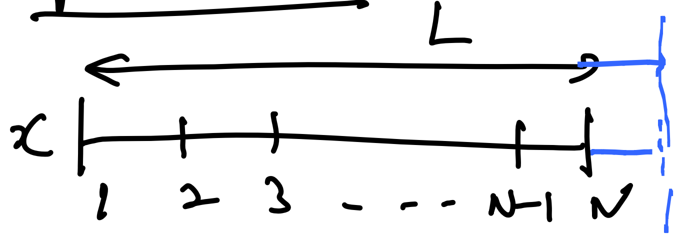
↳ Richardson extrapolation.

6. Introduction to spectral method



(1) Fourier transform

a uniformly spaced set of pts., periodic



discrete Fourier series

$$\begin{cases} f(x_i) = \sum_{q=-N/2}^{N/2-1} \boxed{\hat{f}(k_q)}\, e^{ik_q x_i} \\ \hat{f}(k_q) = \frac{1}{N} \sum_{i=1}^{N} f(x_i)\, e^{-ik_q x_i} \end{cases}$$

↑

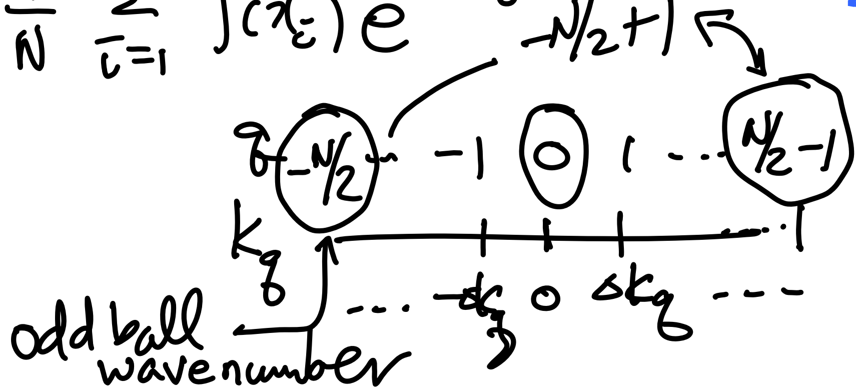
Fourier coeff. of f.

$\Delta k_q \cdot L = 2\pi$ N: even number

$$\Delta k_q = \frac{2\pi}{L} = \frac{2\pi}{N \Delta x}$$

$$k_q = \Delta k_q \cdot q = \frac{2\pi q}{N \Delta x}$$

$q = -N/2, \dots, 0, 1, \dots N/2-1$



$$\frac{df}{dx} = \sum_{q=-N/2}^{N/2-1} \boxed{i k_q \hat{f}(k_q)} e^{i k_q x_i}$$ Fourier coeff. of $\frac{df}{dx}$

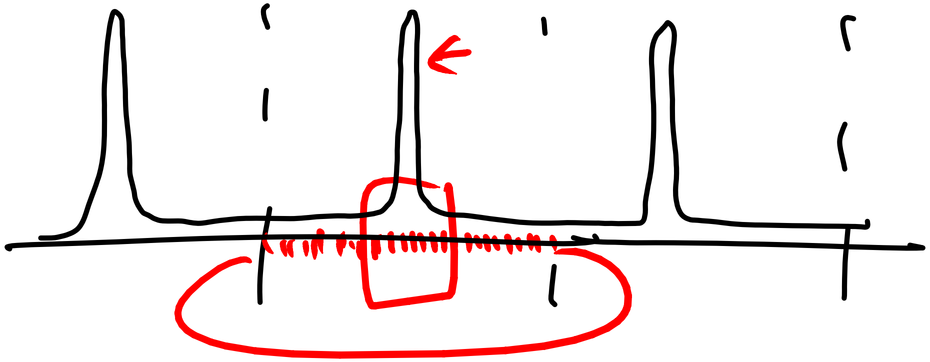
To get df/dx. ① FT of $f(x_i)$ to get $\hat{f}(k_q)$

② obtain $i k_q \hat{f}(k_q)$

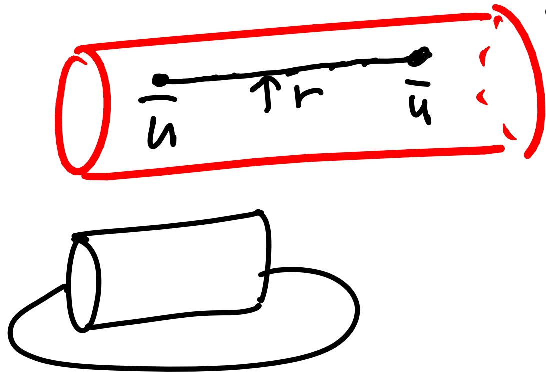
③ IFT to get df/dx

- higher derivatives are easy to obtain $\frac{d^2f}{dx^2} \rightarrow -k_q^2 \hat{f}$
- error decreases exponentially with N when N is large enough.

much more accurate than FD, FE, FV.



pipe flow fully developed flow



but it may be more than FD, FV, FE when N is small.

cost of FT $\longrightarrow O(N^2)$

" FFT $\longrightarrow O(N \log_2 N)$

(2) Modified wavenumber

$$\frac{d\phi}{dx} \longrightarrow \sum i\underset{\sim}{k}\hat{\phi} e^{ikx} \quad \text{(spectral or exact)}$$

• $\phi = e^{ikx}$

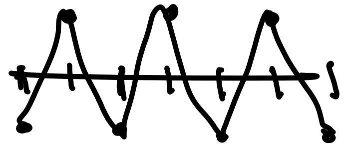
CD2 : $\dfrac{d\phi}{dx} = \dfrac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} = \dfrac{e^{ik(x+\Delta x)} - e^{ik(x-\Delta x)}}{2\Delta x}$

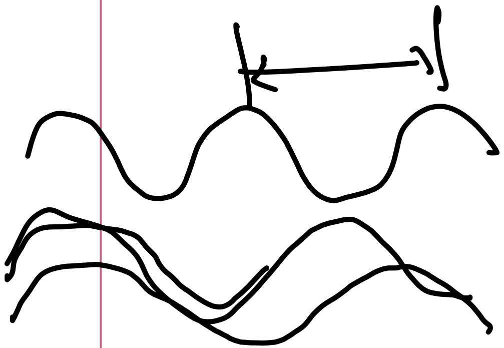
$$= i \underbrace{\frac{\sin k\Delta x}{\Delta x}}_{|||} e^{ikx}$$

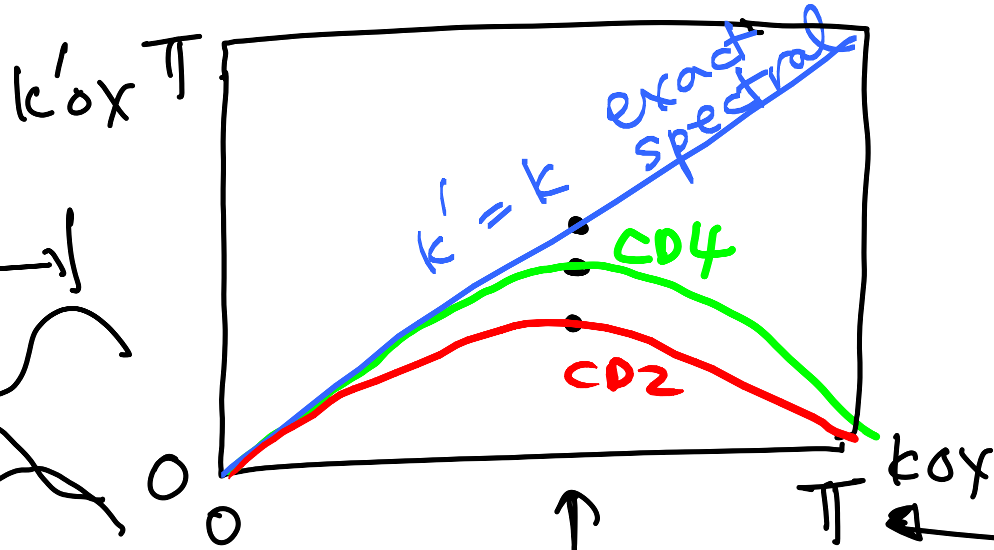
k' : modified wavenumber

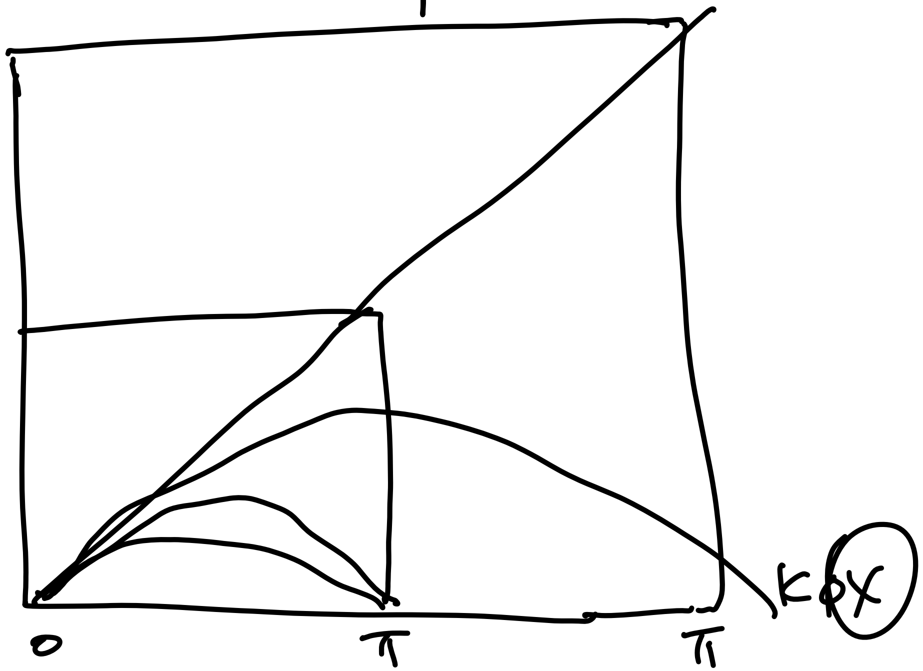
$k'\Delta x = \sin k\Delta x$: (CD2)

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









$$\frac{L}{N}$$

$$\delta x = L/N$$

$$K\cdot(2\delta x) = 2\pi$$

$$K\delta x = \pi$$

upwind scheme

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

$$= i \underbrace{\frac{-i\left(1-e^{-ik\Delta x}\right)}{\Delta x}}_{k'} e^{ikx}$$

k' : complex number

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

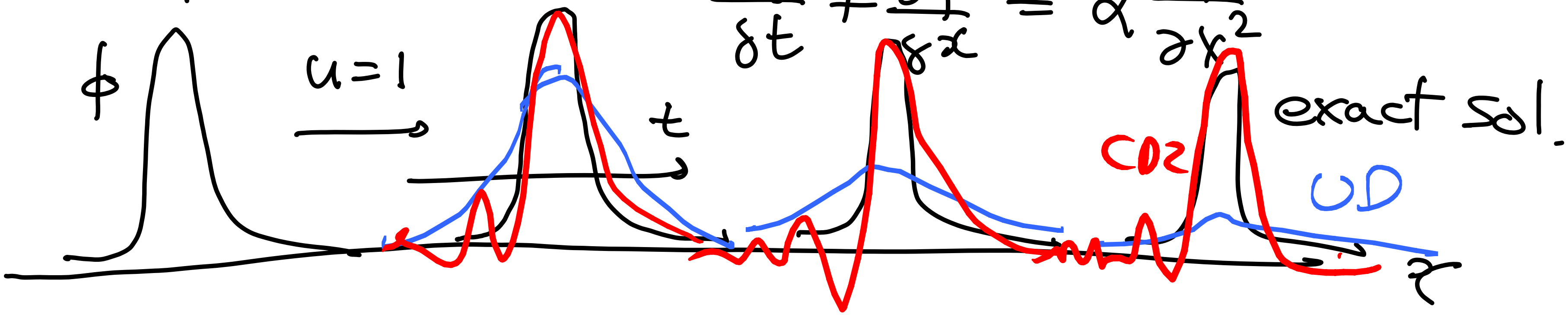
$$= \frac{1}{\Delta x}\left(\sin k\Delta x - i\left(1 - \cos k\Delta x\right)\right) = \frac{\sin k\Delta x}{\Delta x} - \frac{i\left(1-\cos k\Delta x\right)}{\Delta x}$$

$$ik' e^{ikx} = i \frac{\sin k\Delta x}{\Delta x} e^{ikx} + \frac{1 - \cos k\Delta x}{\Delta x} e^{ikx}$$

$\hookrightarrow \frac{d\phi}{dx}\Big|_{UD}$ $\quad \frac{d\phi}{dx}\Big|_{CD}$ $\quad -\frac{d^2\phi}{dx^2}\Big|_{CD}$

dissipation

$$\frac{\partial\phi}{\partial t} + 1\frac{\partial\phi}{\partial x} = 0 \quad \xrightarrow{UD} \quad \frac{\partial\phi}{\partial t} + \frac{\partial\phi}{\partial x} = \alpha\frac{\partial^2\phi}{\partial x^2}$$



7. Examples 1D convection/diffusion eq.

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

ρ, u, Γ const.

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

$$Pe = \rho u L/\Gamma \quad : \text{Peclet number}$$

physics : convection is balanced by diffusion

Almost no flows are in this kind of balance.

Convection is balanced by pressure gradient

$$\frac{\partial}{\partial x}(uu) + \frac{\partial}{\partial y}(uv) = \mu \frac{\partial^2 u}{\partial y^2}$$

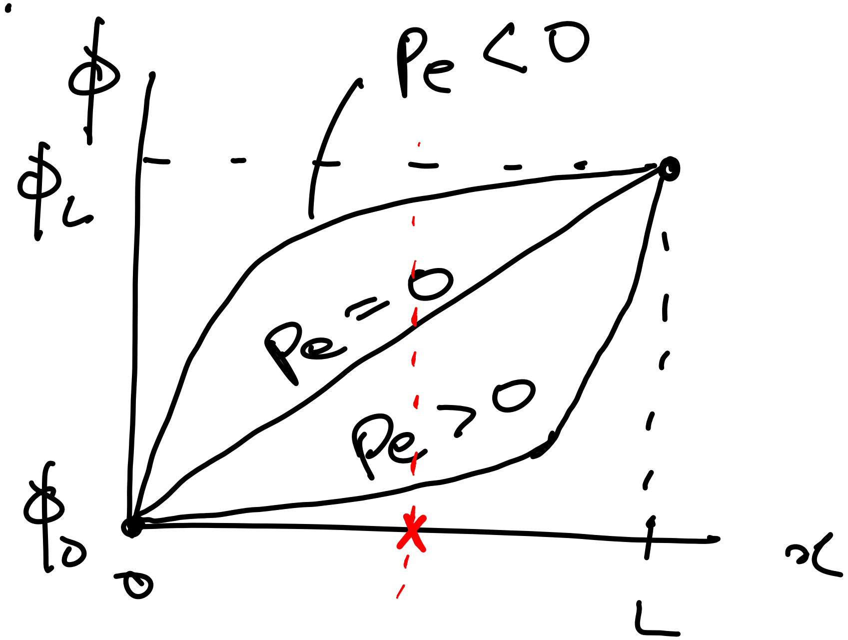
or diffusion in the direction normal to the flow

☆ Thus, it is very misleading to conclude anything from this example.

Anyway, let's do it.

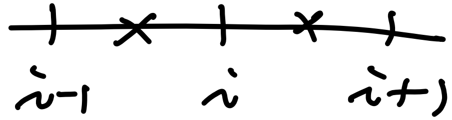
Let $u \geq 0$, $\phi_0 < \phi_L$

$$\left(Pe = \rho u L / \Gamma \right)$$



$$\frac{\partial}{\partial x}(\rho u \phi) = \underline{\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)} \qquad \left(\begin{array}{l} \phi = \phi_0 \text{ at } x = 0 \\ \phi = \phi_L \text{ at } x = L \end{array}\right.$$

Let's do UDS and CDS

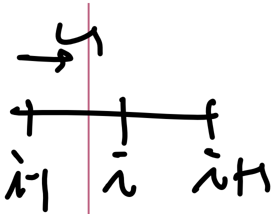


Diffusion term – CDS

$$\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)_i = \frac{1}{\frac{1}{2}(x_{i+1} - x_{i-1})}\left[\Gamma \frac{\partial \phi}{\partial x}\Big|_{i+\frac{1}{2}} - \Gamma \frac{\partial \phi}{\partial x}\Big|_{i-\frac{1}{2}} \right]$$

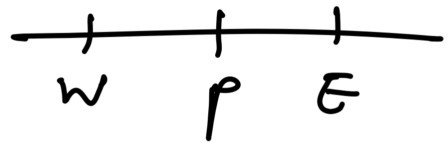
$$\Gamma \frac{\partial \phi}{\partial x}\Big|_{i+\frac{1}{2}} = \Gamma \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \qquad \Gamma \frac{\partial \phi}{\partial x}\Big|_{i-\frac{1}{2}} = \Gamma \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

Convection term $\frac{\partial}{\partial x}(\rho u \phi)$



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

CDS $\quad \frac{\partial}{\partial x}(\rho u \phi) = \rho u \dfrac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}}$



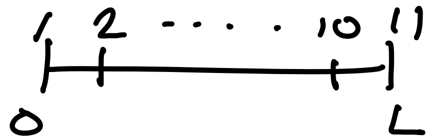
$\Rightarrow$ construct $\quad A_W \phi_W + A_P \phi_P + A_E \phi_E = Q_P$

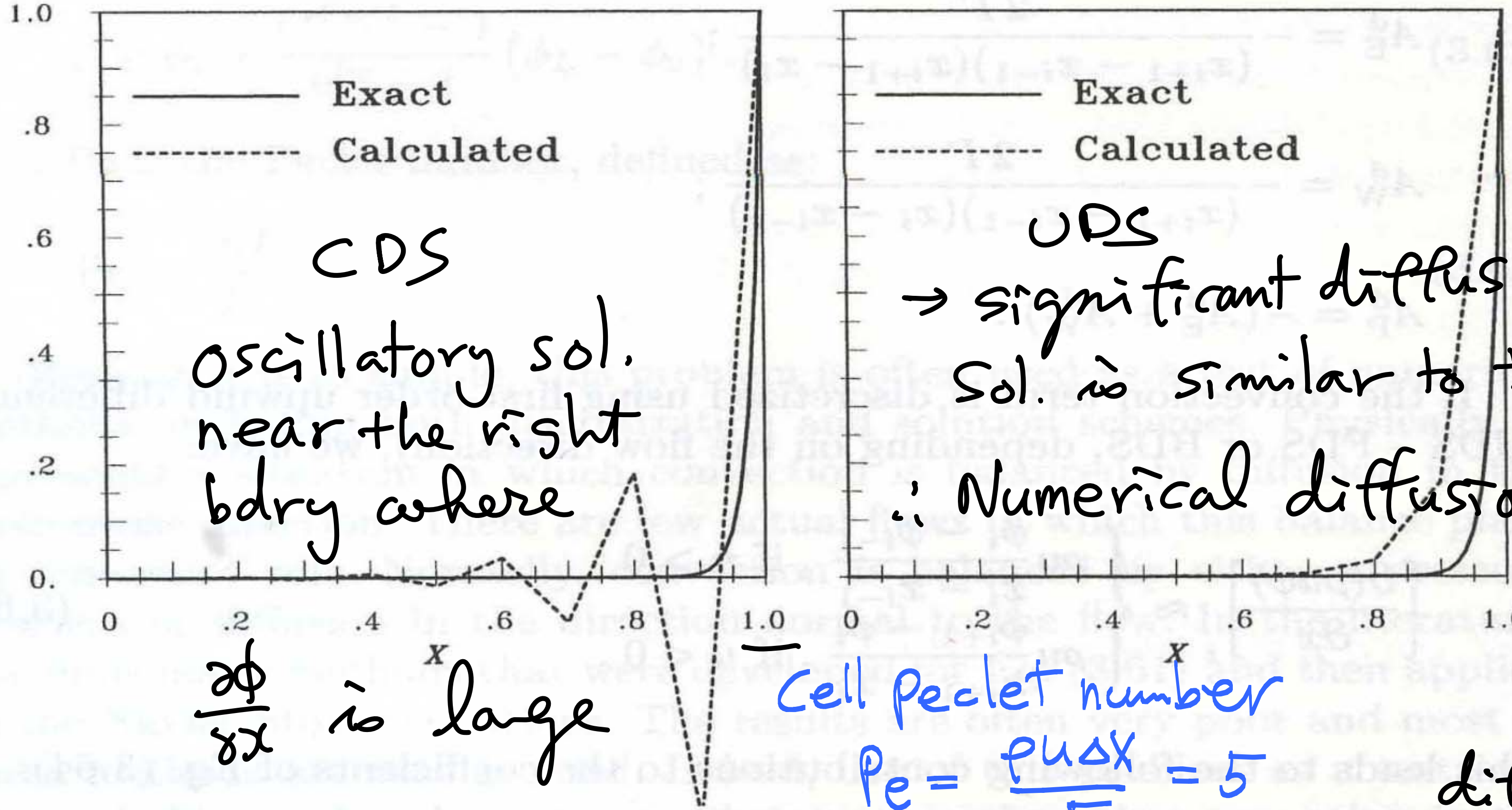
$\Rightarrow$ TDMA $\longrightarrow$ obtain ϕ

⊙ $\underline{L=1}$, $\rho = 1$, $u = 1$, $\Gamma = 0.02$, $\phi_0 = 0$, $\phi_L = 1$

$Pe = \rho u L / \Gamma = 50$

① $N = 11$ including bdry pts.





ϕ

CDS

oscillatory sol. near the right bdry where $\frac{\partial \phi}{\partial x}$ is large

UDS

→ significant diffusion

Sol. is similar to that of $Pe = 18$

∴ Numerical diffusion is bigger than real diffusion

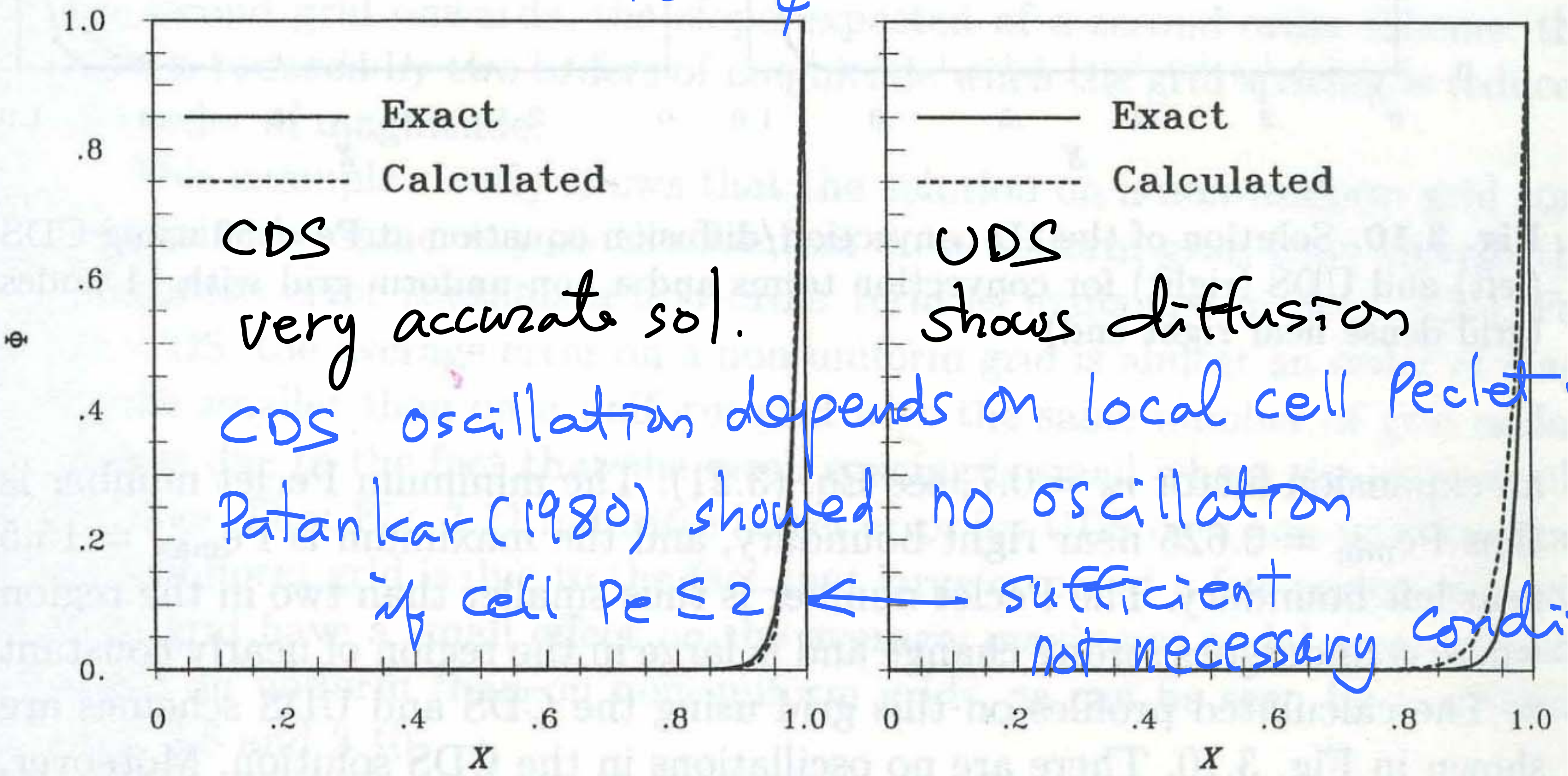
Cell Peclet number

$$Pe = \frac{\rho u \Delta x}{\Gamma} = 5$$

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

② N = 41

cell Pe = $\frac{5}{4}$ = 1.25



CDS very accurate sol.

UDS shows diffusion

CDS oscillation depends on local cell Peclet number.

Patankar (1980) showed no oscillation if cell Pe ≤ 2 ← sufficient condition, not necessary

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

- Hybrid scheme (Spalding 1972)

  switch from CDS to UDS when $Pe > 2$.

  (let diff. coeff $= 0$)

  → too restrictive

  reduces accuracy

Oscillation appears only when sol. changes rapidly in a region of high cell Pe.

③ Non-uniform grids w/ $N = 11$

$\Delta x_{max} = 0.31$, $\Delta x_{min} = 0.0125$; $r_e = 0.75$ expansion factor

$$\frac{\rho u \Delta x}{\Gamma} = Pe_{max} = 15.5 \qquad Pe_{min} = 0.625$$

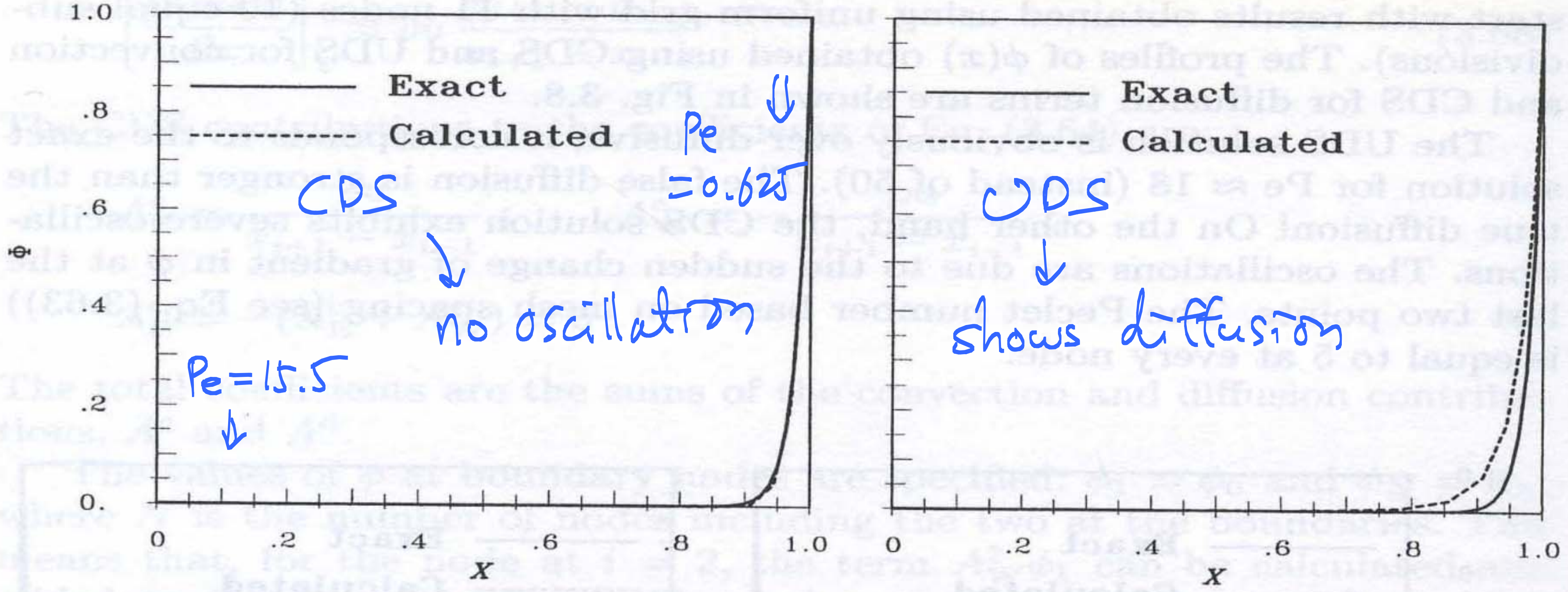


Fig. 3.10. Solution of the 1D convection/diffusion equation at Pe = 50 using CDS (left) and UDS (right) for convection terms and a non-uniform grid with 11 nodes (grid dense near right end)

L_1 norm $\quad \epsilon = \frac{1}{N}\sum_{i=1}^{N} |\phi_i^{exact} - \phi_i| \quad$ L_2 norm $\frac{1}{N}\sum(\ )^2$

HW2

Do it again for $\epsilon = \max |\phi_i^{exact} - \phi_i|$.

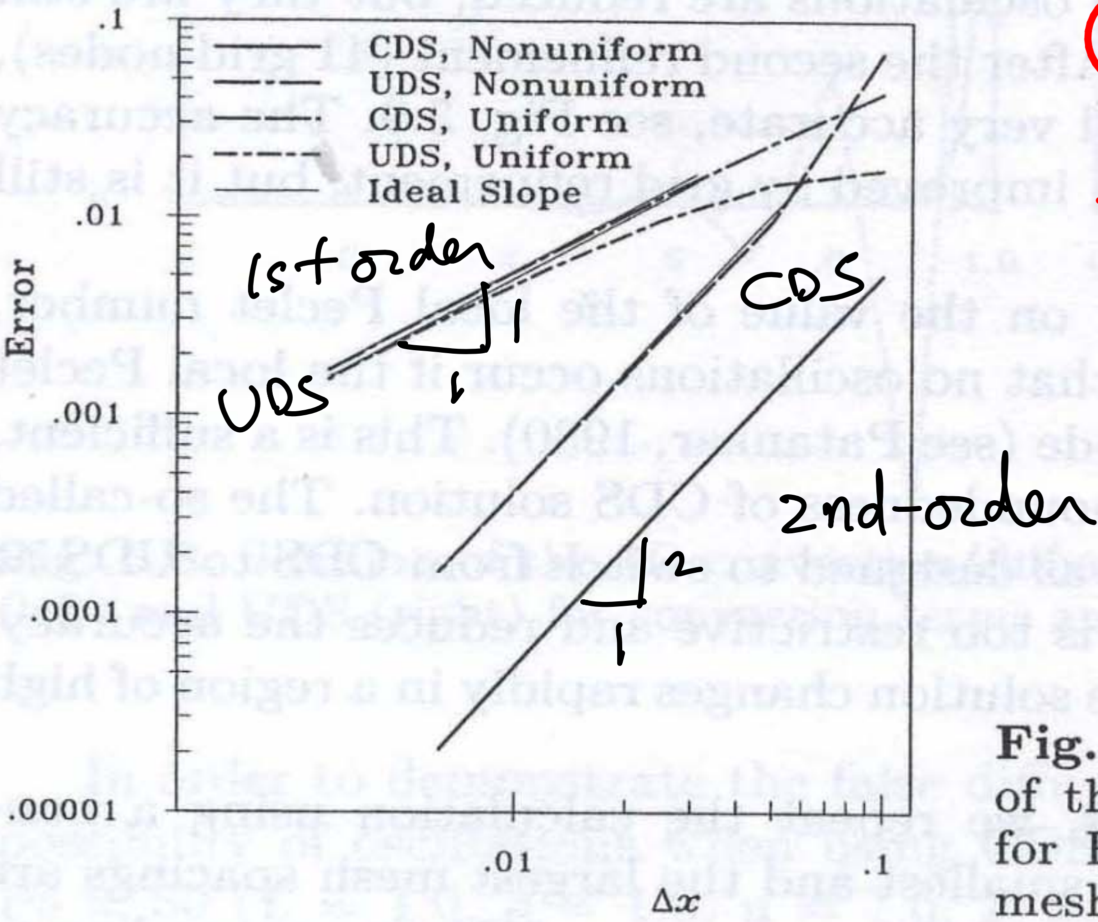
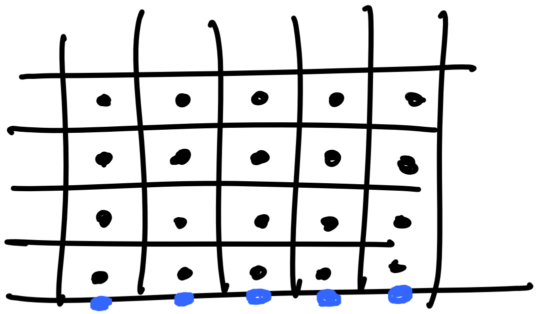


Fig. 3.11. Average error in the solution of the 1D convection/diffusion equation for Pe=50 as a function of the average mesh spacing

Ch. 4 Finite volume methods

FVM → integral form of governing eq.

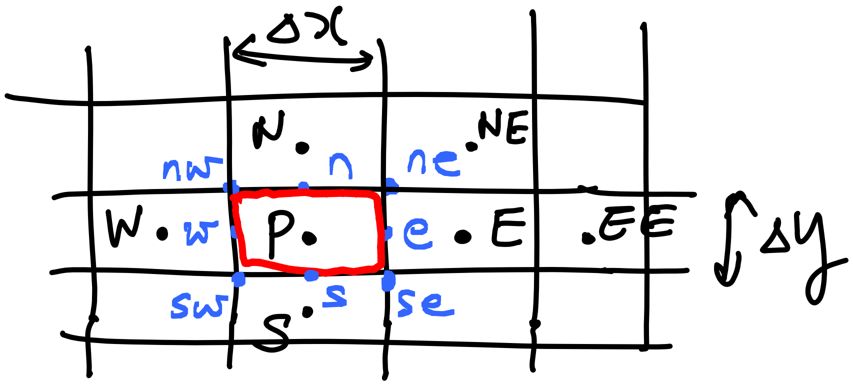
$$\int_S \rho\phi(\underline{u}\cdot\underline{n})\,dS = \int_S \Gamma(\nabla\phi\cdot\underline{n})\,dS + \int_\Omega q_\phi\,d\Omega$$

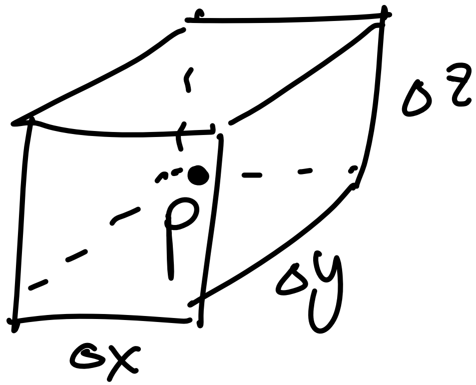


• : location for variables

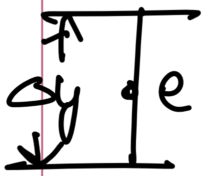
□ : control volume

2D





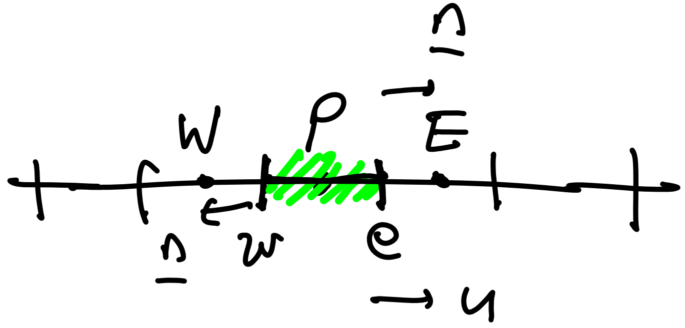
3D



$$\int_{S_e} f\,dS = f_e S_e = f_e \Delta y$$ how to determine?

$O(\Delta y^2)$ – mid-point rule

$$\int_\Omega q\,d\Omega = q_P \Delta\Omega$$



• upwind interpolation (UDS)

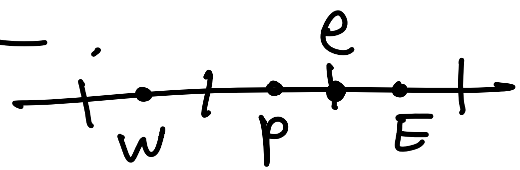
$$\phi_e = \begin{cases} \phi_P & \text{if } (\underline{u}\cdot\underline{n})_e > 0 \\ \phi_E & \text{if } \quad '' \quad < 0 \end{cases}$$

$$\underbrace{\phi_e = \phi_P}_{\text{UDS}} + \underbrace{(x_e - x_P)\left.\frac{\partial\phi}{\partial x}\right|_P}_{\text{leading error } \sim\, \Gamma_e \frac{\partial\phi}{\partial x}} + \frac{(x_e - x_P)^2}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_P + HOT$$

$\Rightarrow \Gamma_e^{num} = (\rho u)_e \dfrac{\Delta x}{2}$

numerical diffusion

$\therefore$ this scheme never yields oscillatory sols., but is numerically diffusive.



- Linear interpolation (CDS)

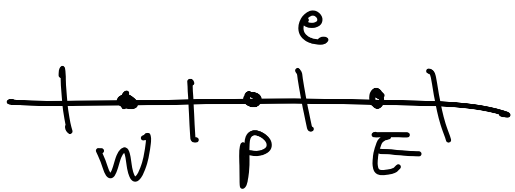
  " " between two nearest nodes

$$\phi_e = \phi_E \lambda_e + \phi_P (1 - \lambda_e) \quad : \quad \text{2nd-order}$$

$$\lambda_e = \frac{x_e - x_P}{x_E - x_P}$$

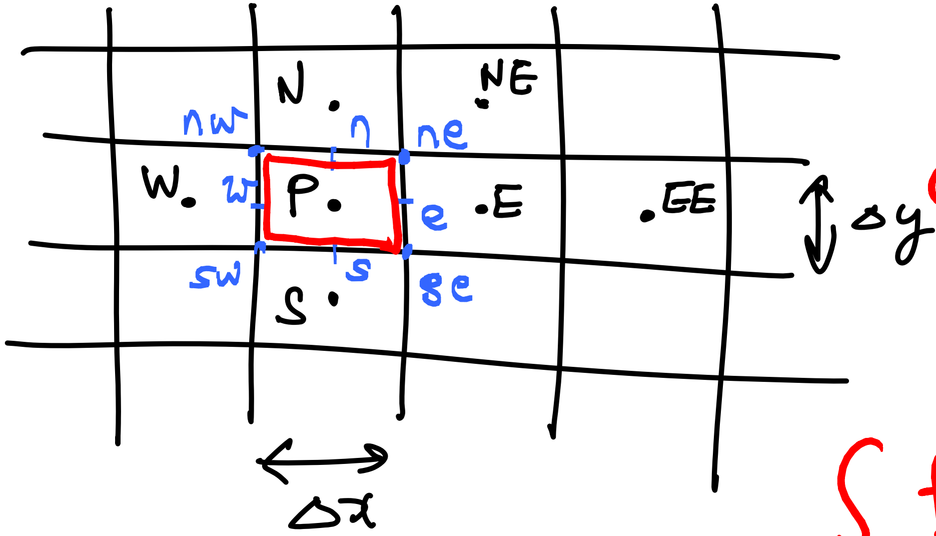
$$\phi_e = \phi_E \lambda_e + \phi_P (1 - \lambda_e) - \frac{(x_e - x_P)(x_E - x_e)}{2} \left.\frac{\partial^2 \phi}{\partial x^2}\right)_P + HOT$$

Viscous term $\longrightarrow$ $\left.\dfrac{\partial \phi}{\partial x}\right|_e$ CDS



$$\left.\frac{\partial\phi}{\partial x}\right|_e = \frac{\phi_E - \phi_P}{x_E - x_P} + \frac{(x_e - x_P)^2 - (x_E - x_e)^2}{2(x_E - x_P)} \left.\frac{\partial^2\phi}{\partial x^2}\right|_e + HOT$$

$$\delta x_{TH} = r_e \delta x_i \rightarrow \text{second-order}$$



$$\int_S \rho\phi(\underline{u}\cdot\underline{n})\,ds = \int_S \Gamma\nabla\phi\cdot\underline{n}\,ds + \int_\Omega q_\phi\,d\Omega$$

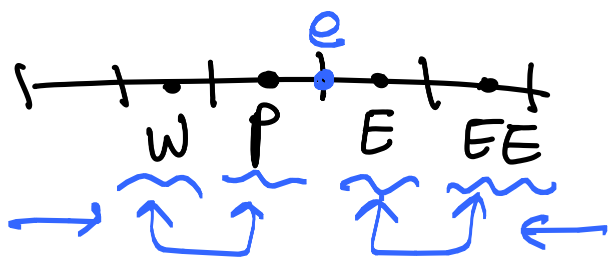
$$\int_{S_e} f\,ds \doteq f_e S_e = f_e \Delta y$$

- QUICK (quadratic upwind interpolation)

  Leonard (1979)

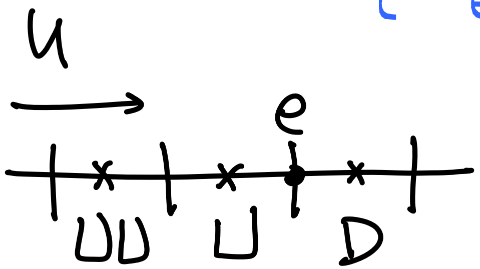
  Quadratic Upwind Interpolation for Convective Kinematics

  → "parabolic" interpolation between P and E to evaluate variables at e.



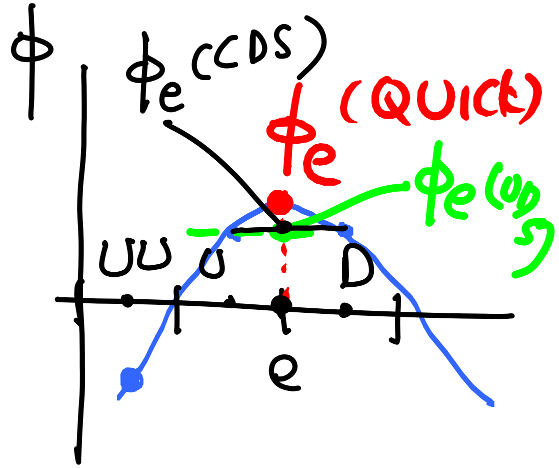
→ need to use data at one more pt.

$$\begin{cases} W & \text{for } u > 0 \\ EE & \phantom{\text{for }} u < 0 \end{cases}$$



$$\boxed{\phi_e = \phi_U + g_1(\phi_D - \phi_U) + g_2(\phi_U - \phi_{UU})}$$

$$\begin{cases} g_1 = \dfrac{(x_e - x_U)(x_e - x_{UU})}{(x_D - x_U)(x_D - x_{UU})} \\[2ex] g_2 = \dfrac{(x_e - x_U)(x_D - x_e)}{(x_U - x_{UU})(x_D - x_{UU})} \end{cases}$$



does not guarantee bounded sols.

For uniform grids,

$$\phi_e = \begin{cases} \frac{3}{8}\phi_E + \frac{6}{8}\phi_P - \frac{1}{8}\phi_W & \text{if } u>0 \\ \frac{3}{8}\phi_P - \frac{1}{8}\phi_{EE} + \frac{6}{8}\phi_E & \text{if } u<0 \end{cases}$$

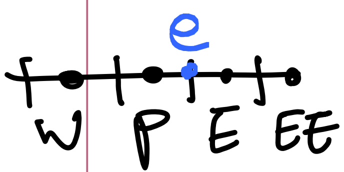
Taylor series exp.

$$\phi_e = \underbrace{\frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}\phi_W}_{\text{QUICK}} - \underbrace{\frac{3(\Delta x)^3}{48}\left(\frac{\partial^3\phi}{\partial x^3}\right)_P}_{\text{3rd-order approx.}} + HOT$$

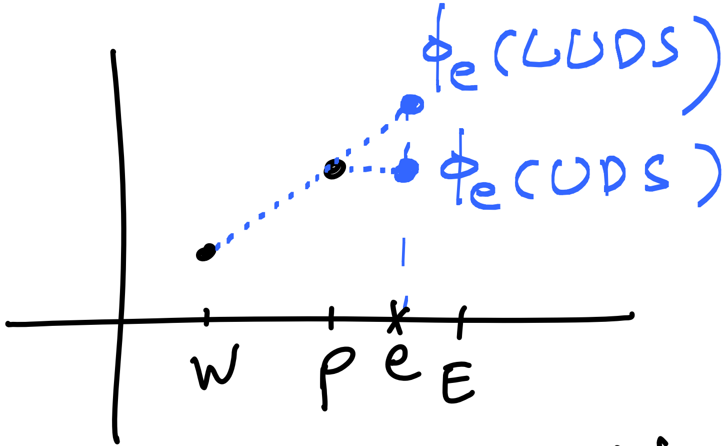
$$\int \phi \, dy \simeq \phi_e \Delta y \rightarrow \text{2nd-order}$$

$\therefore$ overall 2nd-order.

- Linear upwind scheme (LUDS): 2nd-order

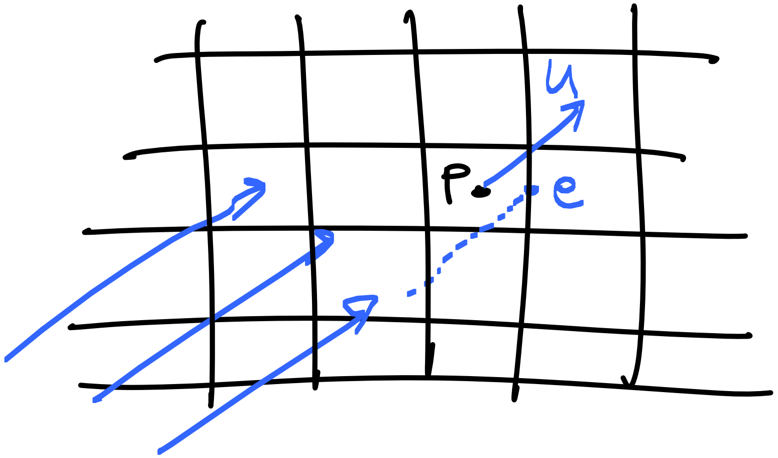


$$\phi_e = \begin{cases} \text{linear interpolation from } \phi_P \text{ and } \phi_W & \text{if } u>0 \\ \quad \text{"} \qquad\qquad \phi_E \text{ and } \phi_{EE} & \text{if } u<0 \end{cases}$$



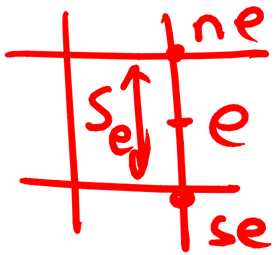
LUDS can produce unbounded sols.

- Skew upwind scheme (Raithby 1976)
  upstream nodes are from streamline rather than from grid line.



complex

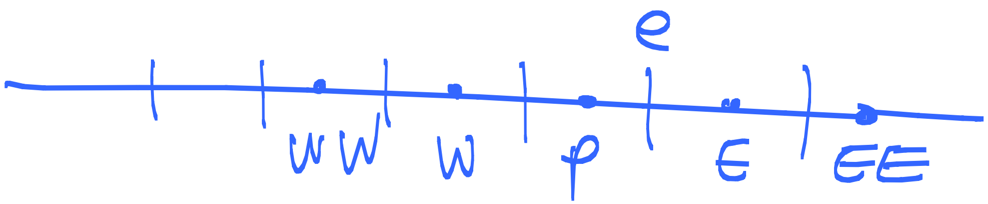
may produce oscillatory sol.



$$\frac{S_e}{6}\left(f_{ne}+4f_e+f_{se}\right)$$

- Higher-order schemes

↳ makes sense only if the integral (i.e. $\int f_e \, dy$) are approximated using higher-order formulae.



uniform mesh

CDS

$$\phi_e = \frac{1}{48}\left(27\phi_P + 27\phi_E - 3\phi_W - 3\phi_{EE}\right) + O(\Delta x^4)$$

$$\left.\frac{\partial \phi}{\partial x}\right|_e = \frac{1}{24\Delta x}\left(27\phi_E - 27\phi_P + \phi_W - \phi_{EE}\right) + \text{''}$$

or, cubic splines

or, Padé (compact) scheme

$$\phi_e = \frac{\phi_P + \phi_E}{2} + \frac{\Delta x}{8}\left[\underset{\displaystyle \frac{\phi_E - \phi_W}{2\Delta x}}{\underset{\|}{\left.\frac{\partial \phi}{\partial x}\right|_P}} - \underset{\displaystyle \frac{\phi_{EE} - \phi_P}{2\Delta x}}{\underset{\|}{\left.\frac{\partial \phi}{\partial x}\right|_E}}\right] + O(\Delta x^4)$$

$$= \quad \text{''} \quad + \frac{\phi_P + \phi_E - \phi_W - \phi_{EE}}{16} + O(\Delta x^4)$$

large stencil size!

- Deferred correction

higher-order interpolation → sparse matrix

$$\phi_e \simeq \phi_e^L + (\phi_e^H - \phi_e^L)^{old}$$

low-order interpolation — usually upwind scheme — L.H.S

high-order interpolation — R.H.S

$$\underline{A}\,\phi = b \longrightarrow (A_1 + (A - A_1))\,\phi = b$$

ϕ_e^H sparse

$$A_1 \phi^{k+1} = (A_1 - A)\,\phi^k + b$$

A_1: upwind, CDS

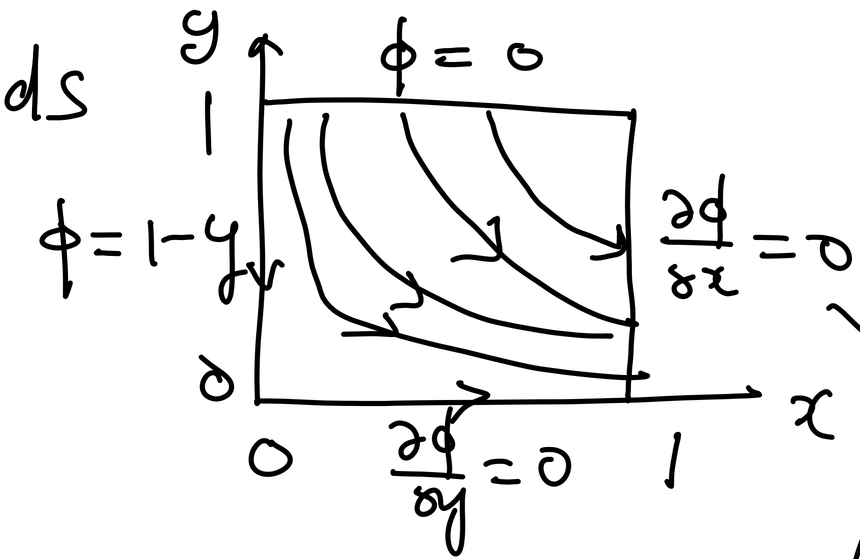
index — k: iteration

Ex. $\int_S \rho\phi(\underline{u}\cdot\underline{n})\,ds = \int_S \Gamma\nabla\phi\cdot\underline{n}\,ds$

HW3 until April 30.

$\underline{u}=(u_x,u_y)$ $u_x = x$, $u_y = -y$

(stagnation flow)

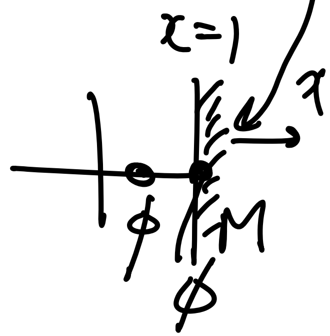


Conv. term : UDS or CDS

viscous term : CDS

@ $x=1$, $\frac{\partial\phi}{\partial x}=0$: one-side difference

@ $y=0$, $\frac{\partial\phi}{\partial y}=0$: // //



40×40 uniform grids, $\rho=1$, $\Gamma = 0.001$ or 0.01

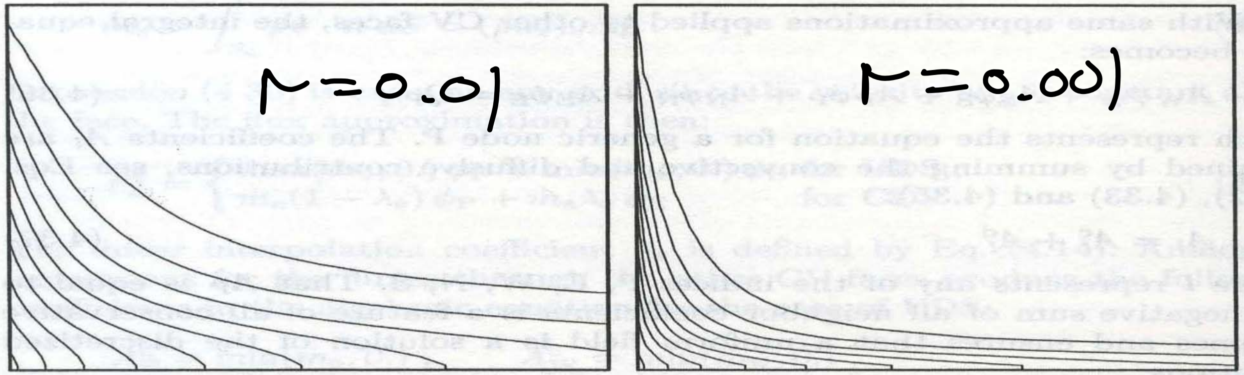


Fig. 4.5. Isolines of ϕ, from 0.05 to 0.95 with step 0.1 (top to bottom), for $\Gamma = 0.01$ (left) and $\Gamma = 0.001$ (right)

CDS

$$\Gamma \frac{\partial \phi}{\partial x}\Big|_{x=0} = Q$$

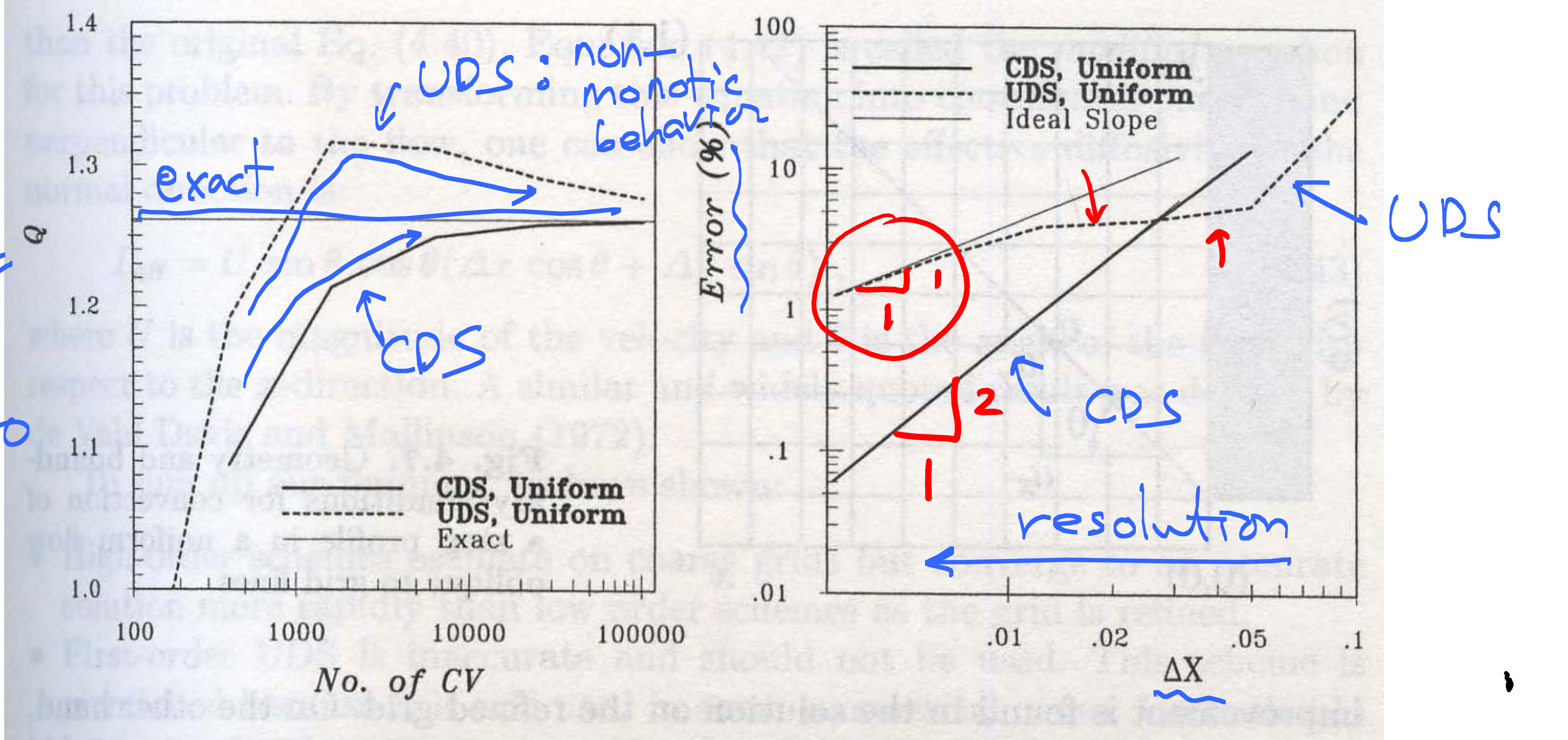
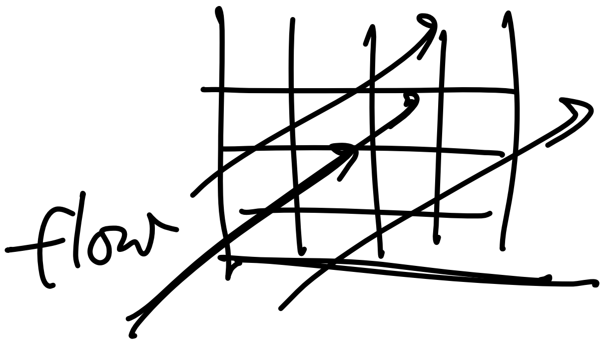


Fig. 4.6. Convergence of total flux of ϕ through the west wall (left) and the error in computed flux as a function of grid spacing, for $\Gamma = 0.001$

Ex. no diffusion

$$u_x \frac{\partial \phi}{\partial x} + u_y \frac{\partial \phi}{\partial y} = 0$$



$$u_x = u_y$$

UDS : $u_x \dfrac{\phi_P - \phi_W}{\Delta x} + u_y \dfrac{\phi_P - \phi_S}{\Delta y} = 0$

$$\phi_P = f(\underbrace{\phi_W , \phi_S}_{\text{known}})$$

→ modified PDE

$$u_x \frac{\partial \phi}{\partial x} + u_y \frac{\partial \phi}{\partial y} = \underbrace{u_x \Delta x \frac{\partial^2 \phi}{\partial x^2} + u_y \Delta y \frac{\partial^2 \phi}{\partial y^2}}_{\text{diffusion !}}$$

CDS : oscillatory sol.

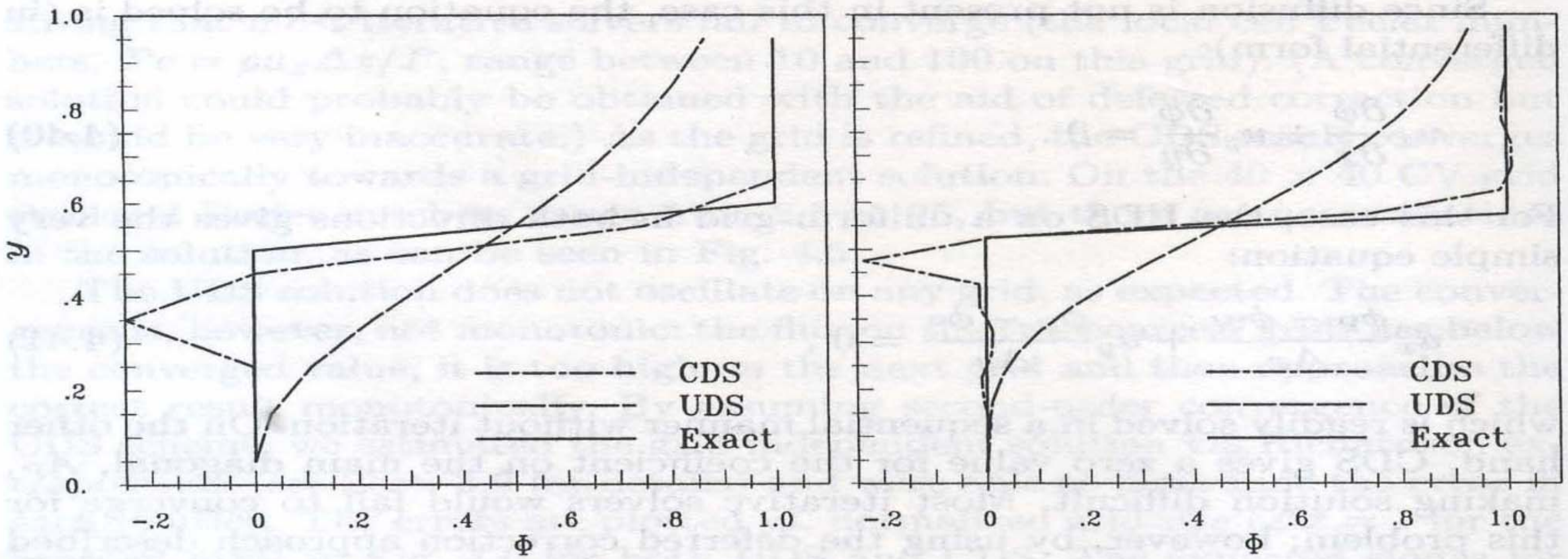


Fig. 4.8. Profile of ϕ at $x = 0.45$, calculated on a 10×10 CV grid (left), and at $x = 0.475$, calculated on a 20×20 CV grid (right)

Summary

1. High-order schemes oscillates on coarse grids but converges to an accurate sol. more rapidly than low order schemes as the grid is refined.
2. First-order UDS is inaccurate and should NOT be used (but still used in commercial codes). High accuracy cannot be obtained on affordable grids w/ this method, especially in 3D.
3. CDS is the simplest scheme of 2nd-order accuracy and offers a good compromise among accuracy, simplicity and efficiency.

⟨ Finite Element Method ⟩

Fletcher I pp. 98–162 참고

Weighted residual method

Heat eq. $\frac{d^2T}{dx^2} + T = F$

Residual : $R = \frac{d^2T}{dx^2} + T - F$

Approx. sol. of $T = \sum_{j=1}^{J} T_j \phi_j(x)$

→ approx. ft
trial ft
interpolating ft
shape ft
basis ft

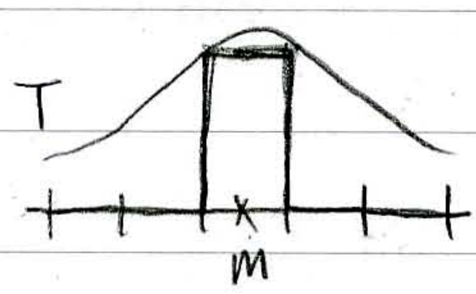
The coefficients T_j are determined by requiring that the integral of the weighted residual over the computational domain is zero.

i.e., $\int w_m(x) R \, dx = 0 \quad (m = 1, 2, \cdots, J)$

↳ weighting ft

determine w_m: ① Subdomain method

$w_m = 1$ in subdomain
$\quad = 0$ otherwise



⇓

Finite Volume Method

② Collocation method

$w_m(x) = \delta(x - x_m)$

$\int w_m R \, dx = 0$ → $R_m = 0$

⇓

Finite Difference Method

③ Least square method

Minimize $\int R^2 dx = Q$

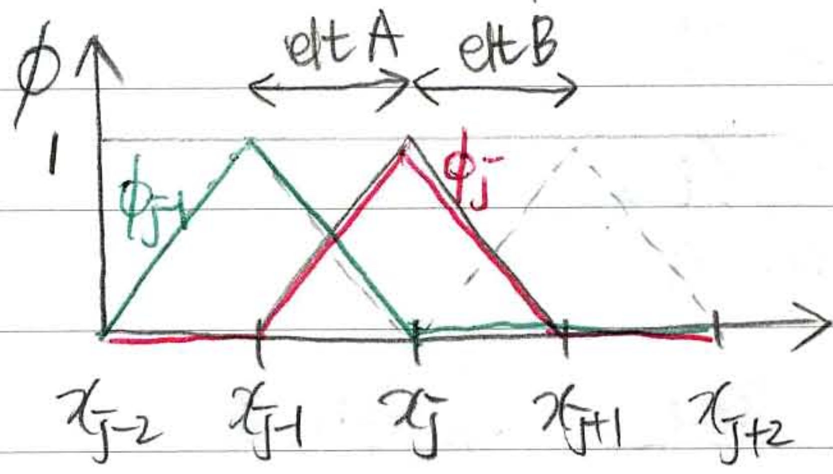
$$\frac{dQ}{dT_m} = \int \underbrace{\left(\frac{\partial R}{\partial T_m}\right)}_{w_m} \cancel{2} R \, dx = 0$$

④ Galerkin method

$w_m = \phi_m \rightarrow$ Standard FEM

1) Linear interpolation

elt: element



$\phi_j(x)$

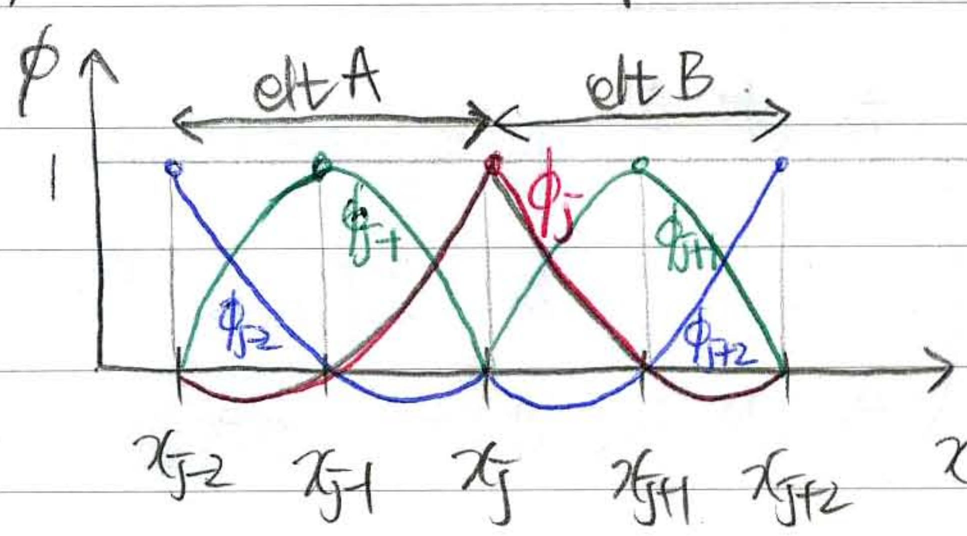
$$
\begin{cases}
\phi_j = 0 & \text{for } x < x_{j-1} \\
\phi_j = \dfrac{x - x_{j-1}}{x_j - x_{j-1}} & \text{for } x_{j-1} \le x \le x_j \\
\phi_j = 1 & \text{for } x = x_j \\
\phi_j = \dfrac{x_{j+1} - x}{x_{j+1} - x_j} & \text{for } x_j \le x \le x_{j+1} \\
\phi_j = 0 & \text{for } x > x_{j+1}
\end{cases}
$$

$T = T_{j-1}\phi_{j-1} + T_j \phi_j$ in elt A

$T = T_j \phi_j + T_{j+1}\phi_{j+1}$ in elt B

2) Quadratic interpolation

parabola (3pts) for basis ft



$\phi_j(x)$

$$
\begin{cases}
\phi_j = 0 & \text{for } x < x_{j-2} \\
\phi_j = \dfrac{x - x_{j-2}}{x_j - x_{j-2}} \cdot \dfrac{x - x_{j-1}}{x_j - x_{j-1}} & \text{for } x_{j-2} \le x \le x_j \\
\phi_j = \dfrac{x - x_{j+1}}{x_j - x_{j+1}} \cdot \dfrac{x - x_{j+2}}{x_j - x_{j+2}} & \text{for } x_j \le x \le x_{j+2} \\
\phi_j = 0 & \text{for } x > x_{j+2}
\end{cases}
$$

FDM이라면 $T=T_j$

$$T = T_{j-2}\phi_{j-2} + T_{j-1}\phi_{j-1} + T_j\phi_j \quad \text{in elt A}$$

$$T = T_j\phi_j + T_{j+1}\phi_{j+1} + T_{j+2}\phi_{j+2} \quad \text{in elt B}$$

$$\phi_{j-2} = \frac{x-x_{j-1}}{x_{j-2}-x_{j-1}} \cdot \frac{x-x_j}{x_{j-2}-x_j}$$

$$\phi_{j-1} = \frac{x-x_{j-2}}{x_{j-1}-x_{j-2}} \cdot \frac{x-x_j}{x_{j-1}-x_j}$$

$$\phi_j = \frac{x-x_{j-2}}{x_j-x_{j-2}} \cdot \frac{x-x_{j-1}}{x_j-x_{j-1}} \quad \text{in elt A.}$$

Roughly,
Linear interpolation → 2nd order FDM
quadratic 〃 → 3rd order 〃

*2D prob. (bilinear interpolation)

$\phi_1 = 0.25(1-x)(1-y)$. $\phi_3 = 0.25(1+x)(1+y)$

$\phi_2 = 0.25(1+x)(1-y)$ $\phi_4 = 0.25(1-x)(1+y)$.

$\boxed{\text{Example}}$

$$\frac{d^2T}{dx^2} + T = F \quad \text{use Galerkin FEM}, \quad \overbrace{T(0)=0, \ \frac{dT}{dx}(1)=0}^{\text{B.C's}}$$

[cf. FDM과 비교

$$\frac{T_{j+1}-2T_j+T_{j-1}}{\Delta x^2} + T_j = F_j$$]

$$T = \sum_{j=1}^{J} T_j \underbrace{\phi_j}_{\text{linear approx.}}$$

in elt A: $\phi_j(\xi) = 0.5(1+\xi)$

$$\xi = 2\left(x - \frac{x_{j-1}+x_j}{2}\right)/\Delta x_j$$

in elt B: $\phi_j(\xi) = 0.5(1-\xi)$

$$\xi = 2\left(x - \frac{x_j+x_{j+1}}{2}\right)/\Delta x_j$$

$$R = \frac{d^2T}{dx^2} + T - F$$

$$\int w_m R\,dx = \int \phi_m R\,dx = 0.$$

$$\rightarrow \int_0^1 \phi_m(x)\left[\frac{d^2T}{dx^2} + T - F\right]dx = 0.$$

$$\int_0^1 \phi_m \frac{d^2T}{dx^2}\,dx = \underbrace{\left[\phi_m \frac{dT}{dx}\right]_0^1}_{0 \text{ from b.c.'s}} - \int_0^1 \frac{d\phi_m}{dx}\frac{dT}{dx}\,dx$$

$T = \sum T_j \phi_j$

$$\rightarrow \underbrace{\sum_{j=1}^{J}\left[\int_0^1 \left(-\frac{d\phi_m}{dx}\frac{d\phi_j}{dx} + \phi_m\phi_j\right)dx\right]}_{b_{mj}\text{ : analytically obtained.}} T_j = \underbrace{\int_0^1 \phi_m F\,dx}_{g_m} \quad (m=1,2,\cdots,J)$$

$\rightarrow$ $BT = G$

TDMA

$$b_{j,j-1} = \frac{1}{\Delta x_j} + \frac{\Delta x_j}{6}$$

$$b_{j,j} = -\left(\frac{1}{\Delta x_j} + \frac{1}{\Delta x_{j+1}}\right) + \frac{\Delta x_j + \Delta x_{j+1}}{3} \quad \text{for } j=1,\cdots,J-1$$

$$b_{j,j+1} = \frac{1}{\Delta x_{j+1}} + \frac{\Delta x_{j+1}}{6}$$

$$b_{J,J-1} = \frac{1}{\Delta x_J} + \frac{\Delta x_J}{6}$$

$$b_{J,J} = -\frac{1}{\Delta x_J} + \frac{\Delta x_J}{3}$$

$$b_{J,J+1} = 0$$

$$g_m = \sum_{j=1}^{J} F_j \int_0^1 \phi_m\phi_j\,dx \quad \text{for } m=1,\cdots,J-1$$

analytically obtained

$$= \frac{\Delta x_m}{6}F_{m-1} + \frac{\Delta x_m + \Delta x_{m+1}}{3}F_m + \frac{\Delta x_{m+1}}{6}F_{m+1}$$

$$g_J = \frac{\Delta x_J}{6}F_{J-1} + \frac{\Delta x_J}{3}F_J$$

For uniform grids,

$$\frac{T_{j-1} - 2T_j + T_{j+1}}{\Delta x^2} + \frac{T_{j-1} + 4T_j + T_{j+1}}{6} = \frac{F_{j-1} + 4F_j + F_{j+1}}{6}$$

2nd-order accuracy (CD2) Simpson's rule. 4th-order accuracy (FDM : T_j, F_j)

Ch. 7 Solution of the Navier-Stokes Eqs.

1. Conservation properties

- mass conservation
- momentum " : convection term, viscous term, pressure gradient term
- energy "

conservative approx. — finite volume method
non- " "

Biggest problem is how to conserve kinetic energy.

incompressible flow → kinetic energy

u, v, w, p (4) cont. & N-S eqs (4)

compressible flow $\rightarrow$ (kinetic energy
thermal "

u, v, w, p, T, ρ (6) $\rightarrow$ (4) + energy eq (1)
+ state eq (1)

- $$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j}\right) - \frac{2}{3}\frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_k}{\partial x_k}\right)\delta_{ij} + \rho b_i$$

u_i $*$ (")

$$\rightarrow \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i u_i\right) + u_i \frac{\partial}{\partial x_j}(\rho u_i u_j) = -u_i \frac{\partial p}{\partial x_i} + u_i \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j}\right)$$

$$- \frac{2}{3} u_i \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_k}{\partial x_k}\right)\delta_{ij} + \rho u_i b_i$$

$$(u^2 = u_i u_i)$$

$$\rightarrow \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2\right) + \frac{\partial}{\partial x_j}\left(\frac{1}{2}\rho u^2 u_j\right) = -\frac{\partial}{\partial x_i}(p u_i) + p\frac{\partial u_i}{\partial x_i}$$

$$+ \frac{\partial}{\partial x_j}\left(u_i \mu \frac{\partial u_i}{\partial x_j}\right) - \frac{\partial u_i}{\partial x_j}\cdot \mu \frac{\partial u_i}{\partial x_j}$$

$$- \frac{2}{3}\frac{\partial}{\partial x_j}\left(u_i \mu \frac{\partial u_k}{\partial x_k}\right)\delta_{ij} + \frac{2}{3}\frac{\partial u_i}{\partial x_j}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij} + \rho u_i b_i$$

$$\int_\Omega \odot \, dV$$

$$\frac{\partial}{\partial t}\int_\Omega \frac{1}{2}\rho u^2 \, dV = -\int_S \frac{1}{2}\rho u^2 u_j n_j \, dA - \int_S p u_i n_i \, dA$$

$$+ \int_S u_i\left(\mu\frac{\partial u_i}{\partial x_j} - \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) n_j \, dA$$

$$+\int_{\Omega} \left(p\frac{\partial u_i}{\partial x_i} - \frac{\partial u_i}{\partial x_j}\left(\mu\frac{\partial u_i}{\partial x_j} - \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) + \rho u_i b_i\right) d\mathcal{V}$$

Discussion

① First 3 terms on RHS : Kinetic energy in Ω is NOT changed by the action of convection and pressure within the control volume.

If no viscosity
no internal energy
no mtm forcing → kinetic energy is then globally conserved

the property that we like to preserve from a numerical method.

② We solve mtm eq. (NOT energy eq.)
Conservative scheme for mtm eq. does not guarantees conservation of energy.
→ difficult to conserve energy numerically.

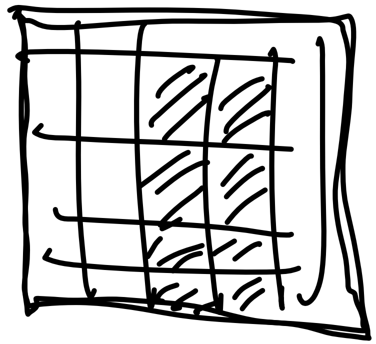
③ If a numerical method is energy conservative, total kinetic energy does not grow in time.

→ vel at every grid pt. in the domain must remain bounded.

→ guarantees numerical stability (NOT accuracy)

→ kinetic energy conservation is important in computing unsteady flow.

④ pressure gradient term



$$u_i \frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_i}(p u_i) - p \frac{\partial u_i}{\partial x_i}$$

If incomp. flow, $\partial u_i / \partial x_i = 0$

$$\int_{\Omega} u_i \frac{\partial p}{\partial x_i} = \int_{\Omega} \frac{\partial}{\partial x_i}(p u_i) = \int_{S} p u_i n_i \, dA$$

$\Rightarrow$ pressure influences the overall kinetic energy budget only by its action at the surface.

$\rightarrow$ We have to retain this property.

$G_i p$: numerical approx. of the press. grad. used in mtm eq.

$\sum u_i \cdot u_i\text{-mtm} \longrightarrow \sum_{i=1}^{N} u_i \underline{G_i p} \, \Delta\Omega$

num. approx. of $\partial u_i/\partial x_i$

$\left(u_i \frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_i}(u_i p) - p \frac{\partial u_i}{\partial x_i} \right) = \sum_S p u_n \Delta S - \sum_N p \underline{D_i u_i} \, \Delta\Omega$

used in the cont. eq.

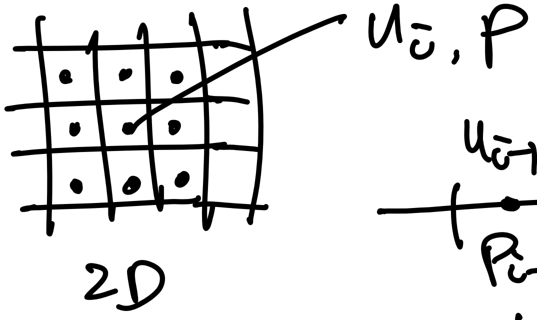
Equality is ensured only if G_i and D_i are compatible.

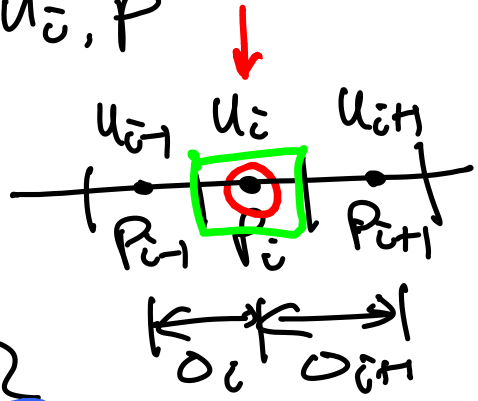
i.e. $\sum_{i=1}^{N} (u_i G_i p + p D_i u_i) \Delta\Omega =$ surface terms.

ex) G_i : backward

D_i : forward

collocated mesh





$$u_i G_i p \Delta\Omega$$

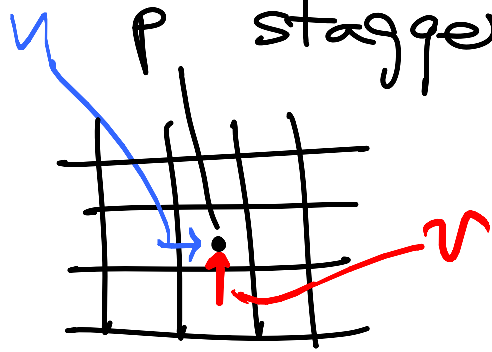
$$= u_i \frac{\cancel{p_i} - p_{i-1}}{\Delta_i} \Delta_i$$

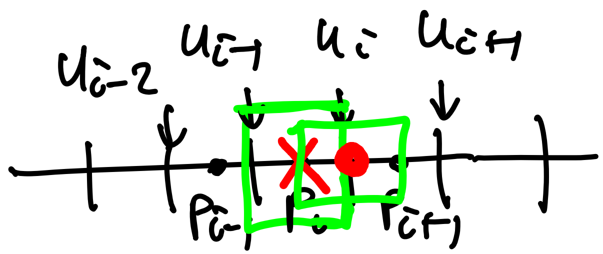
$$+ \quad p D_i u_i \Delta\Omega$$

$$= p_i \frac{u_{i+1} - \cancel{u_i}}{\Delta_{i+1}} \cdot \Delta_{i+1}$$

$$= -u_i p_{i-1} + u_{i+1} p_i$$

staggered mesh





Do the same thing

$$u_i G_i p \Delta\Omega \Big|_{\bullet} =$$

$$p D_i u_i \Delta\Omega \Big|_{\times} =$$

$$\sum_{i=1}^{N} \left(-u_i P_{i-1} + u_{i+1} P_i\right) = -u_1 P_0 + u_{N+1} P_N$$

ok.

⊙ $G_i p$: CD2, $D_i u_i$: CD2 ok only for staggered mesh

not ok for collocated mesh

The requirement that only bdry terms remain when the sum over all c.v's is taken is not easily satisfied for other two terms.

conv. & diffusion

⑤ Pressure $\longrightarrow$ Poisson eq (incomp. flow)

$$\underbrace{\nabla \cdot \underbrace{\nabla p}_{G_i p}}_{D_i G_i p} = q$$

; numerical operators should be consistent if mass conserv. is to obtain.

$$\begin{cases} \dfrac{\partial u_i}{\partial t} = \cdots - \dfrac{\partial p}{\partial x_i} + \cdots \\ \boxed{\nabla^2 p = q} \end{cases}$$

⑥ Incomp. flow w/o body force

$$-\int_{\Omega} \mu \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}\, d\forall < 0$$

dissipation $\rightarrow$ goes to thermal energy

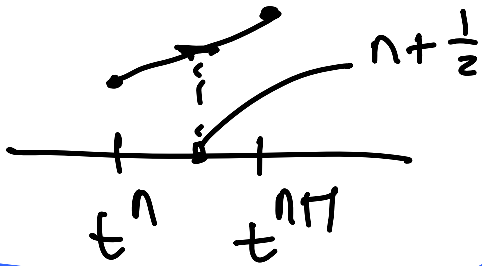
⑦ $\frac{\partial}{\partial t}(\rho u_i) \rightarrow \rho \frac{u_i^{n+1}-u_i^{n}}{\Delta t}\Delta\Omega$ n : time step index

If Crank-Nicolson method is used, $u_i^{n+\frac{1}{2}} = \frac{1}{2}(u_i^{n+1}+u_i^{n})$

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

CN $\Rightarrow$ $\frac{u^{n+1}-u^{n}}{\Delta t} = \frac{1}{2}\left[f(u^{n+1}) + f(u^{n})\right]$

Trapezoidal method



$$u_i \frac{\partial}{\partial t}(\rho u_i) \Rightarrow u_i^{n+\frac{1}{2}} \cdot \rho \frac{u_i^{n+1}-u_i^{n}}{\Delta t} \cdot \Delta\Omega$$

$u_i^{n+\frac{1}{2}}$

$$= \frac{\rho\Delta\Omega}{\Delta t}\left[\frac{1}{2}{u^{n+1}}^2 - \frac{1}{2}{u^{n}}^2\right]$$

$\therefore$ C-N is energy conservative

forward Euler

$u_i^n \cdot \rho \frac{u_i^{n+1}-u_i^{n}}{\Delta t} \cdot \Delta\Omega$

$\downarrow$

not energy conservative

⇒ time difference scheme can destroy the energy conservation property.

$$\frac{\partial u}{\partial t} = f$$

FE $\quad \dfrac{u^{n+1} - u^n}{\Delta t} = f^n \cdot u^n$

BE $\quad \left(u^n \quad f^{n+1} \right) \cdot u^{n+1}$

- Alternative method:
  to use a different form of mtm eq.

$$\underset{\text{conv-term}}{H_i} = \underbrace{\frac{\partial}{\partial x_j}(u_i u_j)}_{\text{divergence form}} = \underbrace{u_j\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(\frac{1}{2}u_j u_j\right)}_{\text{rotational form}} = \underbrace{u_j \frac{\partial u_i}{\partial x_j}}_{\text{convective form}}$$

$$= \frac{1}{2}\left(\frac{\partial u_i u_j}{\partial x_j} + u_j \frac{\partial u_i}{\partial x_j} \right)$$

skew-symmetric form

Kravchenko, . . .

JCP (19** / 20**)

rotational form

$$= \epsilon_{ijk} u_j \omega_k + \frac{\partial}{\partial x_i}\left(\frac{1}{2} u_j u_j\right)$$

vorticity ($\underline{\omega} = \nabla \times \underline{u}$)

$$\begin{pmatrix} \epsilon_{11k} = 0 \\ \epsilon_{123} = 1 \\ \epsilon_{132} = -1 \end{pmatrix}$$

$$\Rightarrow \frac{\partial u_i}{\partial t} + \boxed{\epsilon_{ijk} u_j \omega_k} = -\frac{\partial}{\partial x_i}\left(\frac{p}{\rho} + \underline{\frac{1}{2} u_j u_j}\right) + \nu \frac{\partial}{\partial x_j}\frac{\partial u_i}{\partial x_j}$$

$$u_i \cdot (\qquad\qquad // \qquad\qquad)$$

sym. tensor

$$u_i \epsilon_{ijk} u_j \omega_k = \epsilon_{ijk} \overline{u_i u_j} \omega_k = 0$$

anti-sym. tensor

Thus, nonlinear term has no effect.

However, this eq. is nonconservative form for momentum.

- Kinetic energy conservation
  - turbulence
    weather prediction

  angular mtm conservation – turbomachinery

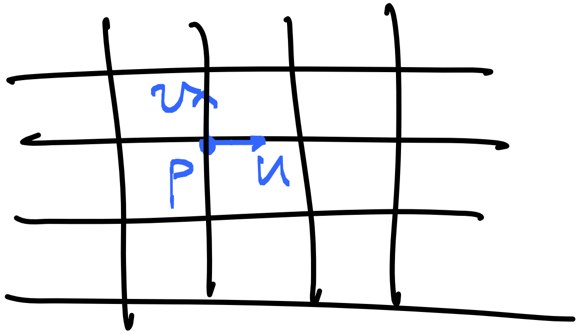
- CDS on staggered mesh → mtm / energy conservation

  CDS is much better than UDS.

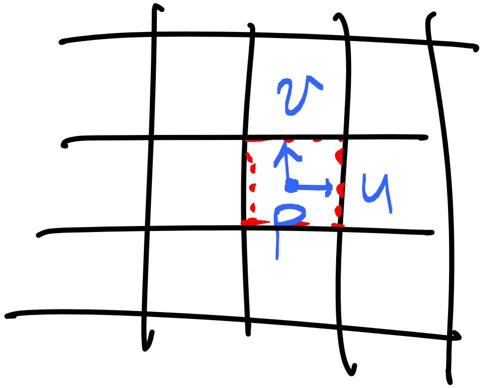
2. Choice of grid system

① Collocated (non-staggered) mesh

FDM

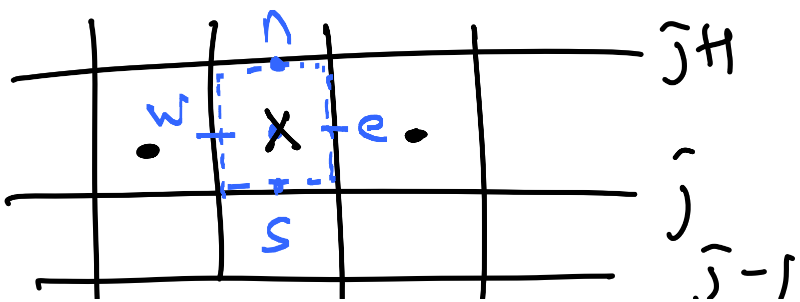


FVM



out of favor for incomp. flow due to difficulties with pressure-velocity decoupling and occurance of oscillations in p.

FVM – collocated mesh



continuity $\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$

$\rightarrow \frac{u_e - u_w}{\Delta x} + \frac{v_n - v_s}{\Delta y} = 0$

$i-1 \quad i \quad i+1$ $\rightarrow$ requires interpolation

$$u_e = \frac{1}{2}(u_{i+1j} + u_{ij})$$
$$u_w = \frac{1}{2}(u_{ij} + u_{i-1j})$$
$\rightarrow$ $u_e - u_w$

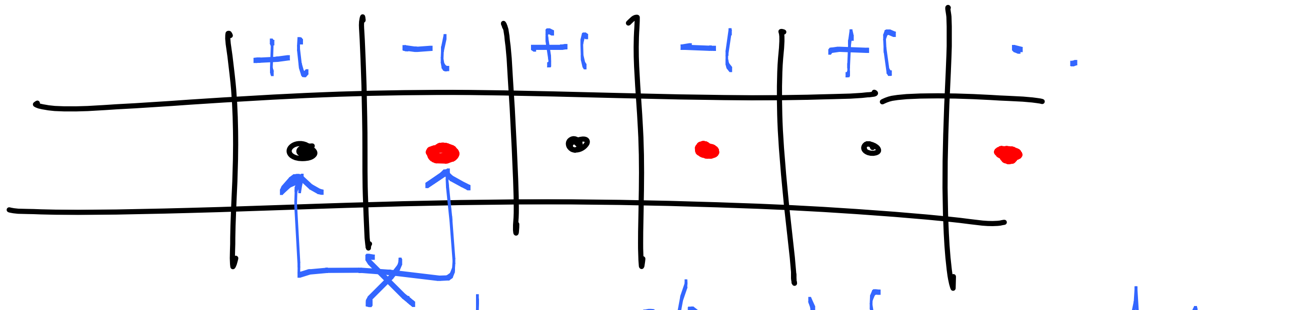
$$= \frac{1}{2}(u_{i+1j} - u_{i-1j})$$

likewise $v_n - v_s = \frac{1}{2}(v_{ij+1} - v_{ij-1})$

no u_{ij} & v_{ij}

x-mtm eq: $\frac{\partial p}{\partial x} = \frac{p_{i+1j} - p_{i-1j}}{2\Delta x}$ $\longrightarrow$ no p_{ij}

$$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

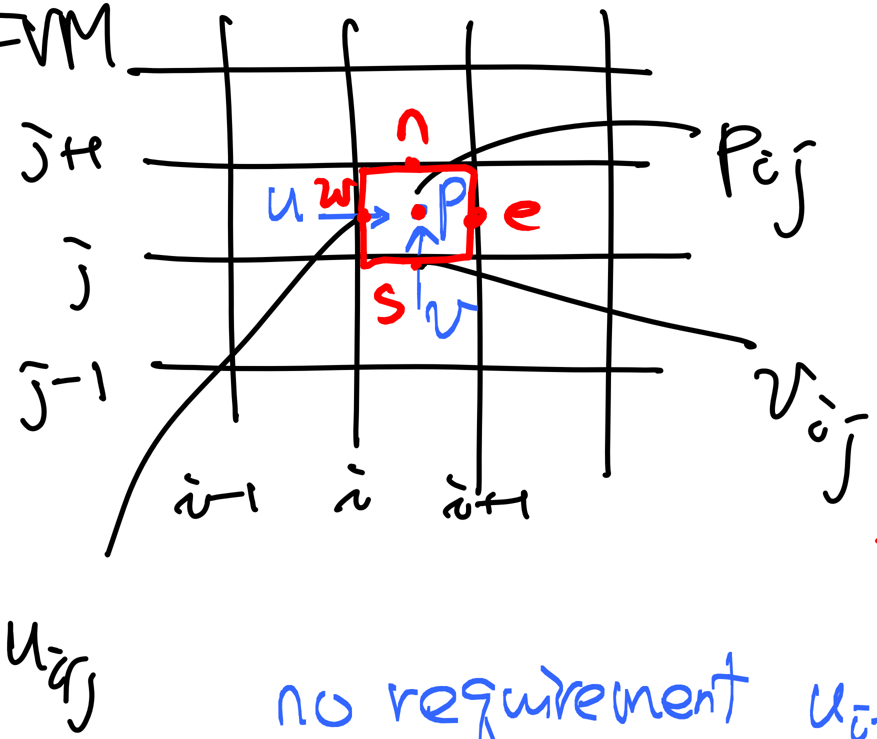


decoupling bet. p and u.

② Staggered mesh ← invented by Harlow & Welch (1965)

Phys. Fluids (2176 citations)

FVM



Continuity $\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$

$\square$ c.v for p.

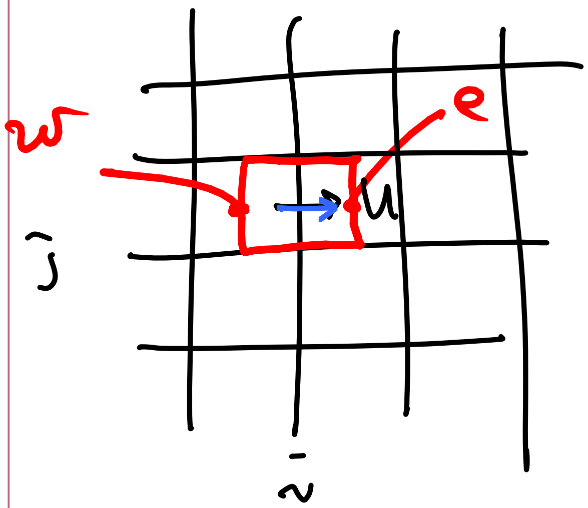
$$\frac{u_e - u_w}{\Delta x} + \frac{v_n - v_s}{\Delta y} = 0$$

$u_{i+1\,j}$ $\quad u_{ij}$ $\quad v_{ij+1}$ $\quad v_{ij-1}$

no requirement of interpolation!

compact!

x-mtm eq : $\dfrac{\partial p}{\partial x}$

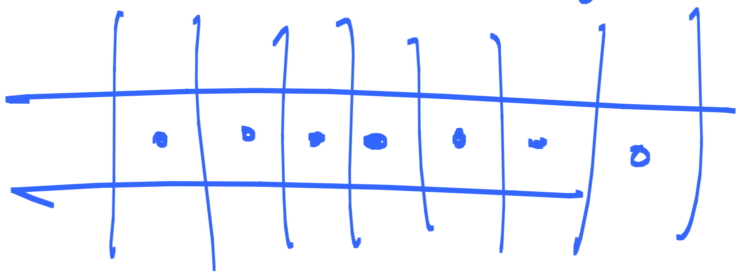


$\square$: c.v for x-mtm eq.

$$\frac{\partial p}{\partial x} = \frac{P_e - P_w}{\delta x}$$

$P_{i,j}$ $\qquad$ $P_{i+1,j}$

compact
no interpolation required!



strong coupling bet. $\underline{u}$ and p.

→ no oscillations in p

→ staggered mesh is dominantly used.

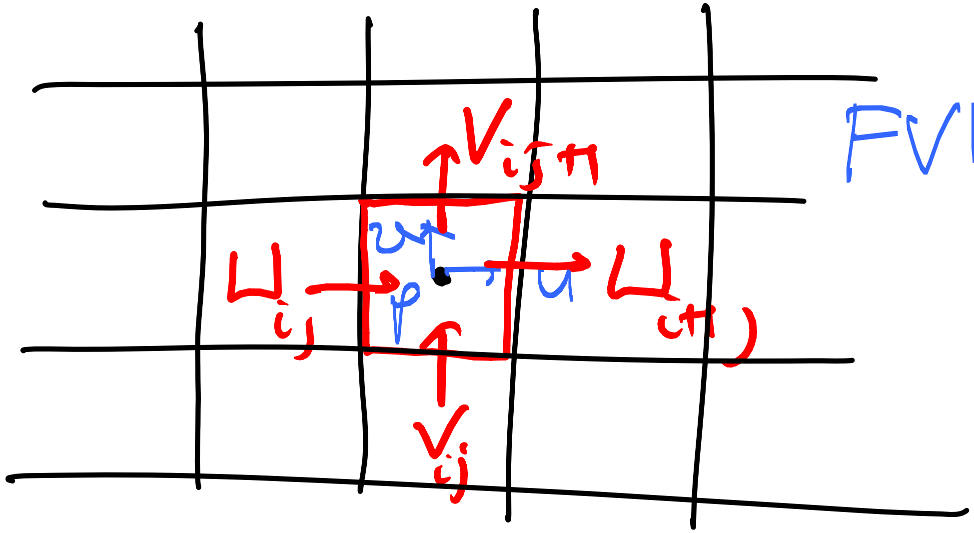
However, for complex geometry, one has to transform N–S in "generalized" coordinates with dependent variables of contravariant vel.
to satisfy $\boxed{\nabla \cdot \underline{u} = 0}$

→ very complicated !

→ back to collcated mesh with improved p–u coupling algorithm since 1980's ↘ getting more popular

* momentum interpolation method invented by Rhie & Chow (AIAA J.) Vol. 21, 1525 (1983)
(1354 citations)

unstructured mesh ← Kim & Choi (JCP, 162, 411) (2000)



FVM

$$\frac{\partial}{\partial x_j}(u u_j)$$

U or V

$$\frac{\partial p}{\partial x} \sim U$$

eliminate the u-p decoupling!

3. Calculation of pressure

Incomp. flow → $\rho \equiv$ const

P ? $\Rightarrow$ a mathematical quantity to enforce the continuity eq.

① pressure eq.

N-S: $\rho \dfrac{\partial u_i}{\partial t} + \rho \dfrac{\partial u_i u_j}{\partial x_j} = -\boxed{\dfrac{\partial p}{\partial x_i}} + \dfrac{\partial}{\partial x_j}\left(\mu \dfrac{\partial u_i}{\partial x_j}\right)$

$\dfrac{\partial u_i}{\partial x_i} = 0$

$\dfrac{\partial}{\partial x_i} \cdot \Big(\qquad \qquad \Big)$

$$\rightarrow \boxed{\underbrace{\frac{\partial}{\partial x_i}}_{\text{continuity eq.}} \underbrace{\boxed{\frac{\partial p}{\partial x_i}}}_{\text{mtm eq}} = - \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}(\rho u_i u_j)}$$

Poisson eq.

use consistent discretization method. otherwise, continuity is not satisfied.

② Simple explicit time advance scheme

$$\frac{\partial(\rho u_i)}{\partial t} = -\frac{\partial}{\partial x_j}(\rho u_i u_j) - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

$$= -\frac{\delta}{\delta x_j}(\rho u_i u_j) - \frac{\delta p}{\delta x_i} + \frac{\delta \tau_{ij}}{\delta x_j} \equiv H_i - \frac{\delta p}{\delta x_i}$$

EE :
$$\frac{(\rho u_i)^{n+1} - (\rho u_i)^n}{\Delta t} = H_i^n - \frac{\delta p^n}{\delta x_i} \quad \text{—— } (*)$$

If we have $\frac{\delta u_i^n}{\delta x_i} = 0$ and some p^n,

then $\frac{\delta(\rho u_i)^{n+1}}{\delta x_i}$ is usually non zero with u_i^{n+1} from $(*)$.

Now, take divergence on $(*)$

$$\frac{\delta}{\delta x_i}(\rho u_i)^{n+1} - \frac{\delta}{\delta x_i}(\rho u_i)^{n} = \Delta t\left[\frac{\delta}{\delta x_i}\left(H_i^n - \frac{\delta p^n}{\delta x_i}\right)\right]$$

If u_i^n is divergence free, $\frac{\delta}{\delta x_i}(\rho u_i)^n = 0$

We require $\underline{\frac{\delta}{\delta x_i}(\rho u_i)^{n+1} = 0}$

$\rightarrow$ $\frac{\delta}{\delta x_i}\left(\frac{\delta p^n}{\delta x_i}\right) = \frac{\delta H_i^n}{\delta x_i}$ $\longrightarrow$ obtain p^n.

$\Rightarrow$ $\frac{\delta}{\delta x_i}(\rho u_i)^{n+1} = 0$ with u_i^{n+1} from (*). $\}$ higher-order method

EE : 1st-order accurate $\rightarrow$ inaccurate.

small Δt $\rightarrow$ implicit method

③ Simple implicit time advance method

Implicit Euler method (backward Euler method)

$$\frac{\partial(\rho u_i)}{\partial t} = -\frac{\partial}{\partial x_j}(\rho u_i u_j) - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + O(\Delta t^1)$$

IE : $$\frac{(\rho u_i)^{n+1} - (\rho u_i)^n}{\Delta t} = -\frac{\delta(\rho u_i u_j)^{n+1}}{\delta x_j} - \frac{\delta p^{n+1}}{\delta x_i} + \frac{\partial \tau_{ij}^{n+1}}{\delta x_j} \quad \text{—} \ (*)$$

We require $\frac{\delta(\rho u_i)^{n+1}}{\delta x_i} = 0$ $\qquad \tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$

Take divergence on $(*)$ (ρu_i^n is divergence free)

$$\frac{\delta}{\delta x_i}\left(\frac{\delta p^{n+1}}{\delta x_i}\right) = \frac{\delta}{\delta x_i}\left[-\frac{\delta(\rho u_i u_j)^{n+1}}{\delta x_j}\right] \quad \text{—} \quad \cancel{**}$$

unknown

Thus, one has to solve $\circledast$ & $\circledast\circledast$ simultaneously.

→ rely on iterative procedure.

Even if we know p^{n+1}, $\circledast$ contains nonlinear term

→ requires iterative procedure.

Or, introduce linearization $u_i^{n+1} = u_i^n + \underbrace{\Delta u_i}_{O(\Delta t)}$

→ $u_i^{n+1} u_j^{n+1} = (u_i^n + \Delta u_i)(u_j^n + \Delta u_j)$

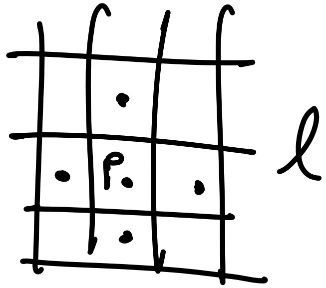
$$= \underbrace{u_i^n u_j^n + u_i^n \Delta u_j + \Delta u_i u_j^n}_{\Downarrow \ \text{linear term}} + \underbrace{\Delta u_i \Delta u_j}_{O(\Delta t^2)}$$

∴ neglect

④ Implicit pressure-correction methods for steady state flow

why implicit method? large Δt!

→ use implicit method and take large Δt.



mtm eq.

$$\Rightarrow \quad A_P^{u_i} u_{i,P}^{n+1} + \sum_l A_l^{u_i} u_{i,l}^{n+1} = Q_{u_i}^{n+1} - \left(\frac{\delta p^{n+1}}{\delta x_i}\right)_P$$

contains all the terms treated explicitly as well as the body force term.

→ iterative solver

$$A_p^{u_i} u_{i,p}^{m*} + \sum_l A_l^{u_i} u_{i,l}^{m*} = Q_{u_i}^{m-1} - \left(\frac{\delta p^{m-1}}{\delta x_i}\right)_p$$

get $u_{i,p}^{m*}$

m: iteration index

- $u_{i,p}^{m*}$ does not satisfy continuity.
- We need continuity enforcement.
  - → vel. has to be corrected.
  - → modification of the press.

$$\hookrightarrow \quad u_{i,P}^{m*} = \underbrace{\frac{1}{A_P^{u_i}}\left(Q_{u_i}^{m-1} - \sum_l A_l^{u_i} u_{i,l}^{m*} \right)}_{\equiv\ \tilde{u}_{i,P}^{m*}} - \frac{1}{A_P^{u_i}}\left(\frac{\delta p^{m-1}}{\delta x_i}\right)_P$$

$\equiv \tilde{u}_{i,P}^{m*}$: one from which the contribution of the press. grad. has been removed.

continuity $\quad \dfrac{\delta}{\delta x_i}(\rho u_i^m) = 0$

$$u_{i,P}^{m} = u_{i,P}^{m*} - \frac{1}{A_P^{u_i}}\left(\frac{\cancel{\delta p^{m}}}{\delta x_i}\right)_P$$

?

$p^m - p^{m-1}$

Let $\quad u_{i,P}^{m} = \tilde{u}_{i,P}^{m*} - \dfrac{1}{A_P^{u_i}}\left(\dfrac{\delta p^{m}}{\delta x_i}\right)_P$

vel. correction

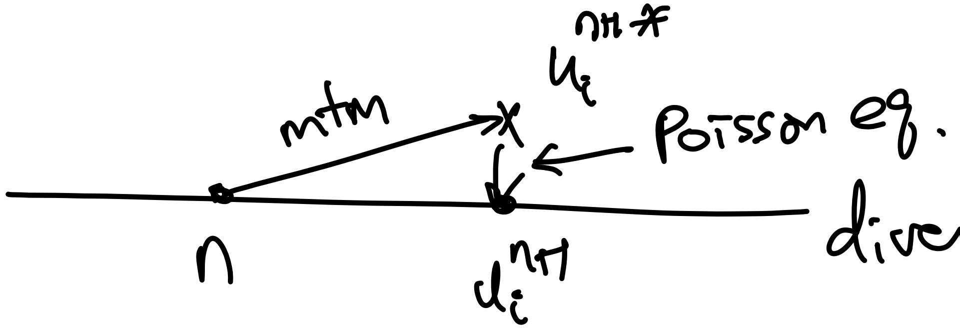
take divergence : $\quad \dfrac{\delta}{\delta x_i}\left[\dfrac{\rho}{A_P^{u_i}}\left(\dfrac{\delta p^m}{\delta x_i}\right)\right]_P = \left(\dfrac{\delta \rho \tilde{u}_i^{m*}}{\delta x_i}\right)_P$

→ obtain p^m

→ update $u_{i,p}^m$

→ keep iteration until converges.

This kind of method is called <u>projection method</u>.



(fractional-step method)

divergence-free vel

$$u_{i,p}^{m} = \tilde{u}_{i,p}^{m*} - \frac{1}{A_p^{u_i}} \frac{\delta p^m}{\delta x_i}\Big)_p \quad ?$$

$$A_p u_{i,p}^{n+1} + \sum_l A_l u_{i,l}^{n+1} = -\frac{\delta p^{n+1}}{\delta x_i}\Big)_p$$

iteration : $A_p u_{i,p}^m + \sum_l A_l u_{i,l}^m = -\frac{\delta p^m}{\delta x_i}\Big)_p$

$$A_p u_{i,p}^{m*} + \sum_l A_l u_{i,l}^{m*} = -\frac{\delta p^{m-1}}{\delta x_i}\Big)_p$$

$$\rightarrow u_{i,p}^{m*} = \underbrace{\frac{1}{A_p}\left(-\sum_l A_l u_{i,l}^{m*}\right)}_{\equiv \tilde{u}_{i,p}^{m*}} - \frac{1}{A_p}\frac{\delta p^{m-1}}{\delta x_i}\Big)_p$$

$$\frac{\delta}{\delta x_i}(\rho u_i^m) = 0$$

$$u_{i,p}^m = \tilde{u}_{i,p}^{m*} - \frac{1}{A_p}\frac{\delta \phi}{\delta x_i}\Big)_p$$

$$\rightarrow u_{i,p}^m = u_{i,p}^{m*} + \frac{1}{A_p}\frac{\delta}{\delta x_i}(p^{m-1} - \phi)\Big)_p$$

$$A_p u_{i,p}^{m*} = \underbrace{A_p \tilde{u}_{i,p}^{m*}}_{= -\sum_l A_l u_{i,l}^{m*}} - \frac{\delta p^{m-1}}{\delta x_i}\Big)_p \qquad u_{i,p}^{m*} = u_{i,p}^{m} + \frac{1}{A_p}\frac{\delta}{\delta x_i}\left(\phi - p^{m-1}\right)_p$$

$$\rightarrow \quad A_p u_{i,p}^{m} + \sum_l A_p u_{i,l}^{m} + \underbrace{\sum_l \frac{A_l}{A_p}\left(\frac{\partial \phi}{\partial x_i} - \frac{\delta p^{m-1}}{\delta x_i}\right)}_{\text{goes to zero when converged.}} = -\frac{\delta \phi}{\delta x_i}\Big|_p$$

$$\Big(\qquad \text{''} \qquad \Big) = -\frac{\delta p^{m}}{\delta x_i}$$

$\Rightarrow$ then, $\phi = p^m$

ⓐ SIMPLE (Semi-Implicit Method for Pressure-Linked Equations)

$$\begin{cases} u_i^m = u_i^{m*} + u_i' \\ p^m = p^{m-1} + p' \end{cases}$$

$$\text{mtm} : \; A_p u_{i,p}^m + \sum_l A_l u_{i,l}^m = \cancel{Q_{u_i,p}^m} - \frac{\delta p^m}{\delta x_i}\Big)_p$$

obtain $u_i^{m*} \leftarrow$

$$- \;\Big|\; A_p u_{i,p}^{m*} + \sum_l A_l u_{i,l}^{m*} = \cancel{Q_{u_i,p}^{m-1}} - \frac{\delta p^{m-1}}{\delta x_i}\Big)_p$$

$$A_p u_{i,p}' + \sum_l A_l u_{i,l}' = - \frac{\delta p'}{\delta x_i}\Big)_p$$

$$u'_{i,P} = \underbrace{\frac{1}{A_P}\left(-\sum_l A_l u'_{i,l}\right)}_{\tilde{u}'_{i,P}} - \frac{1}{A_P}\left(\frac{\delta p'}{\delta x_i}\right)_P$$

$$\nabla \cdot \left(\text{cont}: \ \frac{\delta u_i^m}{\delta x_i} = \frac{\delta u_i^{m*}}{\delta x_i} + \frac{\delta u'_i}{\delta x_i} = 0 \right)$$

press-correction eq.

$$\boxed{\frac{\delta}{\delta x_i}\left[\frac{\rho}{A_P}\left(\frac{\delta p'}{\delta x_i}\right)\right]_P = \left[\frac{\delta}{\delta x_i}(\rho u_i^{m*})\right]_P} + \underbrace{\left(\frac{\delta \tilde{u}'_i}{\delta x_i}\right)_P}_{\text{unknown}}$$

→ obtain p'

→ update $u'_{i,P}$ $\left(= -\frac{1}{A_P}\frac{\delta p'}{\rho \delta x_i}\right)$

no justification ← ∴ neglect!

causes slow convergence

$\rightarrow$ obtain u_i^m and p^m, $\rightarrow$ keep iteration

SIMPLE

$$u_i^m = u_i^{m*} + u_i' \quad , \quad p^m = p^{m-1} + p' \qquad m : \text{iteration index}$$

mtm :

$$A_p u_{i,p}^m + \sum_l A_l u_{i,l}^m = -\frac{\delta p^m}{\delta x_i}\Big)_p + \cancel{Q_{u_i,p}^m}$$

$$\bullet \quad A_p u_{i,p}^{m*} + \sum_l A_l u_{i,l}^{m*} = -\frac{\delta p^{m-1}}{\delta x_i}\Big)_p \Rightarrow \text{obtain } u_i^{m*}$$

①

$$A_p u_{i,p}' + \sum_l A_l u_{i,l}' = -\frac{\delta p'}{\delta x_i}\Big)_p$$

$$u_{i,p}' = \underbrace{\frac{1}{A_p}\left(-\sum_l A_l u_{i,l}'\right)} - \frac{1}{A_p}\frac{\delta p'}{\delta x_i}\Big)_p$$

$$= \tilde{u}'_{i,p}$$

continuity $\frac{\delta u_i^m}{\delta x_i} = \frac{\delta u_i^{m*}}{\delta x_i} + \frac{\delta u_i'}{\delta x_i} = 0$

② $\rightarrow \underbrace{\frac{\delta}{\delta x_i}\left(\frac{\rho}{A_p}\frac{\delta p'}{\delta x_i}\right)_p = \frac{\delta}{\delta x_i}(\rho u_i^{m*})\Big|_p}_{\substack{\Uparrow \\ \text{known}}} + \underbrace{\frac{\delta \rho \tilde{u}_i'}{\delta x_i}\Big|_p}_{\text{unknown}}$

$\rightarrow$ obtain p' $\qquad\qquad\qquad \rightarrow$ neglect

$\rightarrow$ update $u_i' = -\frac{1}{A_p}\frac{\delta p'}{\delta x_i}$ and $\underline{p^m = p^{m-1} + p'}$

$\rightarrow$ obtain $\underline{u_i^m = u_i^{m*} + u_i'}$

ⓑ SIMPLEC

Don't neglect $\frac{\delta}{\delta x_i}(\rho \tilde{u}_i')$.

Do approximate as $\sum_l A_l u'_{i,l} \simeq u'_{i,p} \cdot (\sum_l A_l)$

then, $\tilde{u}'_{i,p} = -\frac{1}{A_p} \sum_l A_l u'_{i,l} \doteqdot - u'_{i,p} \sum_l A_l / A_p$

$$\left[u'_{i,p} = \tilde{u}'_{i,p} - \frac{1}{A_p} \frac{\delta p'}{\partial x_i}\Big)_p \right] \Leftarrow$$

$$\hookrightarrow \; u'_{i,p} = - \frac{1}{A_p + \sum_l A_l} \frac{\delta p'}{\delta x_i}\Big)_p$$

Poisson eq : $\frac{\delta}{\delta x_i} \left[\frac{1}{A_p + \sum_l A_l} \frac{\delta p'}{\partial x_i} \right]_p = \frac{\delta}{\delta x_i} (\rho u_i^{m*}) \Big|_p$

$\to$ obtain p' $\to$ obtain u'_i

$\to$ update u_i^m and p^m

ⓒ SIMPLER

neglect $\frac{\delta}{\delta x_i}(\rho \tilde{u}_i')\Big|_p$ as in SIMPLE

and obtain p' as in SIMPLE

$\rightarrow$ update u_i' $\rightarrow$ obtain u_i^m

How to obtain p^m? ($p^m = p^{m-1} + p'$ in SIMPLE)

$$A_p u_{i,p}^m + \underbrace{\sum_l A_l u_{i,l}^m}_{\equiv -\tilde{u}_i^m} = -\frac{\delta p^m}{\delta x_i}\Big)_p$$

$$\rightarrow \quad \frac{\delta}{\delta x_i}\left[\frac{\rho}{A_p}\frac{\delta p^m}{\delta x_i}\right]_p = \frac{\delta}{\delta x_i}(\rho \tilde{u}_i^m)\Big|_p$$

$\rightarrow$ obtain p^m $\rightarrow$ iterate until convergence.

(d) PISO $u_i^m = u_i^{m*} + u_i' + u_i''$, $p^m = p^{m-1} + p' + p''$

these methods are fairly efficient for solving steady state problems.

4. other methods

(i) Fractional step methods (called projection method)

Kim & Moin (1985)
— 2nd-order accurate in time

Chorin (19 --)
Temam ( )
1st-order accurate

$$\begin{cases} \dfrac{\partial u_i}{\partial x_i} = 0 \\ \dfrac{\partial u_i}{\partial t} + \dfrac{\partial}{\partial x_j}(u_i u_j) = -\dfrac{\partial p}{\partial x_i} + \dfrac{1}{Re}\nabla^2 u_i \end{cases}$$

non-dimensionalized N-S eq.

(Adams - Bashforth method for nonlinear term
and Crank - Nicolson method for viscous term)

$(n \to n+1)$

$$
\begin{cases}
\dfrac{u_i^{n+1} - u_i^n}{\Delta t} + \underbrace{\dfrac{1}{2}\left[3\dfrac{\partial}{\partial x_j}\left(u_i^n u_j^n\right) - \dfrac{\partial}{\partial x_j}\left(u_i^{n-1} u_j^{n-1}\right)\right]}_{AB2} \\[2ex]
\quad = \underbrace{-\dfrac{1}{2}\left(\dfrac{\partial p^{n+1}}{\partial x_i} + \dfrac{\partial p^n}{\partial x_i}\right) + \dfrac{1}{2}\dfrac{1}{Re}\nabla^2\left(u_i^{n+1} + u_i^n\right)}_{\text{implicit}} \\[2ex]
\dfrac{\partial u_i^{n+1}}{\partial x_i} = 0
\end{cases}
$$

explicit

one way to go w/ this formulation

→ direct inverting → very expensive

- fractional step method $\quad \hat{u}_i$: intermediate vel.

① $\dfrac{\hat{u}_i - u_i^n}{\Delta t} + \dfrac{1}{2}\left[3\dfrac{\partial}{\partial x_j} u_i^n u_j^n - \dfrac{\partial}{\partial x_j} u_i^{n-1} u_j^{n-1}\right] = \dfrac{1}{2}\dfrac{1}{Re}\nabla^2\left(\hat{u}_i + u_i^n\right)$

→ second-order approximation of

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_i u_j) = \frac{1}{Re}\nabla^2 u_i$$

obtain $\hat{u}_i$. → $\hat{u}_i$ does not satisfy the continuity.

$$\frac{u_i^{n+1} - \hat{u}_i}{\Delta t} = -\frac{\partial \phi^{n+1}}{\partial x_i}$$

Force u_i^{n+1} to satisfy the continuity.

→ $\nabla^2 \phi^{n+1} = \dfrac{1}{\Delta t}\dfrac{\partial \hat{u}_i}{\partial x_i}$ ②

$\rightarrow$ obtain ϕ^{n+1}

$\rightarrow$ $u_i^{n+1} = \hat{u}_i - \Delta t \dfrac{\partial \phi^{n+1}}{\partial x_i}$ 3 $\rightarrow$ time marching

- Issue on the computational cost for Eq. 1

$$N_i \equiv \frac{\partial}{\delta x_j}(u_i u_j)$$

$$\frac{\hat{u}_i - u_i^n}{\Delta t} + \frac{1}{2}\left(3N_i^n - N_i^{n-1}\right) = \frac{1}{2Re}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right)(\hat{u}_i + u_i^n) + O(\Delta t^2)$$

$$\rightarrow \left[1 - \frac{\Delta t}{2Re}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right)\right](\hat{u}_i - u_i^n)$$

$\left[\delta \hat{u}_i = \hat{u}_i - u_i^n \text{ delta form}\right]$

$$= \frac{\Delta t}{2}\left(-3N_i^n + N_i^{n-1}\right) + \frac{\Delta t}{Re}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right) u_i^n + O(\Delta t^3)$$

$$A_x = \frac{\Delta t}{2Re}\frac{\delta^2}{\delta x^2}, \quad A_y = \frac{\Delta t}{2Re}\frac{\delta^2}{\delta y^2}, \quad A_z = \frac{\Delta t}{2Re}\frac{\delta^2}{\delta z^2}$$

$\rightarrow \underbrace{(1 - A_x - A_y - A_z)}_{\text{Sparse Matrix}} (\hat{u}_i - u_i^n) = R_i + O(\Delta t^3)$

Sparse Matrix → expensive to invert

✓ introduce approximate factorization scheme

$$(1-A_x-A_y-A_z)(\hat{u}_i-u_i^n) = (1-A_x)(1-A_y)(1-A_z)(\hat{u}_i-u_i^n) + O(\Delta t^3)$$

do not lose any accuracy

$$\rightarrow \underbrace{(1-A_x)}_{\text{tri-diagonal matrix}}\underbrace{(1-A_y)(1-A_z)(\hat{u}_i-u_i^n)}_{v_i} = R_i + \underline{O(\Delta t^3)}$$

tri-diagonal matrix

v_i → get v_i

$$(1-A_y)\underbrace{(1-A_z)(\hat{u}_i-u_i^n)}_{w_i} = v_i$$

w_i → get w_i

$$(1-A_z)(\hat{u}_c - \hat{u}_i) = w_i \rightarrow \text{get } \hat{u}_c$$

$O(N)$ operation.

Saves a lot of CPU and memory!

Issue on the numerical stability

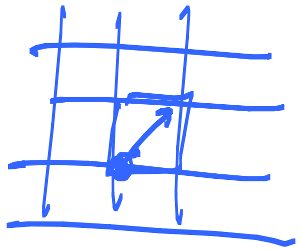
$$\underbrace{AB2}_{\text{explicit}} + \underbrace{CN}_{\text{implicit}} \; : \; \text{semi-implicit method}$$

↓

conditionaly stable

$$CFL = \left(\frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} + \frac{|w|}{\Delta z} \right) \Delta t \le 1$$

$$\Delta t \le \left(\frac{\Delta x}{|u|} + \frac{\Delta y}{|v|} + \frac{\Delta z}{|w|} \right)^{-1}$$



(AB2 + AB2 fully explicit $\Delta t \sim \Delta x^2$ too severe)

problem : not self-starting $\because$ $\dfrac{n \;\&\; n-1}{n-1,\; n,\; n+1}$

AB2+CN spurious root $\because$

↳ better one is

① RK3 + CN

② CN (fully implicit)

$n-1,\ n,\ n+1$

Δt Δt : $n-1$, n, $n+1$

CFL ≤ 1

- AB2 + CN
- RK3 + CN

} semi-implicit methods

Fractional step method using RK3 + CN

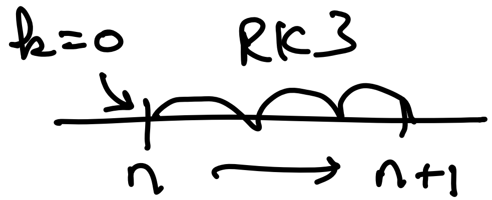
RK3 → N_i - nonlinear

CN → viscous L_i

① $$\frac{\hat{u}_i^k - u_i^{k-1}}{\Delta t} = (\alpha_k + \beta_k) L_i(\underline{u}^{k-1}) + \beta_k L_i(\hat{\underline{u}}^k - \underline{u}^{k-1}) - \gamma_k N_i(\underline{u}^{k-1}) - \zeta_k N_i(\underline{u}^{k-2}) \qquad k = 1, 2, 3$$

② $$+(\gamma_k + \zeta_k)\nabla^2 \phi^k = \frac{1}{\Delta t}\frac{\partial \hat{u}_i^k}{\partial x_i}$$

③ $$u_i^k = \hat{u}_i^k - \Delta t(\gamma_k + \zeta_k)\partial\phi^k/\partial x_i$$



$$\alpha_1 = \beta_1 = \frac{4}{15} \qquad \gamma_1 = \frac{8}{15} \qquad \zeta_1 = 0$$

$$\alpha_2 = \beta_2 = \frac{1}{15} \qquad \gamma_2 = \frac{5}{12} \qquad \zeta_2 = -\frac{17}{60}$$

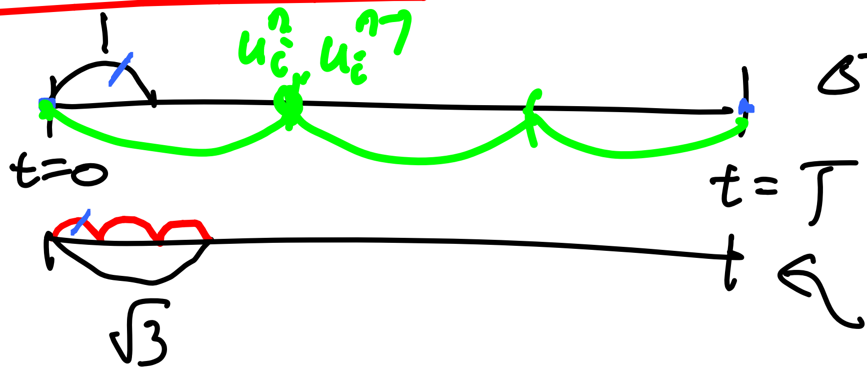
$$\alpha_3 = \beta_3 = \frac{1}{6} \qquad \gamma_3 = \frac{3}{4} \qquad \zeta_3 = -\frac{5}{12}$$

ϕ: pseudo-pressure

$$CFL = \boxed{\left(\frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} + \frac{|w|}{\Delta z} \right)} \Delta t \le \sqrt{3}$$

u_i^n, u_i^{n-1} ← AB2+CN

RK3+CN → self-starting, no spurious root



Δt = const throughout the comp.

$\boxed{\Delta t \text{ can be changed.}}$

- CN only (fully implicit) $\rightarrow$ no limit on Δt.

Choi & Moin (1994, JCP, 113, 1)

$$\begin{cases} \dfrac{u_i^{n+1}-u_i^n}{\Delta t} + \dfrac{1}{2}\dfrac{\partial}{\partial x_j}\left(u_i^{n+1}u_j^{n+1}+u_i^n u_j^n\right) = -\dfrac{\partial p^{n+1}}{\partial x_i} + \dfrac{1}{2Re}\nabla^2\left(u_i^{n+1}+u_i^n\right) \\ \dfrac{\partial u_i^{n+1}}{\partial x_i} = 0 \end{cases}$$

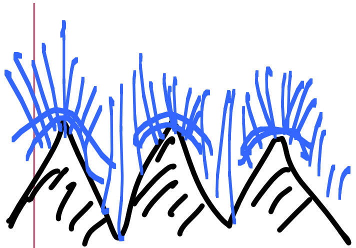
or $-\dfrac{1}{2}\left(\dfrac{\partial p^{n+1}}{\partial x_i}+\dfrac{\partial p^n}{\partial x_i}\right)$

FSM ① $\dfrac{\hat{u}_i-u_i^n}{\Delta t} + \dfrac{1}{2}\dfrac{\partial}{\partial x_j}\left(\hat{u}_i\hat{u}_j+u_i^n u_j^n\right) = -\dfrac{\partial p^n}{\partial x_i} + \dfrac{1}{2Re}\nabla^2\left(\hat{u}_i+u_i^n\right)$

↳ get $\hat{u}_i$ using iterative scheme like Newton iteration or using

② $\dfrac{u_i^*-\hat{u}_i}{\Delta t} = \dfrac{\partial p^n}{\partial x_i}$

③ $\nabla^2 p^{n+1} = \dfrac{1}{\Delta t}\dfrac{\partial u_i^*}{\partial x_i}$



④ $u_i^{n+1} = u_i^{*} - \Delta t \dfrac{\partial p^{n+1}}{\partial x_i}$ linearization

Main difference bet. FSM and SIMPLE :
for unsteady prob.

FSM : Solve the Poisson eq 1~3 times / time step

SIMPLE : solve both the mtm and pressure-correction eqs several times per time step.

Let's go back to AB2+CN

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}+\frac{1}{2}\left[3\frac{\partial}{\partial x_j}u_i^n u_j^n-\frac{\partial}{\partial x_j}u_i^{n-1}u_j^{n-1}\right]$$

$$=-\frac{1}{2}\left(\frac{\partial p^{n+1}}{\partial x_i}+\frac{\partial p^n}{\partial x_i}\right)+\frac{1}{2Re}\nabla^2\left(u_i^{n+1}+u_i^n\right)$$

$$-\frac{\partial p^{n+1}}{\partial x_i}$$

$$-\frac{\partial p^n}{\partial x_i}$$

FSM

$$\frac{\hat{u}_i-u_i^n}{\Delta t}+\frac{1}{2}\left[\quad // \quad\right]=\frac{1}{2Re}\nabla^2\left(\hat{u}_i+u_i^n\right)$$

$$\frac{u_i^{n+1}-\hat{u}_i}{\Delta t}=-\frac{\partial\phi}{\partial x_i}\Rightarrow\boxed{\hat{u}_i=u_i^{n+1}+\Delta t\frac{\partial\phi}{\partial x_i}}$$

$$-\frac{\partial p^n}{\partial x_i}$$

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}+\frac{\partial \phi}{\partial x_i}+\frac{1}{2}\left[\quad '' \quad -\frac{\partial p^n}{\partial x_i}\right]=\frac{1}{2Re}\nabla^2\left(u_i^{n+1}+\Delta t\frac{\partial \phi}{\partial x_i}+u_i^n\right)$$

$$\rightarrow \boxed{\frac{u_i^{n+1}-u_i^n}{\Delta t}+\frac{1}{2}\left[\quad '' \quad\right]=-\frac{\partial \phi}{\partial x_i}+\frac{\Delta t}{2Re}\frac{\partial}{\partial x_i}\left(\nabla^2\phi\right)+\frac{1}{2Re}\nabla^2\left(u_i^{n+1}+u_i^n\right)}$$

$$-\frac{\partial}{\partial x_i}\left(\boxed{\frac{1}{2}\left(p^{n+1}+p^n\right)}\right)=-\frac{\partial}{\partial x_i}\left(\boxed{\phi-\frac{\Delta t}{2Re}\nabla^2\phi}\right)$$

p^{n+1} $\quad$ $p^n +$

$$\rightarrow p^{n+1}=\boxed{-p^n}+2\phi-\frac{\Delta t}{Re}\nabla^2\phi$$

p^n $\quad$ $p^{n+1}=\phi-\frac{\Delta t}{2Re}\nabla^2\phi$

Q: following Kim & Moin (1985),

what is the b.c. for $\hat{u}_i$? $\qquad$ $\hat{u}_i = u_i^{n+1}$?

$\rightarrow \hat{u}_i = u_i^{n+1} + \Delta t \dfrac{\partial \phi^n}{\partial x_i}$ (b.c.)

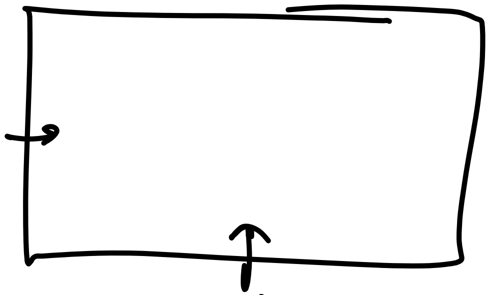
w/ explicit press. grad. $\quad -\dfrac{\partial p^n}{\partial x_i} \rightarrow$ 1st step of FSM $\Rightarrow \hat{u}_i = u_i^{n+1}$ (b.c)

$$\frac{u_i^{n+1} - \hat{u}_i^n}{\Delta t} = -\frac{\partial \phi}{\partial x_i} \rightarrow \boxed{\nabla^2 \phi = \frac{1}{\Delta t}\frac{\partial \hat{u}_i^n}{\partial x_i}}$$

b.c for ϕ ?

$$\frac{u^{n+1}-\hat{u}}{\delta t}\Big|_{bd} = \frac{\partial \phi}{\partial x}$$

$$= 0$$



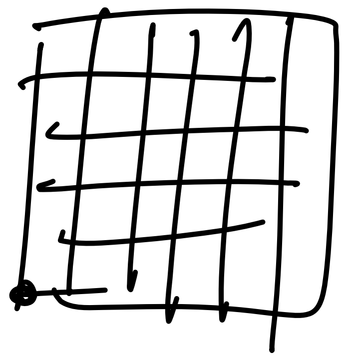
$$\frac{\partial \phi}{\partial y} = (v^{n+1}-\hat{v})/\delta t\,\Big|_{bdry} = 0 \quad \left(w/\ -\frac{\partial p^n}{\partial x_i}\right)$$

$$= 0 \quad (w/o \quad '' \quad)$$

$$\frac{\partial p}{\partial y}\Big|_{bdry} \neq 0 \qquad \frac{1}{Re}\nabla^2 v\Big|_{wall}$$

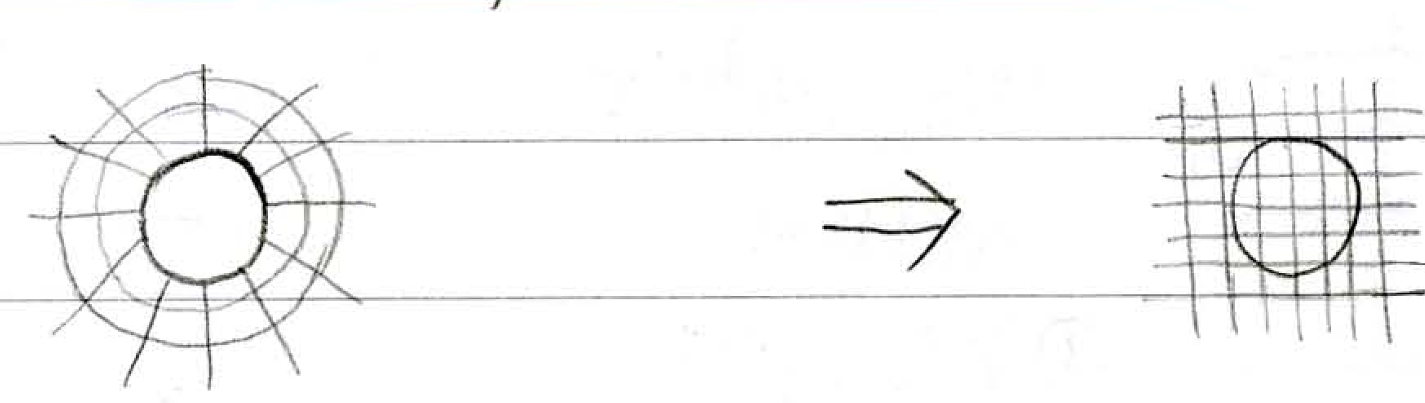
$$\boxed{\nabla^2 \phi = r \quad w/\ \frac{\partial \phi}{\partial n} = 0} \Rightarrow \phi$$

$$\phi + c$$



$\phi(1,1) = 0$

Immersed Boundary method (IB method)

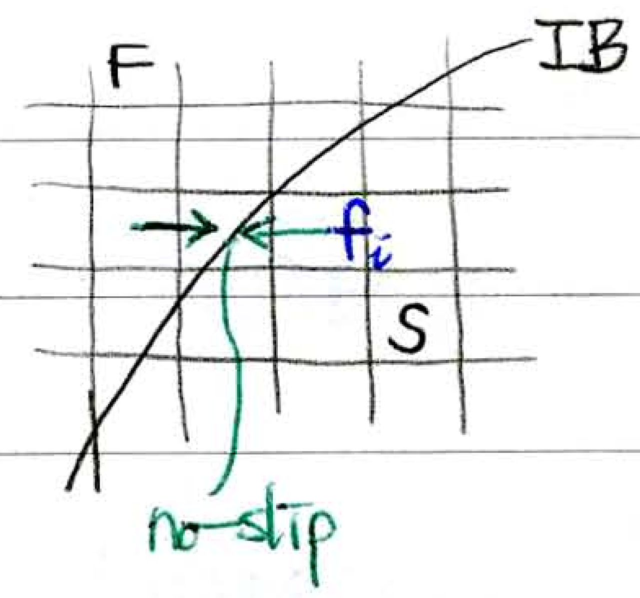


Body-fitted grid IB method

Kim et al. (2001, JCP)

* Peskin (1982): Original Development

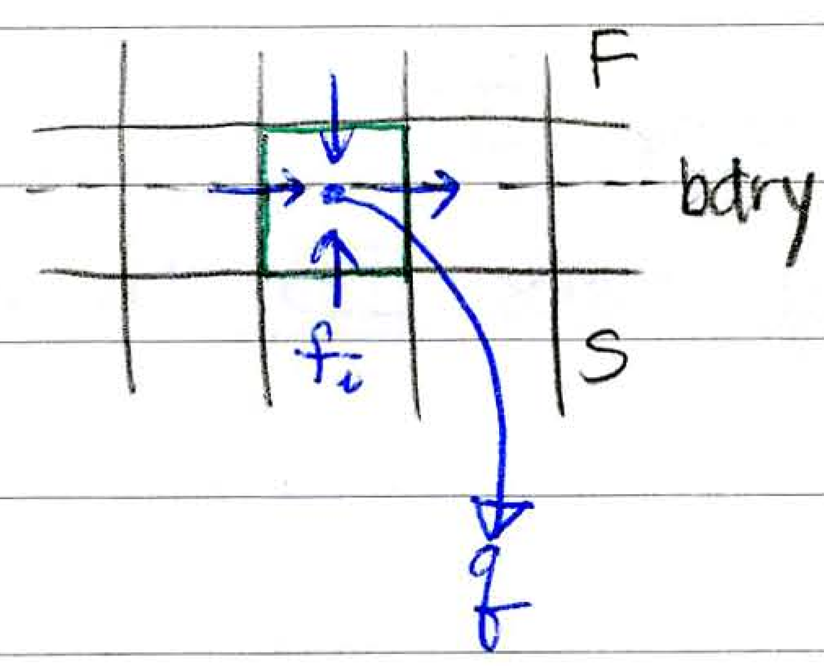
F: fluid
S: Solid



$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} u_i u_j = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\nabla^2 u_i + \underbrace{f_i}_{\substack{\text{mtm forcing} \\ \text{(Peskin)}}}$$

$$\frac{\partial u_i}{\partial x_i} - \underbrace{q}_{\text{mass source/sink (Kim et al.)}} = 0$$

for continuity



→ Provides mass source/sink q for cell containing IB

$$\frac{\partial u_i}{\partial x_i} - q = 0$$

Fractional Step method (RK3 + CN2)

④ $$\frac{\hat{u}_i^k - u_i^{k-1}}{\Delta t} = \alpha_k L(\hat{u}_i^k) + \alpha_k L(u_i^{k-1}) - 2\alpha_k \frac{\partial p^{k-1}}{\partial x_i} - \gamma_k N(u_i^{k-1}) - \rho_k N(u_i^{k-2}) + \underbrace{f_i^k}$$

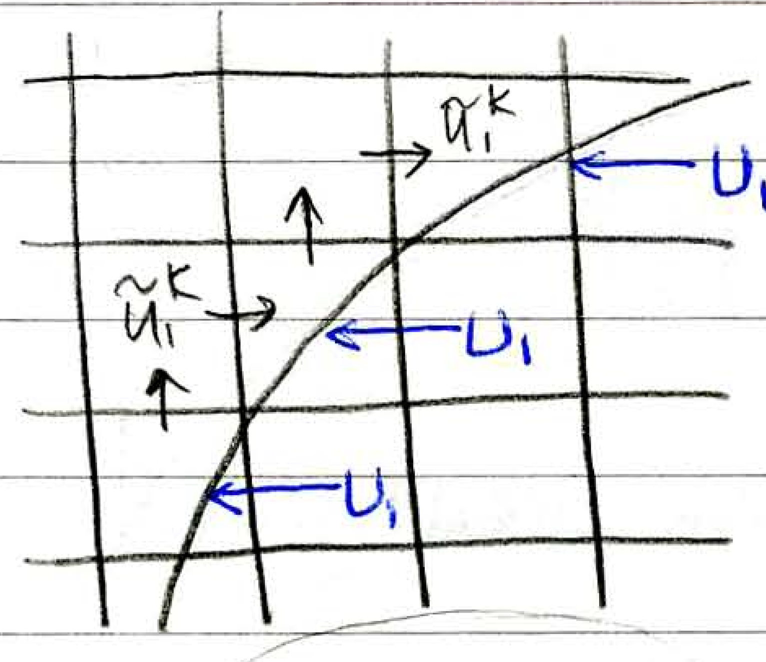
⑥ $$\nabla^2 \phi^k = \frac{1}{2\alpha_k \Delta t}\left(\frac{\partial \hat{u}_i^k}{\partial x_i} - \underbrace{q^k}\right)$$

⑦ $$u_i^k = \hat{u}_i^k - 2\alpha_k \Delta t \frac{\partial \phi^k}{\partial x_i}$$

⑧ $$p^k = p^{k-1} + \phi^k - \frac{\alpha_k \Delta t}{Re}\nabla^2 \phi^k$$

k-1 → k
시간전진
① ~ ⑧

- How to obtain f_i?



We update N-S eq. with explicit numerical method.

① $$\frac{\tilde{u}_i^k - u_i^{k-1}}{\Delta t} = \underbrace{2\alpha_k L(u_i^{k-1})}_{EE} - 2\alpha_k \frac{\partial p^{k-1}}{\partial x_i} \underbrace{- \gamma_k N(u_i^{k-1}) - \rho_k N(u_i^{k-2})}_{RK3}$$

By interpolating the provisional vel. near IB $\tilde{u}_i^k$,
We obtain U_i^k

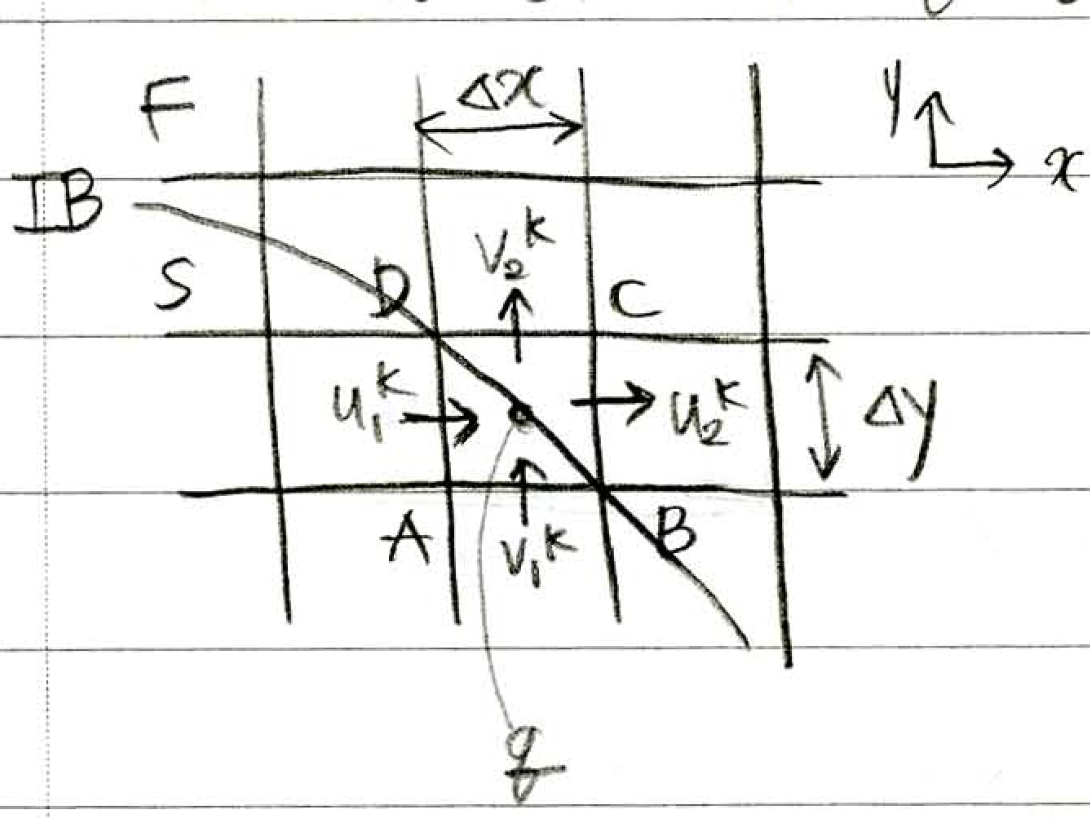
(1D, 2D, 3D (Kim et al.)

② $$\frac{U_i^k - u_i^{k-1}}{\Delta t} = 2\alpha_k L(u_i^{k-1}) - 2\alpha_k \frac{\partial p^{k-1}}{\partial x_i} - \gamma_k N(u_i^{k-1}) - \rho_k N(u_i^{k-2}) + f_i$$

③ $$f_i = \frac{U_i^k - u_i^{k-1}}{\Delta t} - 2\alpha_k L(u_i^{k-1}) + 2\alpha_k \frac{\partial p^{k-1}}{\partial x_i} + \gamma_k N(u_i^{k-1}) + \rho_k N(u_i^{k-2})$$

$\tilde{u}_i$: Provisional velocity near IB $\xrightarrow{\text{intp.}}$
U_i : Interpolated velocity inside IB to obtain f_i

- How to obtain q^k?



$\triangle BCD$: $u_2^k \Delta y + v_2^k \Delta x = 0$

$\square ABCD$: $u_2^k \Delta y + v_2^k \Delta x = u_1^k \Delta y + v_1^k \Delta x + \Delta x \Delta y\, q^k$

⑤ $$q^k = -\frac{u_1^k}{\Delta x} - \frac{v_1^k}{\Delta y} = -\frac{\hat{u}_1^k}{\Delta x} - \frac{\hat{v}_1^k}{\Delta y}$$

Kim et al. 기준

f_i : always inside IB
q : inside / outside IB

"Other" methods

① Fractional step methods

② Immersed boundary methods → direct forcing, discrete forcing
by Peskin

③ Stream function - vorticity methods
ψ - ω

→ $u = \frac{\partial \psi}{\partial y}$, $v = -\frac{\partial \psi}{\partial x}$ only (2D) ⇐ weakness

$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \Rightarrow \boxed{\nabla^2 \psi = -\omega}$ ①

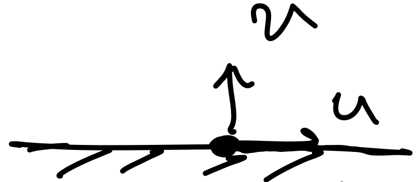
$\nabla \times$ (N-S eqs)

$$\rightarrow \boxed{\rho \frac{\partial \omega}{\partial t} + \rho u \frac{\partial \omega}{\partial x} + \rho v \frac{\partial \omega}{\partial y} = \mu \nabla^2 \omega} \quad (2)$$

3 eqs (cont + N-S) $\longrightarrow$ $\boxed{\text{2 eqs}}$

* continuity is identically satisfied !

no pressure in governing eqs.



$$\omega = \underbrace{\cancel{\frac{\partial v}{\partial x}}}_{0} - \frac{\partial u}{\partial y}\Big|_w$$

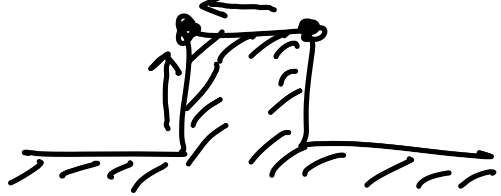
problems : 2-D flows only for

boundary condition of ω @ the wall

- usually one-side difference
- vorticity is singular at sharp corners.

$\psi - \omega$ approaches are less popular nowadays.

not continuous



④ Artificial compressibility method

by Chorin (1967) JCP Vol. 2, 12.

for steady flow, less efficient for unsteady flow

good

incompressible

$$\frac{\partial \rho u_i}{\partial x_i} = 0 \longrightarrow \frac{1}{\beta}\frac{\partial p}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0$$

(background)

$a^2 = \left.\frac{\partial p}{\partial \rho}\right|_s = \gamma RT$ for perfect gas

speed of sound

$$p = \rho R T = \rho R \frac{a^2}{\gamma R} = \rho \cdot \frac{a^2}{\gamma} \equiv \rho \beta$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \rightarrow \frac{1}{\beta}\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

explicit method → restriction in Δt

use implicit method → take large Δt.

β : parameter to be given a priori

large β → more like incompressible

↓

(use IE. . . . . . .)

it corresponds to SIMPLE w/o (under-relaxation)

SIMPLE $\left(\begin{array}{l} u^{n+1^m} = u^{*^m} + u' \\ p^{n+1^m} = p^{*^m} + p' \end{array} \right] \to u^*$

of the press-correction

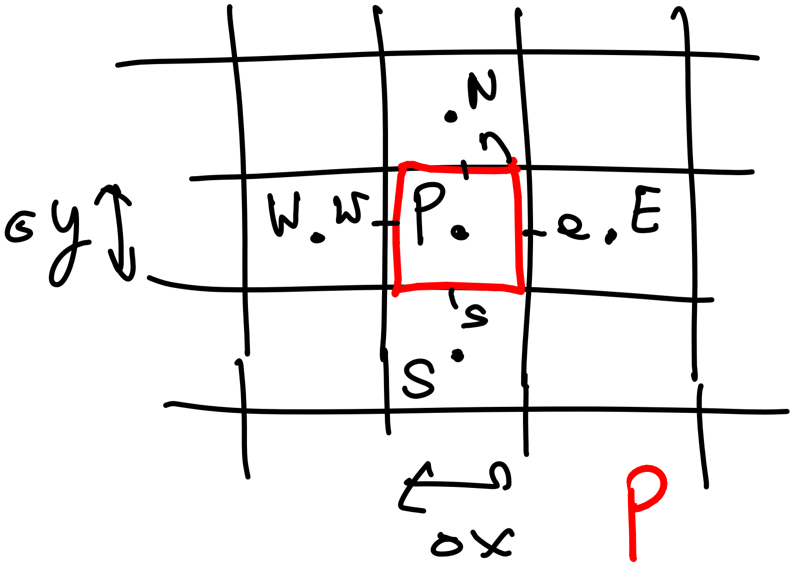
$u^* = \alpha u^*_{old} + (1-\alpha) u^*_{new}$

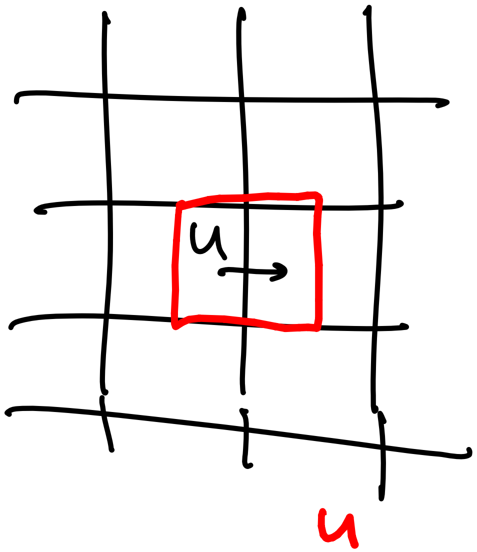
$(0 \le \alpha < 1)$

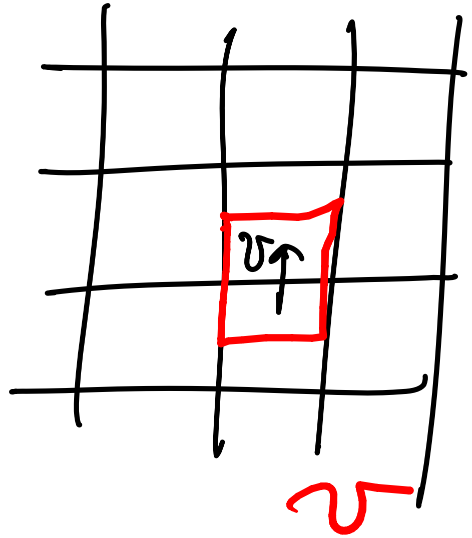
Kwak et al. (1986) AIAA J. 24, 390.

5. Solution methods for the N-S eqs.

5.1 Implicit scheme using pressure-correction and a staggered grid (FVM)







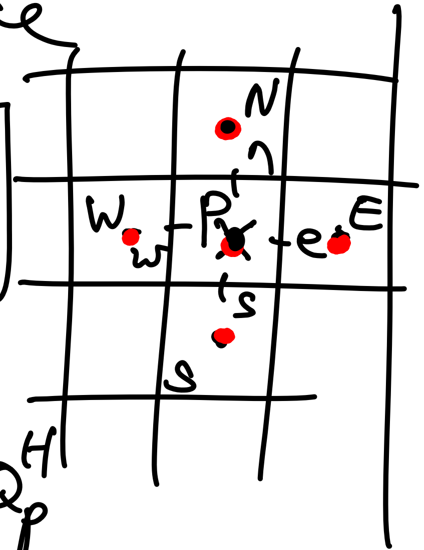
$$\int \frac{\partial}{\partial x}(uu)\, dV = O_w + O_e \ldots$$

5.2 Treatment of pressure for colocated variables

$$\frac{\delta}{\delta x_i}\left(\frac{\delta p^n}{\delta x_i}\right) = \frac{\delta H_i^n}{\delta x_i}, \qquad H_i^n = -\frac{\delta}{\delta x_j}\left(\rho u_i^n u_j^n\right) + \frac{\delta \tau_{ij}^n}{\delta x_j}$$

grad. operater) should be consistent
divergence operater) for energy conserving scheme.

e.g. (foward difference for gradient
(backward " for divergence



then, $\frac{1}{\delta x}\left[\left(\frac{\delta p^n}{\delta x}\right)_p - \left(\frac{\delta p^n}{\delta x}\right)_w\right] + \frac{1}{\delta y}\left[\left(\frac{\delta p^n}{\delta y}\right)_p - \left(\frac{\delta p^n}{\delta y}\right)_s\right]$

$$= \frac{1}{\delta x}\left[H_{x,p}^n - H_{x,w}^n\right] + \frac{1}{\delta y}\left[H_{y,p}^n - H_{y,s}^n\right] \equiv Q_p^H$$

And then

$$\frac{1}{\delta x}\left[\frac{1}{\delta x}\right]\left[\left(P_E^n - P_P^n\right) - \left(P_P^n - P_W^n\right)\right] + \frac{1}{\delta y}\frac{1}{\delta y}\left[\left(P_N^n - P_P^n\right) - \left(P_P^n - P_S^n\right)\right] = Q_P^H$$

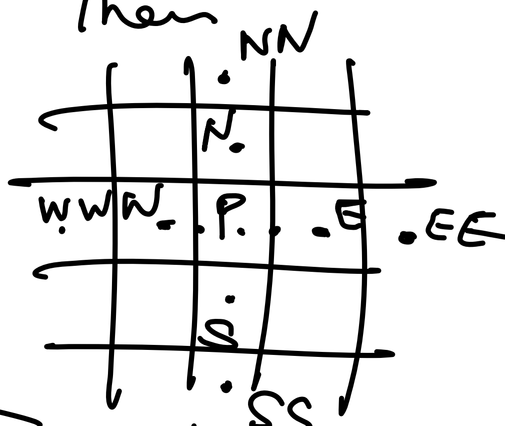
$$\rightarrow \quad A_P^P P_P^n + \sum_{l} A_l^P P_l^n = -Q_P^H$$

Same form as the one obtained on a staggered grid w/ central difference.

However, mtm eq : $-\frac{\delta p}{\delta x_i} \rightarrow$ forward difference

better to use higher order approx. $\leftarrow$ 1st order approx.

Now, CDS for div. & grad. operators. Then



$$\frac{1}{2\Delta x}\left[\left(\frac{\delta p}{\delta x}\right)^n_E - \left(\frac{\delta p}{\delta x}\right)^n_W\right] + \frac{1}{2\Delta y}\left[\left(\frac{\delta p}{\delta y}\right)^n_N - \left(\frac{\delta p}{\delta y}\right)^n_S\right]$$

$$= \frac{1}{2\Delta x}\left[H^n_{x,E} - H^n_{x,W}\right] + \frac{1}{2\Delta y}\left[H^n_{y,N} - H^n_{y,S}\right] \equiv Q_P^H$$

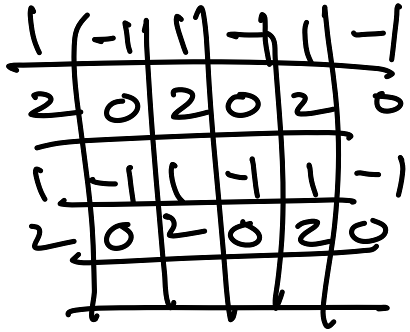
$$\to \frac{1}{2\Delta x}\frac{1}{2\Delta x}\left[(p^n_{EE} - p^n_P) - (p^n_P - p^n_{WW})\right]$$

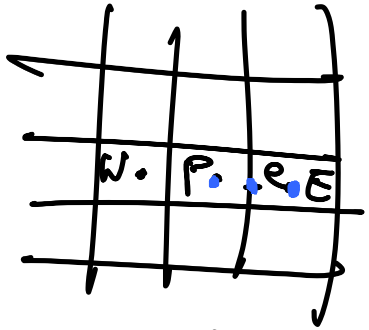
$$+ \frac{1}{2\Delta y}\frac{1}{2\Delta y}\left[(p^n_{NN} - p^n_P) - (p^n_P - p^n_{SS})\right] = Q_P^H$$

$$\to A_P^p\, p_P^n + \sum_l A_l^p\, p_l^n = -Q_P^H, \quad l = EE, WW, NN, SS$$

This eq. involves nodes which are $2\Delta x$ apart.

→ may create a checkerboard press. distribution.





Cure?

We could evaluate $\left.\frac{\partial p}{\delta x}\right|_e$ using CDS $\frac{\partial}{\delta x}\left(\frac{\partial p}{\delta x}\right)$

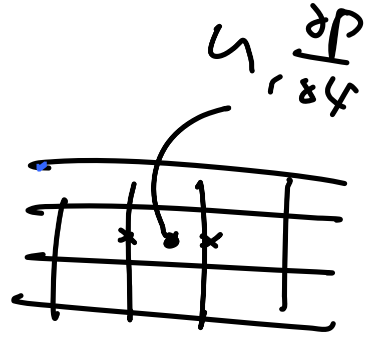
$$\left.\frac{\delta p^n}{\delta x}\right)_e \simeq \frac{P_E - P_P}{\delta x} \qquad \frac{1}{\delta x}\left(\left.\frac{\partial p}{\delta x}\right|_e^n - \left.\frac{\partial p}{\delta x}\right|_w\right.$$

$$\Rightarrow \frac{1}{\delta x^2}\left(P_E^n - 2P_P^n + P_W^n\right) + \frac{1}{\delta y^2}\left(P_N^n - 2P_P^n + P_S^n\right) = Q_P^H$$

$$= \frac{1}{\delta x}\left(H_{x,e}^n - H_{x,w}^n\right) + \frac{1}{\delta y}\left(H_{y,n}^n - H_{y,s}^n\right)$$

by interpolation

this approx. eliminates the oscillation in P



But no energy conservation.

why? $\longrightarrow$ mtm: $-\frac{\partial p}{\partial x_i}$ $\rightarrow$ $\frac{\partial p}{\delta x} = \frac{1}{\delta x}(P_e - P_w)$

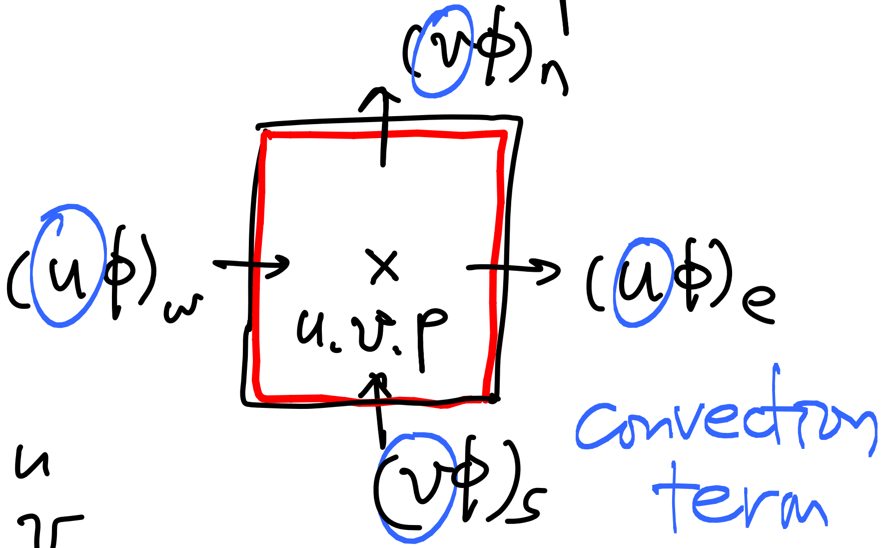
P_e, P_w: ? ? undefined

$$\frac{\partial p}{\delta x} = \frac{1}{2\delta x}(P_E - P_W)$$

inconsistent.

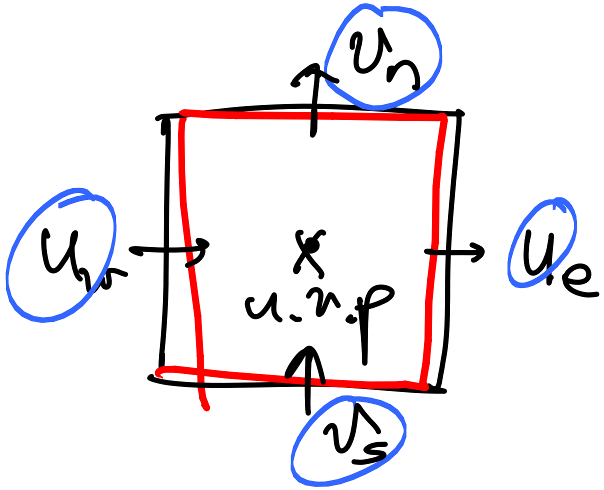
$\Rightarrow$ momentum interpolation method.

- Momentum interpolation method - collocated grid



ϕ: u, v

mtm eq.



cont. eq

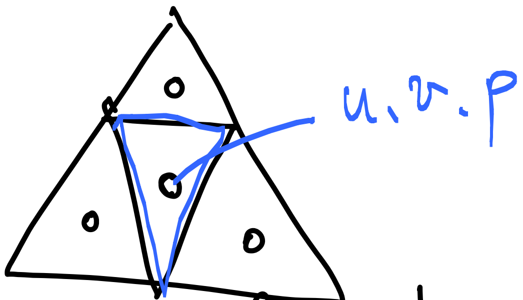
So, in mtm eq., it is important to use u & v at cell faces that satisfy the continuity.

Rhie & Chow (AIAA J. <u>21</u>, 1525 (1983)) for steady flow

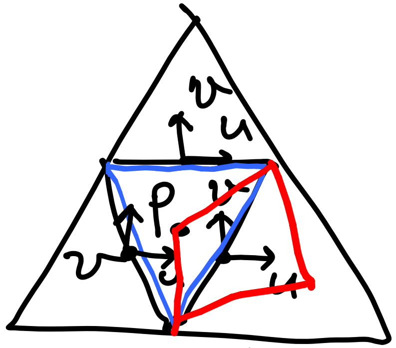
Zang et al. (JCP, <u>114</u>, 18 (1994)) for unsteady flow on structured grids

Kim & Choi (JCP, <u>162</u>, 411 (2000)) for unsteady flow on <u>un</u>structured grids

- Kim & Choi's MIM.

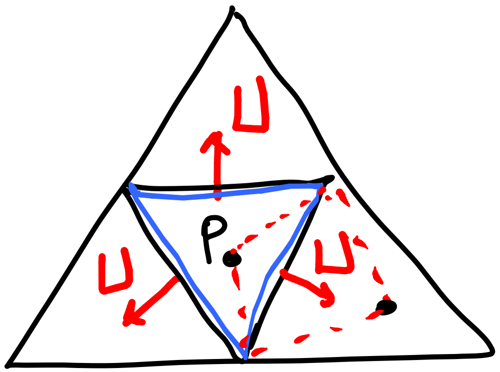


traditional unstructured



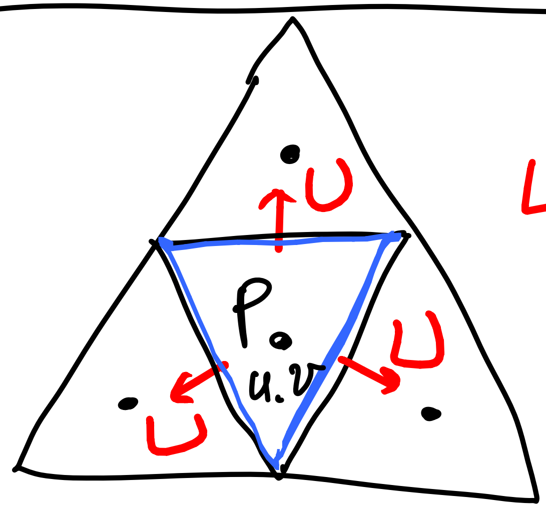
staggered mesh

mesh



staggered mesh
with face-normal
velocity component

with Cartesian
velocity comps.



$U = (u_i)_{face} n_i$

Collocated mesh
w/ face-normal vel. comp.

$U = (u_i)_{face}\, n_i$ $\quad (u_i)_{face}$: Cartesian velocity

n_i : outward-normal unit vector on the cell face

N-S eq
C-N

$$\longrightarrow \frac{u_i^{n+1} - u_i^n}{\delta t} + \boxed{\frac{1}{2}\frac{\partial}{\partial x_j}\left(\underline{u_i^{n+1} u_j^{n+1}} + u_i^n u_j^n\right)} = -\frac{\partial p^{n+1}}{\partial x_i} + \frac{1}{2}\frac{1}{Re}\nabla^2\left(u_i^{n+1} + u_i^n\right)$$

nonlinear eq.

$\hookrightarrow$ linearization

$u_i^{n+1} u_j^n + u_i^n u_j^{n+1} - u_i^n u_j^n + O(\delta t^2)$

Beam & Warming

(AIAA J. 16, 393 (1978))

$$\parallel$$

$$\frac{1}{2}\frac{\partial}{\partial x_j}\left(u_i^{n+1} u_j^n + u_i^n u_j^{n+1}\right)$$

$$\text{L} \quad \frac{\partial u_i^{n+1}}{\partial x_i} = 0$$

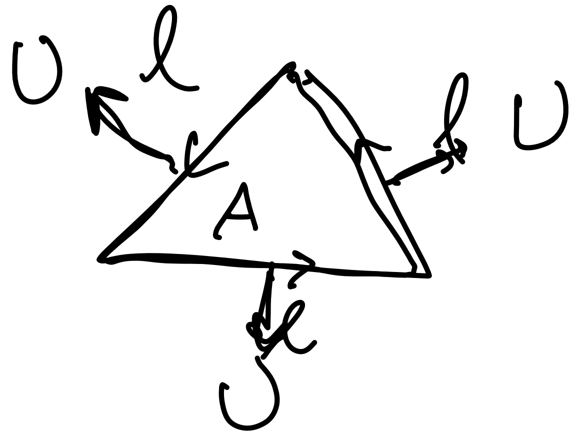
FSM (Choi & Moin):

$$\frac{\hat{u}_i - u_i^n}{\Delta t} + \frac{1}{2}\frac{\partial}{\partial x_j}\left(\hat{u}_i u_j^n + u_i^n \hat{u}_j\right) = -\frac{\partial p^n}{\partial x_i} + \frac{1}{2Re}\nabla^2\left(\hat{u}_i + u_i^n\right)$$

$$\frac{u_i^* - \hat{u}_i}{\Delta t} = \frac{\partial p^n}{\partial x_i}$$

$$\frac{\partial}{\partial x_i}\frac{\partial p^{n+1}}{\partial x_i} = \frac{1}{\Delta t}\frac{\partial u_i^*}{\partial x_i}$$

$$\frac{u_i^{n+1} - u_i^*}{\Delta t} = -\frac{\partial p^{n+1}}{\partial x_i}$$

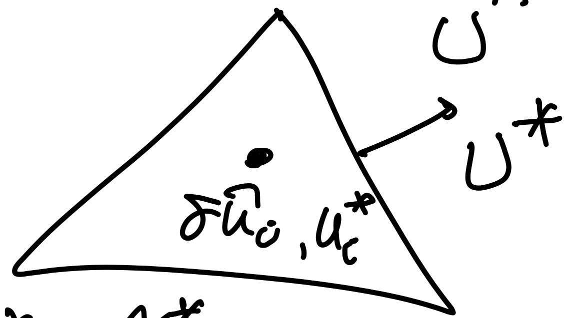


Integrate these eqs over each cell area A and apply the divergence theorem:

$$\delta \hat{u}_i = \hat{u}_i - u_i^n$$

$$\frac{\delta \hat{u}_i}{\Delta t} + \frac{1}{A}\oint_l \frac{1}{2}\left(U^n \delta\hat{u}_i + u_i^n n_j \delta\hat{u}_j + 2u_i^n U^n\right) dl$$

$$= -\frac{1}{A}\int_A \frac{\partial p^n}{\partial x_i}\, dA + \frac{1}{A}\oint \frac{1}{2Re}\frac{\partial}{\partial n}\left(\delta\hat{u}_i + 2u_i^n\right) dl$$



$$u_i^* - \hat{u}_i = \Delta t \frac{\partial p^n}{\partial x_i}$$

$$\frac{1}{A}\oint \frac{\partial p^{n+1}}{\partial n} dl = \frac{1}{A\Delta t}\oint U^* dl \rightarrow \text{get } p^n$$

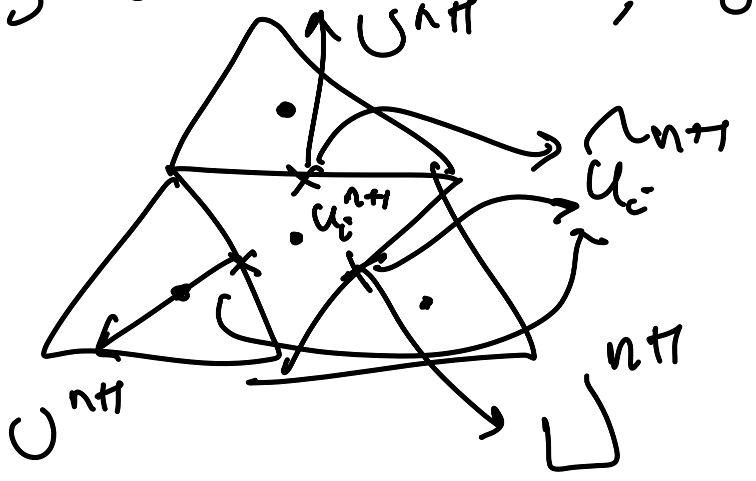
$$u_i^{n+1} - u_i^* = -\Delta t \frac{\partial p^{n+1}}{\partial x_i} \rightarrow \text{obtain } u_i^{n+1}$$

$$U^{n+1} - U^* = -\Delta t \frac{\partial p^{n+1}}{\partial n}$$

$$U^* = \tilde{u}_i^* n_i$$

interpolated from neighboring cell.

$\rightarrow \oint \tilde{u}_i^{n+1} n_i \, dl \neq 0$, $\oint U^{n+1} dl = 0$



the divergence-free velocity U^{n+1} is used for the calculation of the convective fluxes.

$\rightarrow$ eliminate press. oscillations due to strong coupling bet. U and p.

⊙ Note on pressure and incompressibility

To prove that the press. is a mathematical quantity for the continuity.

$\exists\ \underline{v}^*$ s.t. $\nabla\cdot\underline{v}^* \neq 0$.

Want to create $\underline{v}$ s.t. $\nabla\cdot\underline{v} = 0$ & $\underline{v} \simeq \underline{v}^*$.

Set $\tilde{R} = \frac{1}{2}\int_\Omega [\underline{v}(\underline{r}) - \underline{v}^*(\underline{r})]^2 d\Omega$

$\nabla\cdot\underline{v} = 0$

Find $\underline{v}$ minimizing $\tilde{R}$.

$\longrightarrow$ Calculus of variation

$$R = \frac{1}{2}\int_\Omega [\underline{v}(\underline{r}) - \underline{v}^*(\underline{r})]^2 d\Omega - \int_\Omega \lambda(\underline{r})\, \nabla\cdot\underline{v}(\underline{r})\, d\Omega$$

Suppose $\exists\ \underline{v}^{+}$ s.t. $R_{min} = \frac{1}{2}\int_{\Omega}[\underline{v}^{+}(\underline{r}) - \underline{v}^{*}(\underline{r})]^2 d\Omega$ ↳ Lagrange multiplier

& $\underline{\nabla}\cdot\underline{v}^{+} = 0$

Let $\underline{v} = \underline{v}^{+} + \delta\underline{v}$

$$\delta R = R - R_{min} = \int_{\Omega}\delta\underline{v}(\underline{r})\cdot[\underline{v}^{+}(\underline{r}) - \underline{v}^{*}(\underline{r})]d\Omega - \int_{\Omega}\lambda(r)\nabla\cdot\delta\underline{v}(\underline{r})\, d\Omega$$

$$= \int_{\Omega}\delta\underline{v}(\underline{r})\cdot[\underline{v}^{+}(\underline{r}) - \underline{v}^{*}(\underline{r}) + \nabla\lambda(\underline{r})]\, d\Omega$$

$$+ \underbrace{\int_{S}\lambda(\underline{r})\,\delta\underline{v}(\underline{r})\cdot\underline{n}\, dS}$$

↳ make it zero by a natural way or by changing λ.

For arbitrary $\delta \underline{v}$, we need $\delta R = 0$

$$\rightarrow \quad \underline{v}^{+}(\underline{r}) - \underline{v}^{*}(\underline{r}) + \nabla\lambda(\underline{r}) = 0$$

$$\nabla\cdot(\,) \longrightarrow \quad \nabla^2\lambda(\underline{r}) = \nabla\cdot\underline{v}^{*}(\underline{r})$$

$\therefore$ Lagrange multiplier plays the role of p and thus the ft. of p is to allow the continuity to be satisfied.

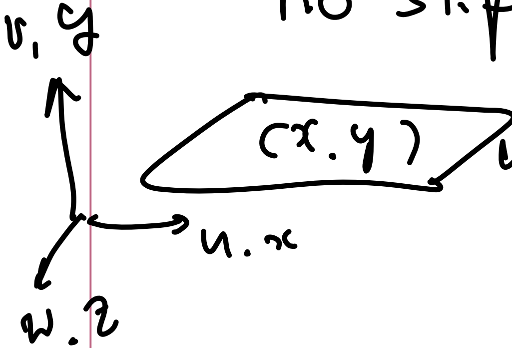
Term project: → Kim^2 & Choi, JCP (2001), this ○, —.

IB method & code explanation: Friday 1pm – 6pm
#301 – 302

7. Boundary condition for N-S eqs.

① wall (x.y.z)

no slip : $u = v = w = 0$ → $v = 0$



wall → $\left.\dfrac{\partial u}{\partial x}\right|_w = 0 \quad \left.\dfrac{\partial w}{\partial z}\right|_w = 0 \Rightarrow$ cont $\boxed{\dfrac{\partial v}{\partial y} = 0}$

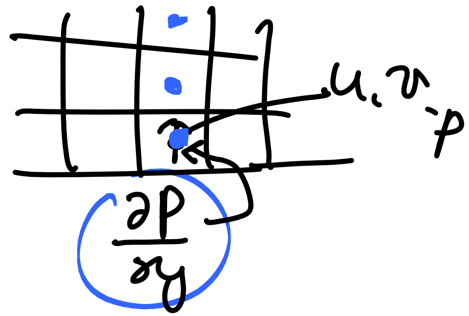
two b.c's

→ One cannot satisfy both b.c's simultaneously

no press. b.c. for staggered mesh

but " " for collacated "

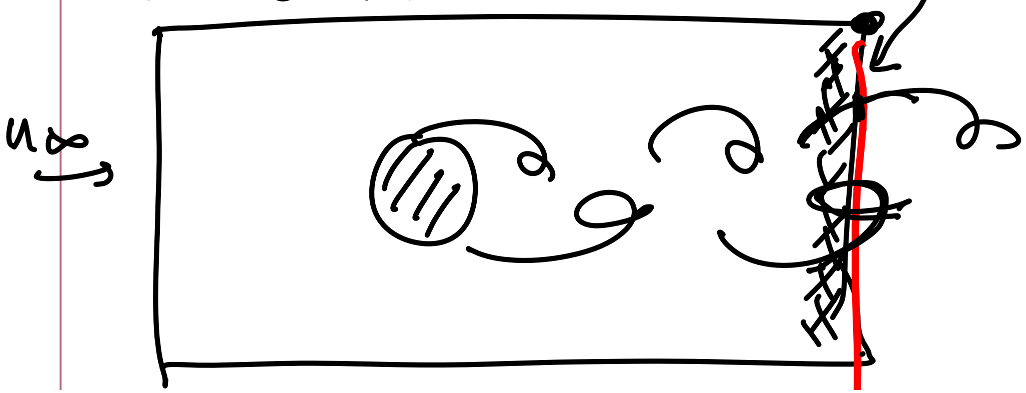
↳ linear extrapolation



② symmetry

$v = 0, \quad \frac{\partial u}{\partial y} = 0$

③ exit



$\frac{\partial u_i}{\partial x} = 0$ Neumann b. c.

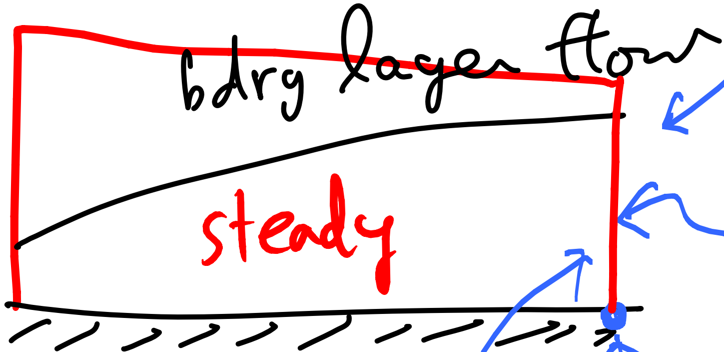
$\rightarrow \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = 0$] two b.c.'s for v

cont. ↳ $\frac{\partial v}{\partial y} = 0$

unsteady flow $\rightarrow$ $\dfrac{\partial u_i}{\partial t} + c\,\dfrac{\partial u_i}{\partial x} = 0$ convective outflow b.c.

c $\rightarrow$ local vel $u(y,t)$

mean vel $\bar{u}^y(t)$ $\Leftarrow$



$\dfrac{\partial u_i}{\partial x} = 0 \rightarrow \dfrac{\partial u}{\partial x} = \dfrac{\partial v}{\partial x} = 0$

$\downarrow$

$\dfrac{\partial v}{\partial y} = 0$

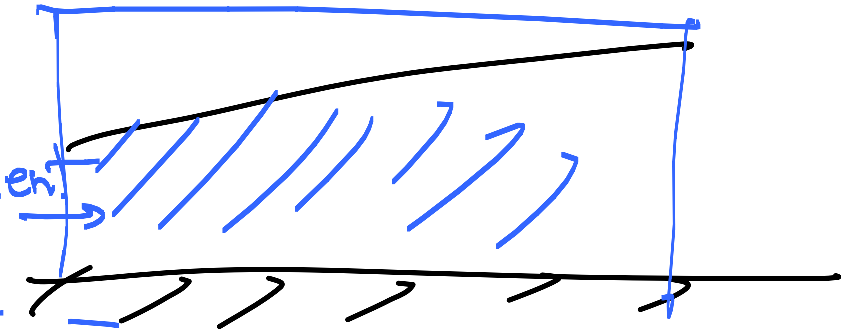
$v = 0$

$\rightarrow v \equiv 0$ at exit

$\dfrac{\partial^2 u}{\partial x^2} = \dfrac{\partial^2 v}{\partial x^2} = 0$

④ inlet → too clear $u = u_\infty,\ v = 0$

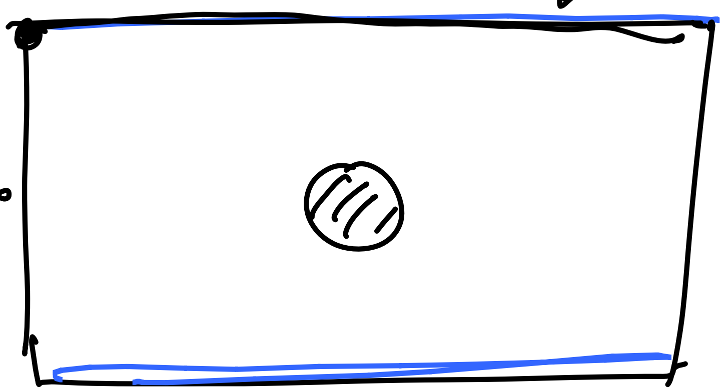
turb. flow



you know $\bar{u}, \bar{v}, \bar{w}$

don't " $u', v', w'(y, z, t)$ ← Lund et al., JCP, (1998)

⑤ far-field ?



- $u = u_\infty,\ v = 0$ → $\frac{\partial u}{\partial x} = 0$ → $\frac{\partial u}{\partial y} = 0$
- $u = u_\infty,\ \frac{\partial u}{\partial y} = 0$
- $\frac{\partial u}{\partial y} = 0,\ \frac{\partial v}{\partial y} = 0$ → $\frac{\partial u}{\partial x} = 0$

$u = u_\infty|_{\text{inlet}}$

$u = u_\infty|_{\text{far-field}}$

- $\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 0$, $u = u_\infty$

$\frac{\partial u}{\partial y} = 0$

- Another formulation of N-S eqs.
  representation

Kim, Moin & Moser (1987) JFM

$$\begin{cases} \frac{\partial u_i}{\partial t} = -\frac{\partial p}{\partial x_i} + H_i + \frac{1}{Re}\nabla^2 u_i, \quad H_i = -u_j \frac{\partial u_i}{\partial x_j} \\ \frac{\partial u_i}{\partial x_i} = 0 \end{cases}$$

vector identity $\nabla^2 \underline{q} = \nabla(\nabla \cdot \underline{q}) - \nabla \times (\nabla \times \underline{q})$

$$(\underline{q} \cdot \nabla)\underline{q} = \frac{1}{2}\nabla(\underline{q} \cdot \underline{q}) - \underline{q} \times (\nabla \times \underline{q})$$

$$\Rightarrow \quad \underline{H}_i = -(\underline{u}\cdot\nabla)\underline{u} = -\frac{1}{2}\nabla(\underline{u}\cdot\underline{u}) + \underline{u}\times(\nabla\times\underline{u})$$

$$= -\nabla\left(\frac{1}{2}\underline{u}\cdot\underline{u}\right) + \underline{u}\times\underline{\omega}$$

Then, $$\frac{\partial \underline{u}}{\partial t} = \underbrace{\underline{u}\times\underline{\omega} - \nabla\left(\frac{1}{2}\underline{u}\cdot\underline{u}\right)}_{\underline{H}} - \nabla p + \frac{1}{Re}\nabla^2\underline{u}$$

$$\frac{\partial}{\partial t}(\nabla^2\underline{u}) = \nabla^2\underline{H} - \nabla^2(\nabla p) + \frac{1}{Re}\nabla^4\underline{u}$$

$$= \nabla(\nabla\cdot\underline{H}) - \nabla\times(\nabla\times\underline{H}) - \nabla^2(\nabla p) + \frac{1}{Re}\nabla^4\underline{u}$$

$$= -\nabla\times(\nabla\times\underline{H}) + \frac{1}{Re}\nabla^4\underline{u} + \nabla(\nabla\cdot\underline{H} - \nabla^2 p)$$

$$\nabla\cdot(NS) \longrightarrow \frac{\partial}{\partial t}\cancel{(\nabla\cdot\underline{u})}^{0} = -\nabla^2 p + \nabla\cdot\underline{H} + \frac{1}{Re}\nabla^2\cancel{(\nabla\cdot\underline{u})}^{0}$$

$$\rightarrow \frac{\partial}{\partial t}(\nabla^2 \underline{u}) = \underbrace{-\nabla\times(\nabla\times\underline{H})}_{\equiv h_{\underline{u}}} + \frac{1}{Re}\nabla^4 \underline{u}$$

eliminate p
but w/ higher derivatives

v component:

$$\boxed{\frac{\partial}{\partial t}(\nabla^2 v) = h_v + \frac{1}{Re}\nabla^4 v} \quad (1)$$

4th-order PDE
→ needs high accurate numerical method
spectral method

$\nabla^2\phi \rightarrow -k^2\phi$

$\nabla^4\phi \rightarrow k^4\phi$

where $h_v = -\frac{\partial}{\partial y}\left(\frac{\partial H_1}{\partial x} + \frac{\partial H_3}{\partial z}\right) + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)H_2$

Also, $\frac{\partial}{\partial z}\left(\frac{\partial u}{\partial t}\right) - \frac{\partial}{\partial x}\left(\frac{\partial w}{\partial t}\right)$:

$$\boxed{\frac{\partial}{\partial t}g = h_g + \frac{1}{Re}\nabla^2 g} \quad (2)$$

$$\boxed{g = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}} = \omega_y \quad (3)$$

$$h_g = \frac{\partial H_1}{\partial z} - \frac{\partial H_3}{\partial x}$$

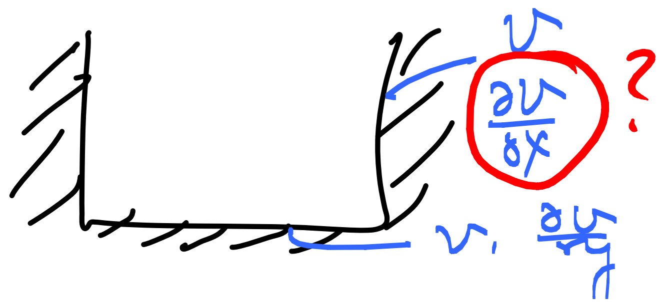
Also, $f \equiv \frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \rightarrow \boxed{f + \frac{\partial v}{\partial y} = 0}$ — (4)

i) solve Eq. (1) to get v → b.c's : $v\big|_w = \frac{\partial v}{\partial y}\Big|_w = 0$

ii) solve Eq. (2) to get g. → " : $g\big|_w = 0$

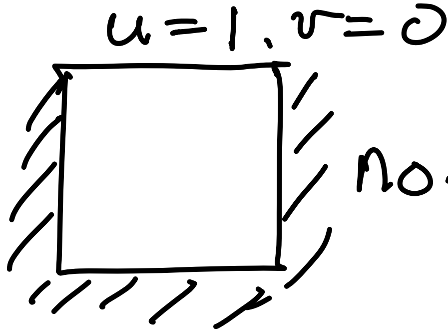
iii) solve Eq. (3) & (4) to get u & w.

→ this formulation has limit in that b.c's are not well defined in most geometries except channel flow



8. Examples

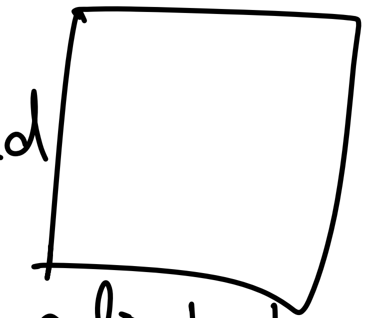
① Lid-driven cavity flow



Ghia, Ghia & Shim (1982)

JCP, 48, 387.

② Buoyancy-driven cavity flow



Hortmann, Perić & Scheuerer (1990)

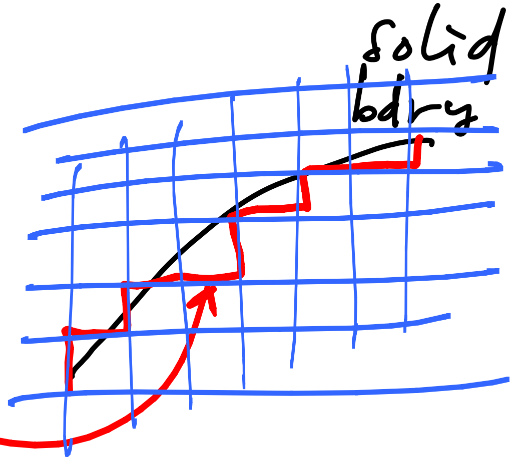
Int. J. Num. Methods Fluids 11, 189.

Ch. 8 Complex geometries

노트 제목 2012-05-14

1. Choice of grid

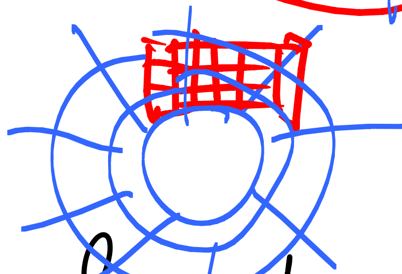
① stepwise approx. using regular grids



provide b.c's here

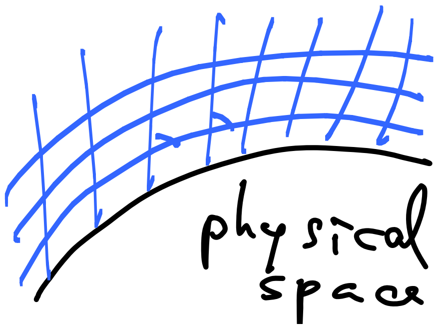
② overlapping grids

ex) chimera grids



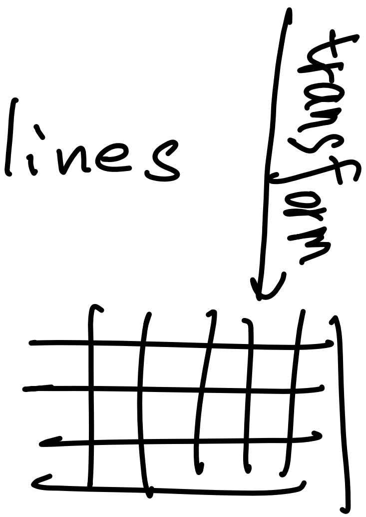
③ boundary-fitted non-orthogonal grids

advantage : can be adapted to any geometry



good for b.c.

grid lines can follow the streamlines



disadvantage:

transformed eqs contain more terms

difficulty of programming

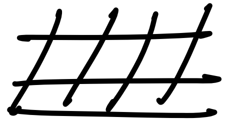
increases cost of solving eqs.

2. Grid generation - very important issue

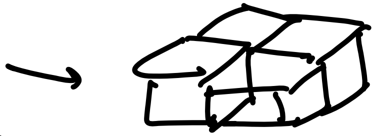
Thompson et al. (1985)

① make grids as nearly orthogonal as possible

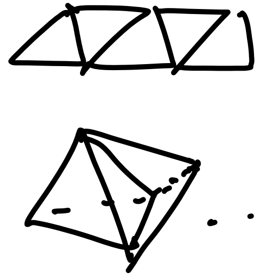
② cell topology



in general, quadrilaterals in 2D are better
hexahedra in 3D



than triangles in 2D
tetrahedra in 3D



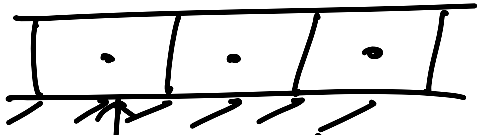
...

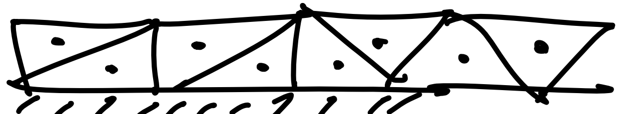
if

i) midpoint rule integral approx.
linear interpolation
central difference

are used

ii) very near the wall

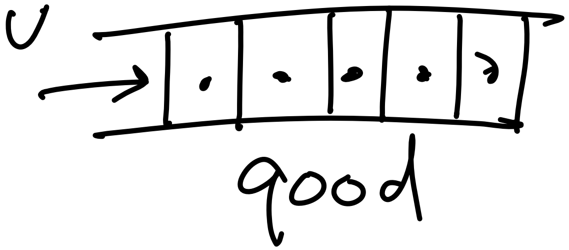


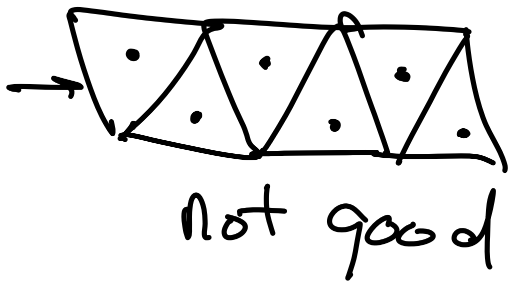


each cell has a same role.

iii) for convection terms

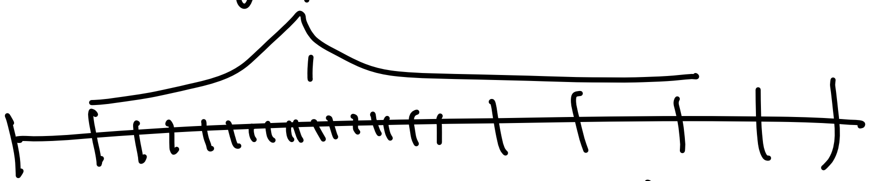
(accuracy is improved if grid lines follow the stream lines)





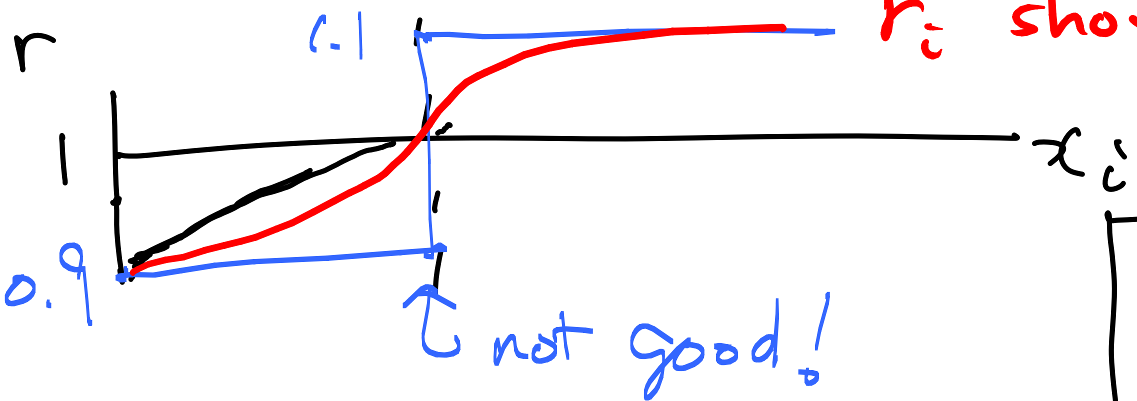
③ non-uniform grids

more grids near the region of rapid variation

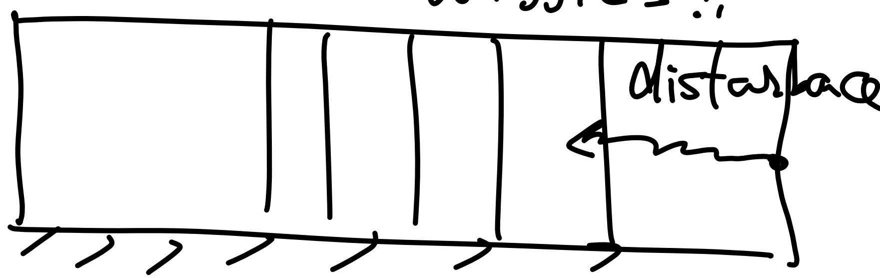


$r_i = \dfrac{\Delta x_{i+1}}{\Delta x_i}$ ratio

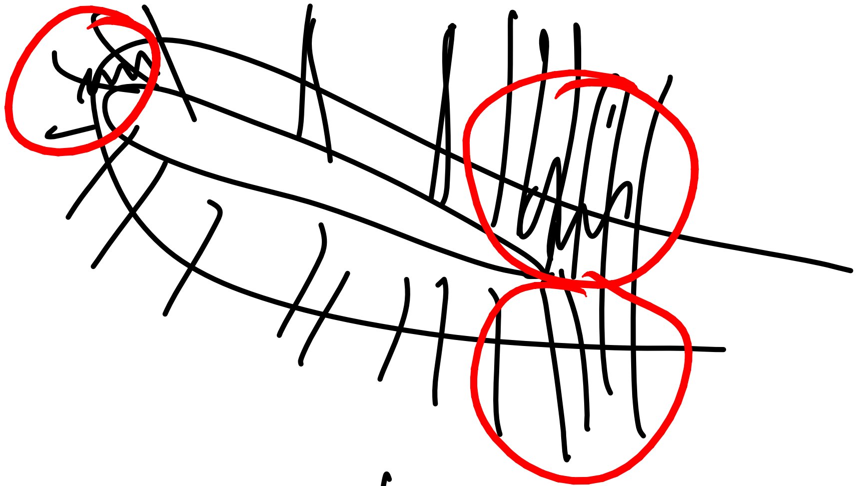
r_i should be kept under control



wiggles!!



Hahn & Choi (JCP, 199? ?)

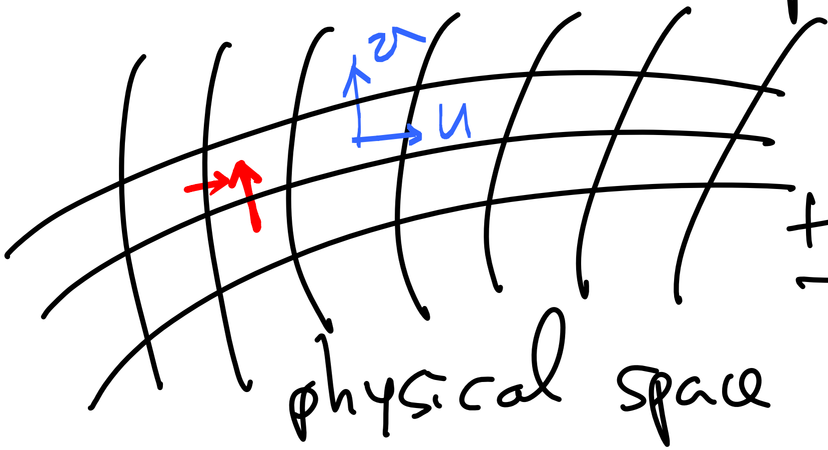


3. Choice of velocity components

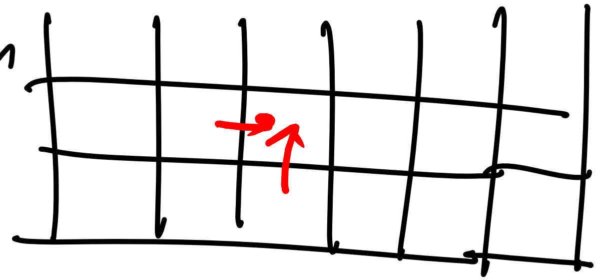
① Grid-oriented vel. components

satisfy the continuity very well.

contravariant vel!



transform



very complicated. Choi, Moin & Kim (1993, JFM)

(1D cartesian
2D generalized coord.

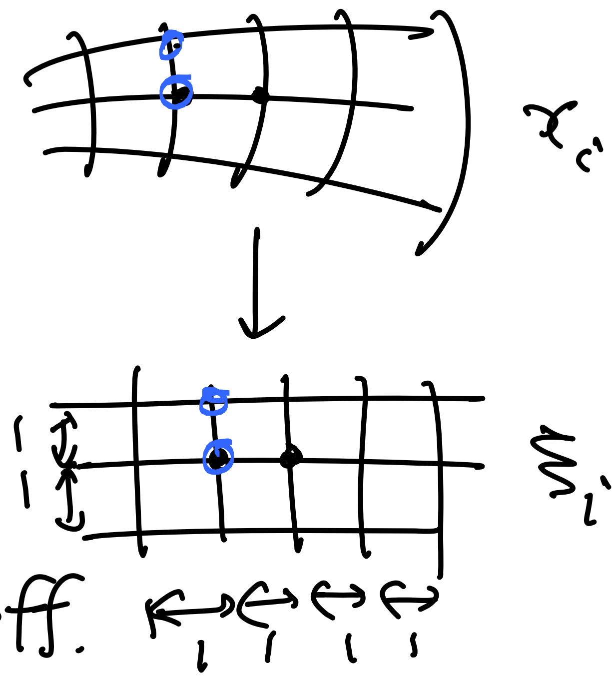
② Cartesian vel comps.

(unstructured
generalized body-fitted.

4. choice of variable arrangement

① staggered ② Collocated

5. FDM → coordinate transformation

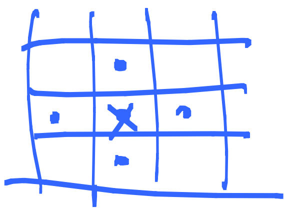


$$x_i \longrightarrow \xi_i$$

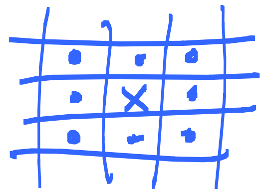
$$\frac{\partial \phi}{\partial x_i} = \frac{\partial \phi}{\partial \xi_j} \underbrace{\frac{\partial \xi_j}{\partial x_i}}_{\text{called metric coeff.}}$$

$$J = \det\left(\frac{\partial x_i}{\partial \xi_j}\right) \quad \text{Jacobian}$$

- Transformation usually provides cross derivative terms



$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \longrightarrow \frac{\partial^2 \phi}{\partial \xi^2}, \quad \frac{\partial^2 \phi}{\partial \eta^2}, \quad \frac{\partial^2 \phi}{\partial \xi \partial \eta}$$



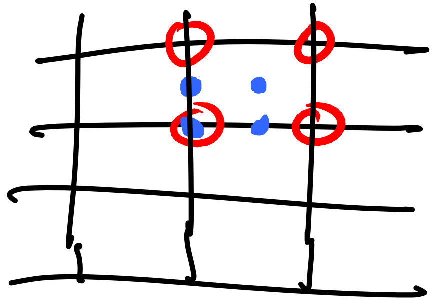
ADI? No!

$= 0$ for orthogonal grids

$\neq 0$ for non-orthogonal grids

- need to store metric coeffs.
- easy to discretize in the transformed space.
- no interpolation of metric coeffs.

  → Interpolation breaks conservation.
  (see Thompson et al. 1985)



- skewness (non-orthogonal grid) and large aspect ratio give poor convergence or oscillations in the solution

skewed grid

large aspect ratio

6. FVM

$$\frac{\partial}{\partial t}\int_\Omega \rho\phi\, d\Omega + \int_S \rho\phi\, \underline{v}\cdot\underline{n}\, dS = \int_S \Gamma\, \nabla\phi \cdot \underline{n}\, dS + \int_\Omega q_\phi\, d\Omega$$

- no need to transform
- need to get ϕ or $\nabla\phi$ at cell surface
  by interpolation or some other methods.

7. FEM — natural method for complex geometries

8. Pressure-correction eq. — covered already

9. Axi-symmetric problems $-(r, \theta, z)$

centrifugal force $\quad -\underline{\Omega} \times \underline{\Omega} \times \underline{x}$

Coriolis force $\quad -2\underline{\Omega} \times \underline{u}_r$

appear in the mtm eq.

$\boxed{\text{N-S eqs}} \quad \boxed{-\underline{\Omega}\times\underline{\Omega}\times\underline{x} - 2\underline{\Omega}\times\underline{u}_r}$

non-conservative form

$\downarrow$

transform to fully conservative form

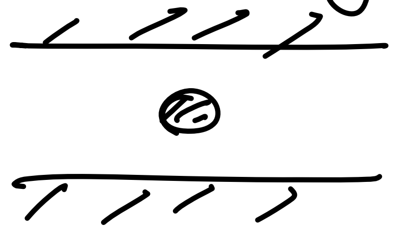
Kim & Choi (JCP, ___) $\leftarrow$

D. Kim $\quad$ see the reference therein.

10. Implementation of boundary conditions

11. Examples

flow around a circular cylinder in a channel.



Ch. 9. Turbulent Flows

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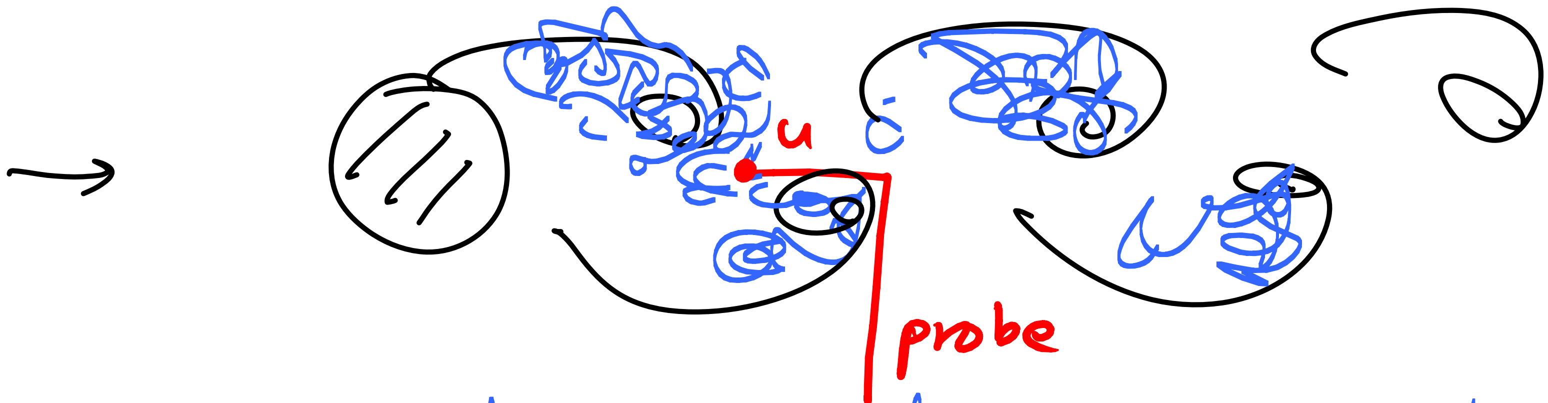
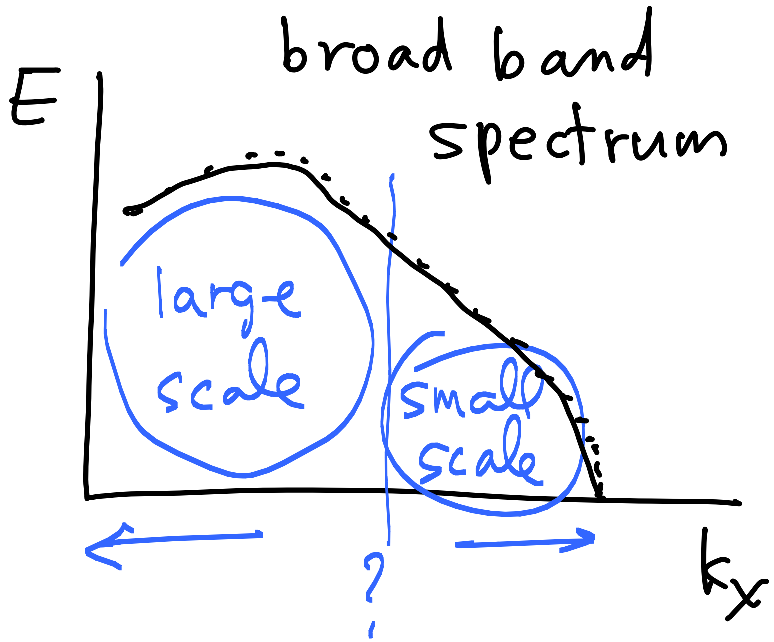
↳ are unsteady 3-D.

contain a variety of spatial and temporal scales from large to small motions.



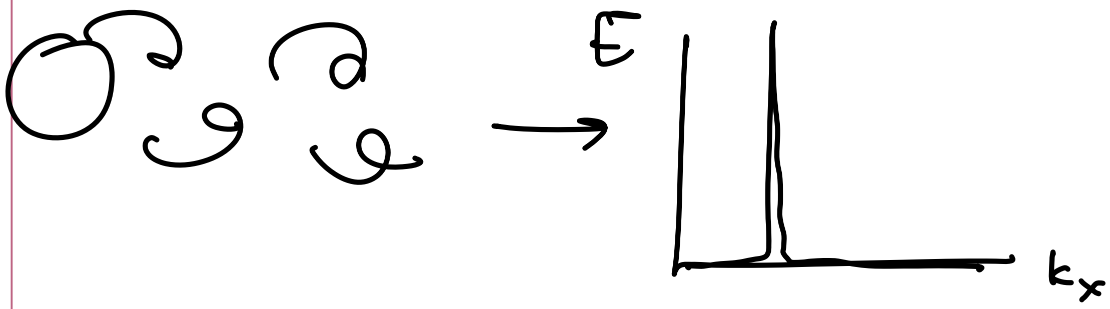
⇒ makes the prediction of turbulent flow very difficult.



$$\begin{tikzcd}
u(t) \arrow[r] \arrow[d, "FT"'] & u(x) \arrow[r, "FT"] & \hat{u}(k_x) \arrow[d] \\
\hat{u}(\omega) \arrow[d] & & E(k_x) = \hat{u}\,\hat{u}^* \\
E(\omega) = \hat{u}\,\hat{u}^* & &
\end{tikzcd}$$

Taylor hypothesis

$$\frac{\partial}{\partial t} \rightarrow c\,\frac{\partial}{\partial x}$$



- Prediction methods for turbulent flow

① RANS (Reynolds averaged Navier-Stokes eq.) technique

② LES (Large Eddy Simulation)

③ DNS (Direct Numerical Simulation)

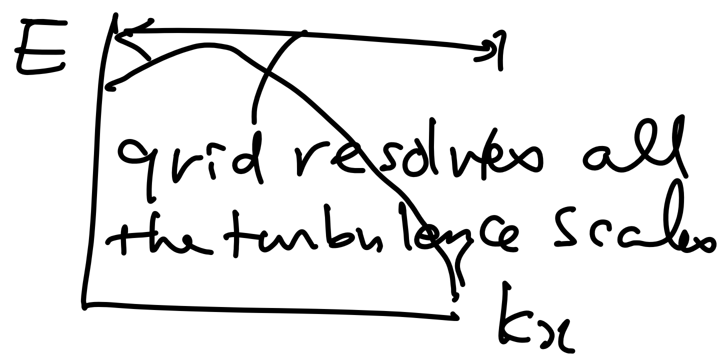
④ Wall-modeled LES or Hybrid LES/RANS

time

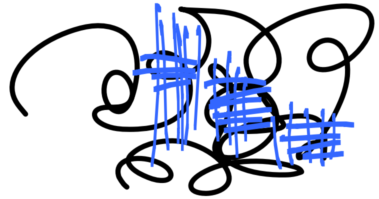
Ⓐ Direct numerical simulation — no model for turbulence

$$\begin{cases} \dfrac{\partial u_i}{\partial x_i} = 0 \\[2ex] \dfrac{\partial u_i}{\partial t} + \dfrac{\partial u_i u_j}{\partial x_j} = -\dfrac{1}{\rho}\dfrac{\partial p}{\partial x_i} + \nu \dfrac{\partial^2 u_i}{\partial x_j \partial x_j} \end{cases}$$

unsteady and 3D.



- grid resolves all the turbulent scales → no model
- highly accurate
- Since 1980's



- Number of grid points requirement

  smallest scale in turbulence — Kolmogorov length scale

  DNS should resolve the Kolmogorov scale.

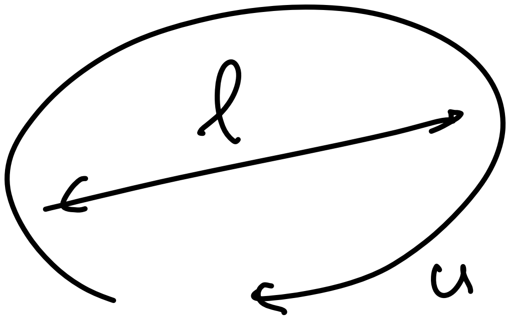
$$\underset{\text{grid resolution}}{\Delta} \sim \eta = \left(\nu^3/\varepsilon\right)^{\frac{1}{4}}$$

ν : kinematic viscosity

ε : dissipation rate

$\Delta \sim O(1)\,\eta \sim (1\sim 10)\,\eta$

in real simulation



N

(number of grid pts in 1-direction)

ℓ: largest turbulent length scale

u: " " velocity scale

$$N = \frac{\ell}{\Delta} \div \frac{\ell}{\eta} = \ell\left(\frac{\varepsilon}{\nu^3}\right)^{\frac{1}{4}} \sim \ell\left(\frac{P}{\nu^3}\right)^{\frac{1}{4}}$$

$$\left(P \sim -\overline{u_i u_j}\,\frac{\partial \overline{U_i}}{\partial x_j} \sim u^3/\ell\right)$$

$$\left(Re_\ell = \frac{u\ell}{\nu}\right)$$

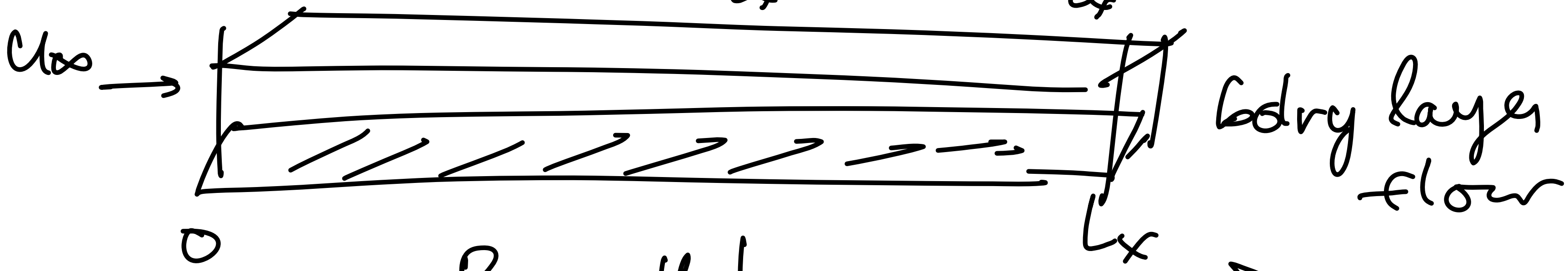
$$Re_\ell^{\frac{3}{4}} = \left(\frac{u^3\ell^3}{\nu^3}\right)^{\frac{1}{4}} = \ell\left(\frac{u^3/\ell}{\nu^3}\right)^{\frac{1}{4}}$$

total # of grid pts in 3D $\boxed{N^3 = Re_\ell^{\frac{9}{4}}}$ $\Longrightarrow$ computationally expensive but very useful for academic purpose.

rarely used for eng. applications.

Choi & Moin (2012, PoF)

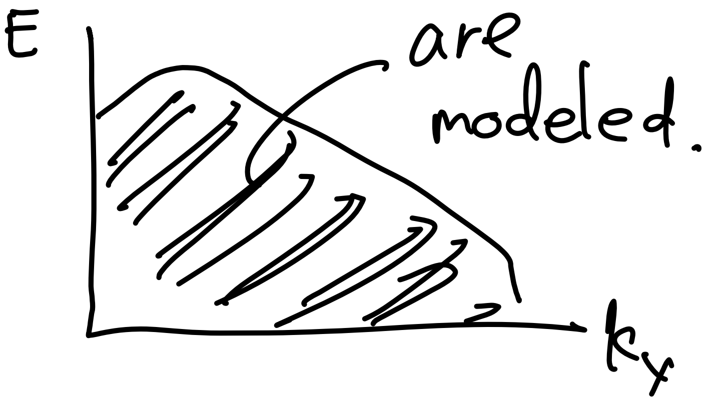
$$N^3 \sim Re_{Lx}^{\frac{37}{14}} \sim Re_{\delta_{Lx}}^{\frac{37}{12}} \sim Re_{\tau_{Lx}}^{\frac{37}{11}}$$



$$Re_{Lx} = \frac{u_\infty L_x}{\nu}, \quad Re_{\delta_{Lx}} = \frac{u_\infty \delta_{Lx}}{\nu}$$

$$Re_{\tau_{Lx}} = \frac{u_{\tau_{Lx}} L_x}{\nu}$$

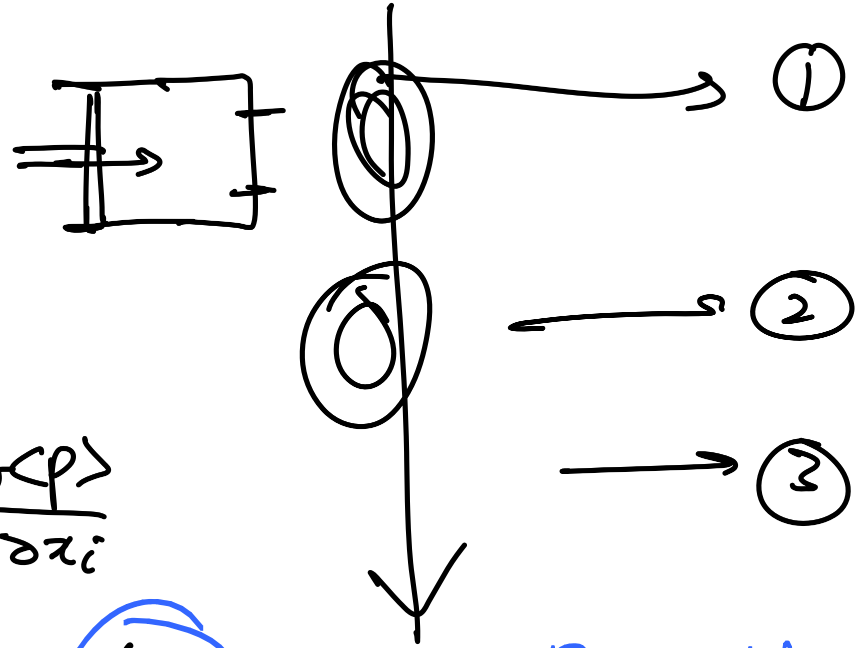
Ⓑ RANS



ensemble averaging

$$u_i = \langle u_i \rangle + u_i' \qquad \text{Reynolds decomposition}$$

$$\left(= \overline{u_i} + u_i'\right)$$



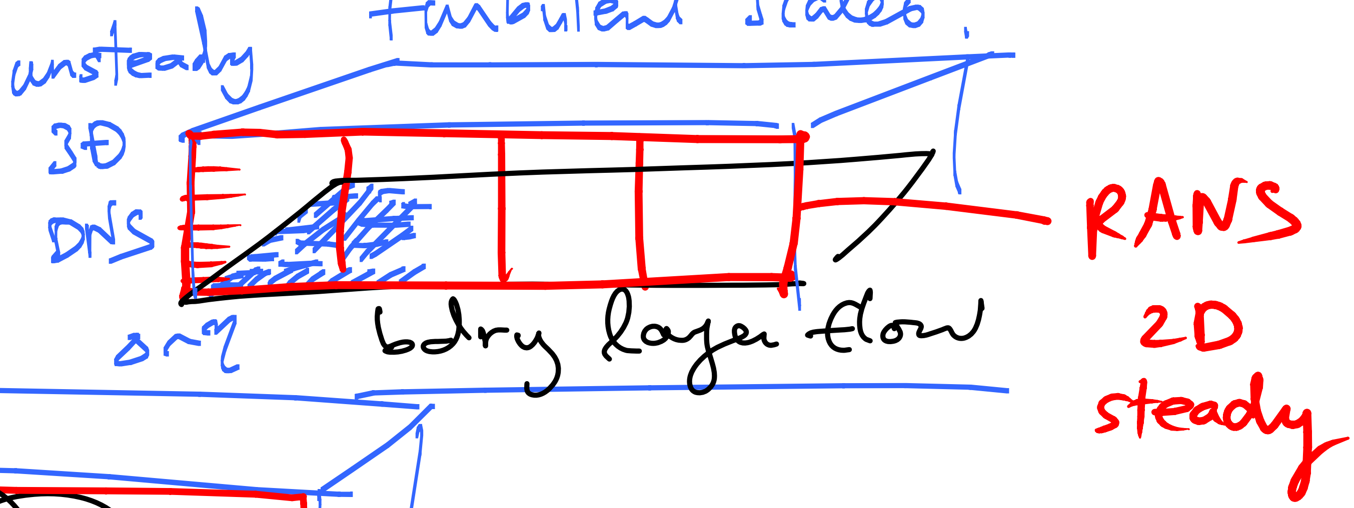
$$\begin{cases} \dfrac{\partial \langle u_i \rangle}{\partial x_i} = 0 \\[2ex] \dfrac{\partial \langle u_i \rangle}{\partial t} + \dfrac{\partial \langle u_i \rangle \langle u_j \rangle}{\partial x_j} = -\dfrac{1}{\rho} \dfrac{\partial \langle p \rangle}{\partial x_i} \end{cases}$$

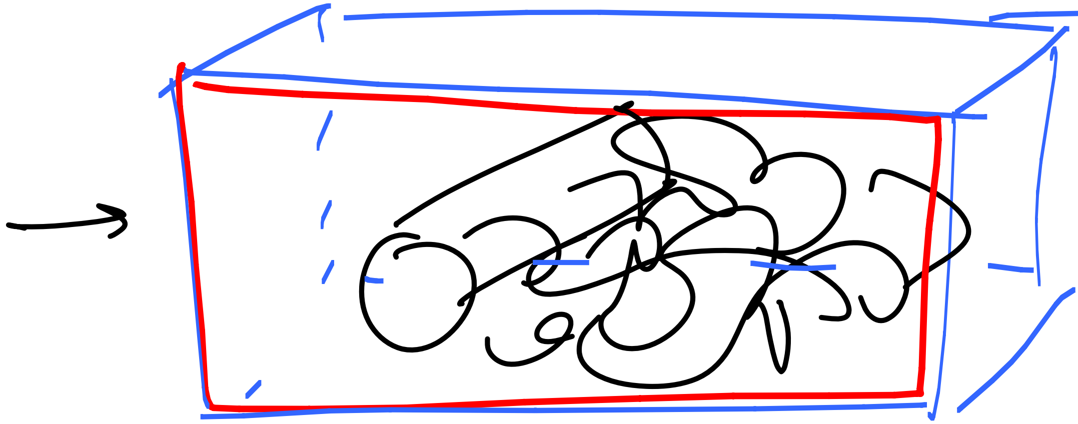
$$+ \nu \frac{\partial^2 \langle u_i \rangle}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} \langle u_i' u_j' \rangle$$

Reynolds stress

is obtained by modeling whole turbulent scales.

- low cost!





- inaccurate for the prediction of massively separated flow or flow w/ high curvature.

- How to model the Reynolds stress term $\langle u_i' u_j' \rangle$?

Boussinesq eddy viscosity hypothesis

in laminar flow, $\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = 2\nu S_{ij}$ ff. of fluid

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\rightarrow \quad -\langle u_i' u_j' \rangle + \frac{2}{3} k \delta_{ij} = 2\nu_T \langle S_{ij} \rangle$$

eddy viscosity

ff. of flow

$$k = \frac{1}{2}\langle u_i u_i \rangle$$

$$\frac{\partial}{\partial x_j}\left(\tau_{ij} - \rho\langle u_i' u_j' \rangle\right)$$

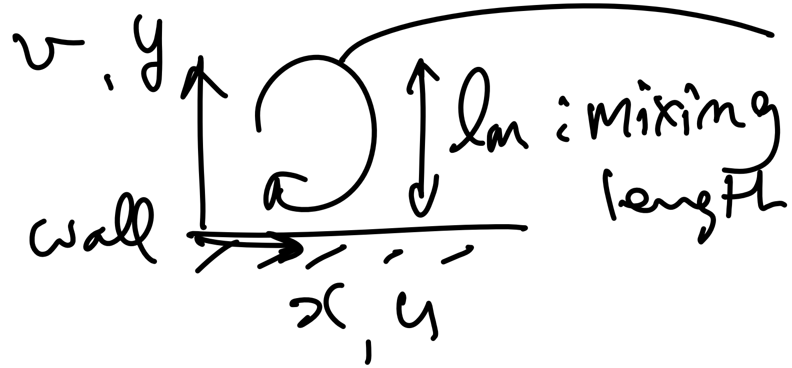
• Eddy viscosity ν_T (m^2/s) [L^2T^{-1}]

$\nu_T \sim l$ (length scale) $\times$ u (velocity scale)

what are the most relevant length and vel. scales?

① zero-equation model : no transport eq.

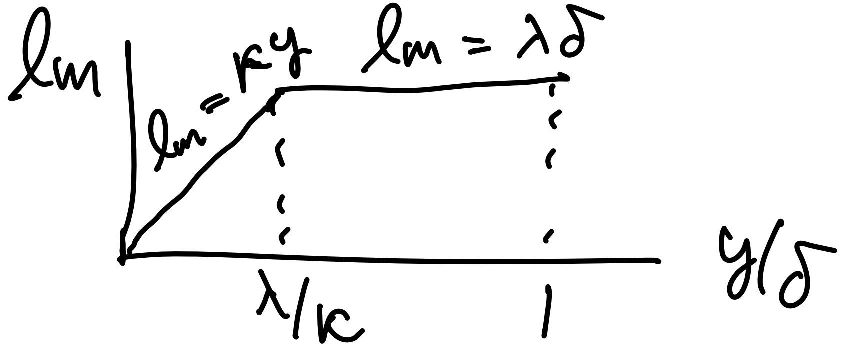
mixing length model (Prandtl, 1925)



$$u = l_m \frac{\partial \langle u \rangle}{\partial y}$$

$$\nu_T = l u = l_m^2 \left| \frac{\partial \langle u \rangle}{\partial y} \right| > 0$$

bdry layer flow



$\kappa = 0.435$

$\lambda = 0.09$

② One-equation model : one transport eq.

ex) k-eq : modeling of the velocity scale only

$$u \sim \sqrt{k} \quad , \quad \nu_T = C_\mu' \sqrt{k}\, l$$

$$\frac{\partial k}{\partial t} + \langle u_j \rangle \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\nu_T}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + \nu_t \left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i}\right)\frac{\partial \langle u_i \rangle}{\partial x_j} - C_D \frac{k^{\frac{3}{2}}}{l}$$

$l = l_m \longrightarrow$ limitation !

ex) Spalart-Allmaras model

$$\nu_T = \tilde{\nu} f_{v_1}$$

$$\frac{D\tilde{\nu}}{Dt} = C_{b_1} \tilde{S} \tilde{\nu} + \frac{1}{\sigma} \left\{ \nabla \cdot \left[(\nu + \tilde{\nu}) \nabla \tilde{\nu} \right] + C_{b_2} (\nabla \tilde{\nu})^2 \right\}$$

$$- C_{w_1} f_w \left[\frac{\tilde{\nu}}{d} \right]^2$$

d : wall distance

$$f_{v_1} = \frac{\chi^3}{\chi^3 + C_{v_1}^3}, \quad \chi = \frac{\tilde{\nu}}{\nu}$$

$\nu_t = v \times l$

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- Two equation model : two transport eqs

$u \sim \sqrt{k}$, l ? $\rightarrow$ $\varepsilon = 2\nu \langle s_{ij} s_{ij} \rangle \sim k^{\frac{3}{2}}/l$

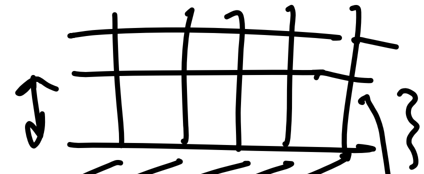
$\nu_T = C_\mu \frac{k^2}{\varepsilon}$

$s_{ij} = \frac{1}{2}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)$

k-eq : $\frac{\partial k}{\partial t} + \langle u_j \rangle \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + \nu_t\left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i}\right)\frac{\partial \langle u_i \rangle}{\partial x_j} - \varepsilon$

ε-eq : $\frac{\partial \varepsilon}{\partial t} + \langle u_j \rangle \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) + C_{1\varepsilon}\frac{\varepsilon}{k}\nu_T\left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i}\right)$

$$- C_{2\varepsilon}\frac{\varepsilon^2}{k}$$



b.c's : high Re # model : $\frac{\partial k}{\partial n} = 0$

$$\varepsilon = C_\mu^{3/4} k^{3/2}/(\kappa y)$$

$$\tau_w = \rho C_\mu^{1/4} \kappa \sqrt{k}\, \bar{u}/\ln(y^+ E)$$

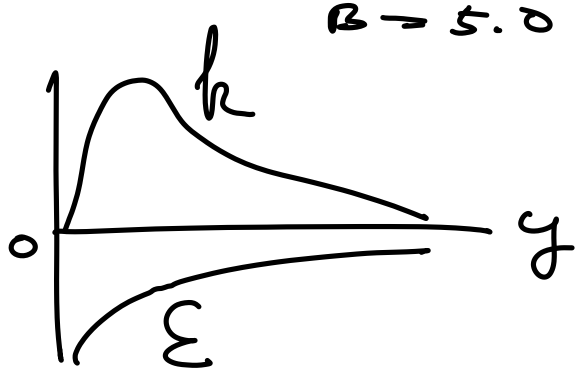
$$E = e^{\kappa B}$$

$$B = 5.0$$

DNS - low Re #

low Re # model : $k = 0$

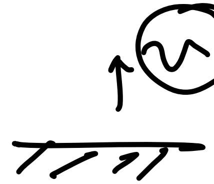
$$\frac{\partial \varepsilon}{\partial n} = 0$$



Other turbulence models

✓ SST k-ω model (Menter, 1993 or 1994)

k-ε-v^2-f model (Durbin, ___)

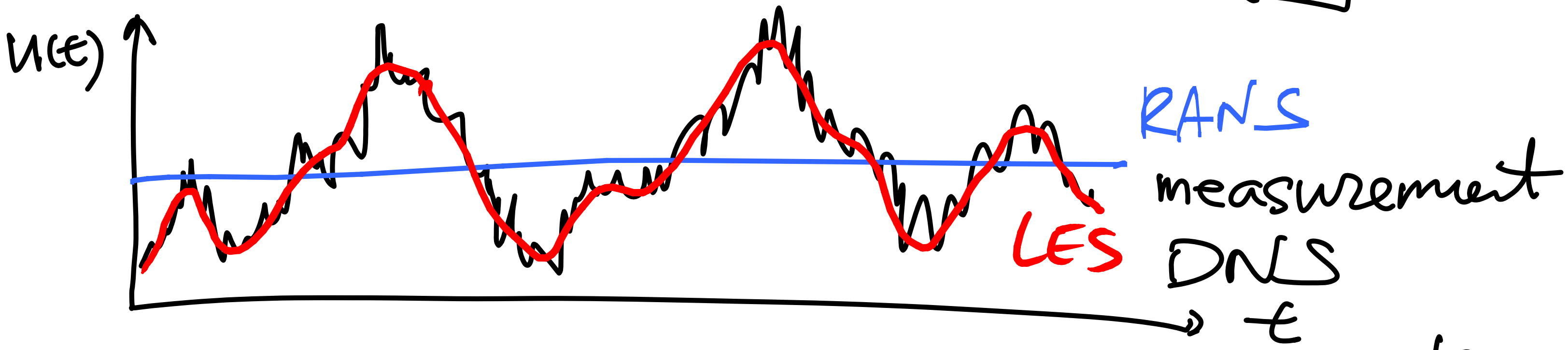


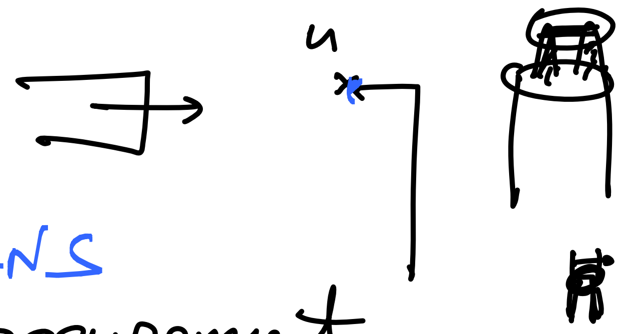
Reynolds stress model (Launder, Reece & Rodi, _ _)

$\overline{uu}$, $\overline{ww}$, $\overline{v^2}$, $\overline{uv}$ $\overline{uw}$ $\overline{vw}$

⇒ RANS models have been widely used for the prediction of turbulent flows in engineering applications. RANS, however, fails to predict massively separated flow and flows with high curvatures

④ Large eddy simulation



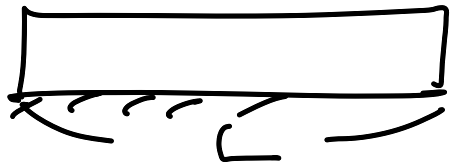


Kim, M M (1987)

The premise of LES is that the motions that are resolved are the dynamically important ones and the errors introduced by modeling the small scale motions are significantly smaller than those incurred in RANS where the entire turbulence stresses are modeled.

LES - unsteady & 3D simulation

Choi & Moin (2012, PoF) turb. boundary layer



DNS : $N_{DNS} \sim Re_L^{37/14}$

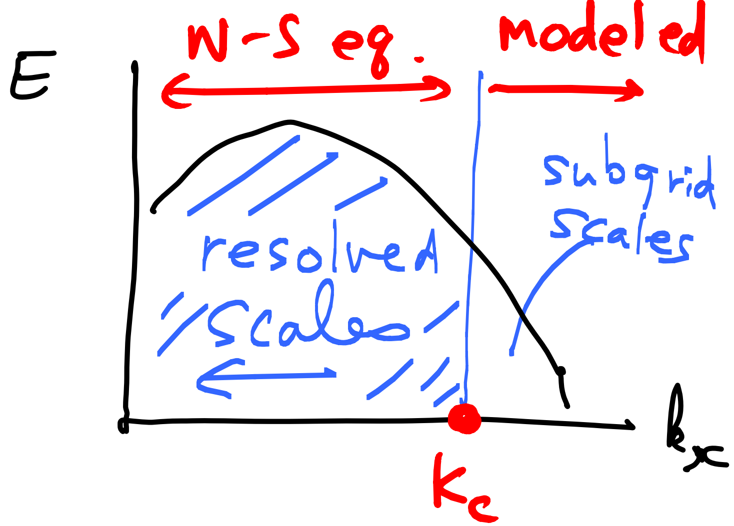
LES : $N_{LES} \sim Re_L^{13/7}$ (w/o wall modeling)

or Re_L (w/ " ")

RAN : $N_{RANS} \sim Re_L^{0}$

- Filtering:

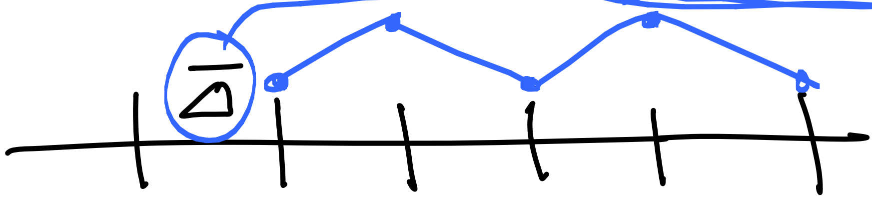
an operation which damps out all the spatial fluctuations of flow variables smaller than a



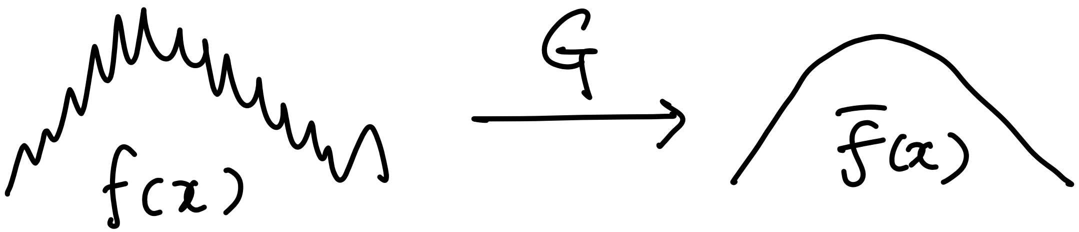
prescribed length scale (filter width)

cutoff wavenumber

$$k_c = \pi / \bar{\Delta}$$



$$k_c \cdot 2\bar{\Delta} = 2\pi$$



$$\boxed{\bar{f}(x) = \int f(\underline{x}')\, G(\underline{x}, \underline{x}')\, d\underline{x}'}$$

FVM
FDM
FEM
Spectral method

- Box filter: $G(\underline{x}, \underline{x}') = \begin{cases} 1 & \text{for } x_i - \bar{\Delta}/2 < x_i' < x_i + \bar{\Delta}/2 \\ 0 & \text{otherwise} \end{cases}$
- Gaussian filter: $G(\underline{x}, \underline{x}') = \left(\frac{6}{\pi \bar{\Delta}}\right)^{3/2} \exp\left[\frac{-6(x_i - x_i')^2}{\bar{\Delta}^2}\right]$
- Sharp cutoff filter: $G(\underline{x}, \underline{x}') = 2\sin\left[\pi(x_i - x_i')/\bar{\Delta}\right] / \pi(x_i - x_i')$

removes modes at $k > k_c = \pi/\bar{\Delta}$.

- Governing equations for LES

Filtered (spatially filtered) continuity & Navier-Stokes eqs.

$$\int \left(\frac{\partial u_i}{\partial x_i} = 0 \right) G \, d\underline{x}' \longrightarrow \frac{\partial \bar{u}_i}{\partial x_i} = 0$$

$\bar{u}_i$: filtered velocity

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_i \bar{u}_j) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}\tau_{ij}$$

$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$: subgrid-scale (SGS) stresses

$\llcorner$ modeling SGS stresses!

- Smagorinsky eddy viscosity model (1963 ; SM)

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_T \overline{S}_{ij} \quad \text{(eddy viscosity hypothesis)}$$

$$\nu_T = (C_s \overline{\Delta})^2 |\overline{S}|, \quad |\overline{S}| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}, \quad \overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)$$

Smagorinsky constant coefficient $\quad 0.1 \sim 0.3$

However, C_s is not universal
and requires damping ft. near the wall,

$$\downarrow$$

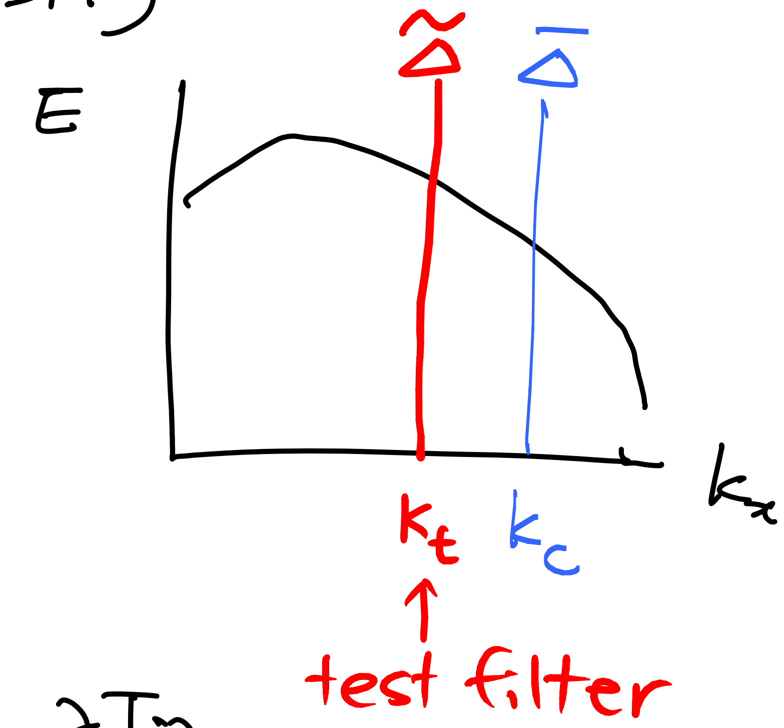
1982 Channel flow LES (Moin & Kim) $\quad C_s(1-e^{-\bigcirc y})$ $\quad y$

→ C_s should be given a priori depending on the flow field.

- Dynamic Smagorinski model (DSM)

  Germano et al. (1991)

  ↑ Moin



Apply another (test) filter : $\sim$

$$\frac{\partial \hat{\tilde{u}}_i}{\partial x_i} = 0$$

$$\frac{\partial \hat{\tilde{u}}_i}{\partial t} + \frac{\partial \hat{\tilde{u}}_i \hat{\tilde{u}}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \hat{\tilde{p}}}{\partial x_i} + \nu \frac{\partial^2 \hat{\tilde{u}}_i}{\partial x_j \partial x_j} - \frac{\partial T_{ij}}{\partial x_j}$$

$$T_{ij} = \widetilde{\overline{u_i u_j}} - \tilde{\bar{u}}_i \tilde{\bar{u}}_j \qquad \tilde{\tau}_{ij} = \widetilde{\overline{u_i u_j}} - \widetilde{\bar{u}_i \bar{u}_j}$$

$$\underline{T_{ij} - \tilde{\tau}_{ij}} = \widetilde{\bar{u}_i \bar{u}_j} - \tilde{\bar{u}}_i \tilde{\bar{u}}_j \equiv \underline{L_{ij}}$$

Germano identity

$$\tilde{\tau}_{ij} - \frac{1}{3}\delta_{ij}\tilde{\tau}_{kk} = -2\,\widetilde{(C_s\bar{\Delta})^2 |\bar{S}|\, \bar{S}_{ij}}$$

$$T_{ij} - \frac{1}{3}\delta_{ij} T_{kk} = -2\,(C_s\tilde{\Delta})^2 |\tilde{\bar{S}}|\, \tilde{\bar{S}}_{ij}$$

$$\Rightarrow \quad \underbrace{-2(C_s\tilde{\Delta})^2 |\tilde{\bar{S}}|\, \tilde{\bar{S}}_{ij} + 2\,\widetilde{(C_s\bar{\Delta})^2 |\bar{S}|\, \bar{S}_{ij}}}_{} = L_{ij} - \frac{1}{3}\delta_{ij} L_{kk}$$

$$-2(C_s\bar{\Delta})^2\left[\left(\frac{\tilde{\Delta}}{\bar{\Delta}}\right)^2 |\tilde{\bar{S}}|\, \tilde{\bar{S}}_{ij} - \widetilde{|\bar{S}|\, \bar{S}_{ij}}\right] = L_{ij} - \frac{1}{3}\delta_{ij} L_{kk}$$

$$\underbrace{\qquad\qquad\qquad}_{M_{ij}}$$

$$\rightarrow \quad L_{ij} - \frac{1}{3}\delta_{ij} L_{kk} + 2(C_s\bar{\Delta})^2 M_{ij} = 0$$

6 eqs but 1 C_s. $\Rightarrow$ least square error method

$$Q = \left[L_{ij} - \frac{1}{3}\delta_{ij} L_{kk} + 2(C_s\bar{\Delta})^2 M_{ij} \right]^2$$

Lilly et al. (1992)

$$\frac{\partial Q}{\partial C_s^2} = 0 \quad \Rightarrow \quad \boxed{(C_s\bar{\Delta})^2 = -\frac{1}{2}\frac{L_{ij}M_{ij}}{M_{ij}M_{ij}}}$$

C_s is a fct of space and time, and is obtained at each time step during computation

→ called, dynamic Smagorinskiy model.

Dynamic Smagorinsky model (DSM) — continued

$$\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = -2\underline{(C_s\bar{\Delta})^2|\bar{S}|}\,\bar{S}_{ij}$$

$$\rightarrow (C_s\bar{\Delta})^2 = -\frac{1}{2}\frac{L_{ij}M_{ij}}{M_{ij}M_{ij}}, \qquad L_{ij} = \widehat{\bar{u}_i\bar{u}_j} - \hat{\bar{u}}_i\hat{\bar{u}}_j$$

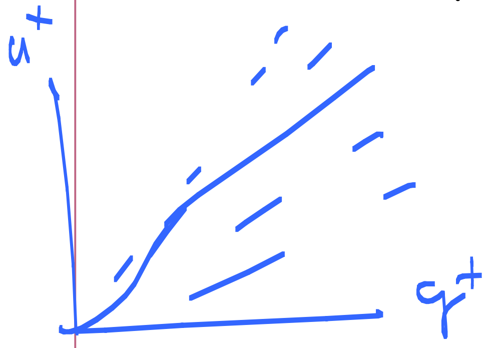
$$M_{ij} = \left(\frac{\hat{\Delta}}{\bar{\Delta}}\right)^2 |\hat{\bar{S}}|\hat{\bar{S}}_{ij} - \widehat{|\bar{S}|\bar{S}_{ij}}$$

→ do computation!

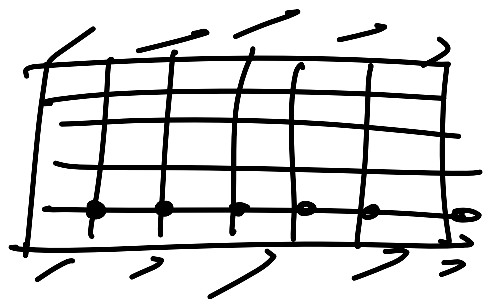
$\Rightarrow (C_s)^2 < 0$ at some grids.

↳ numerical instability

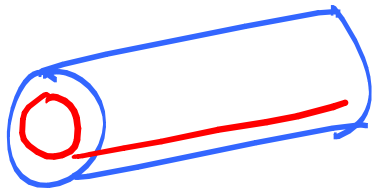
$\Rightarrow$ requires an averaging over homogeneous direction(s) and/or ad hoc clipping: $C_s = 0$ if $C_s < 0$

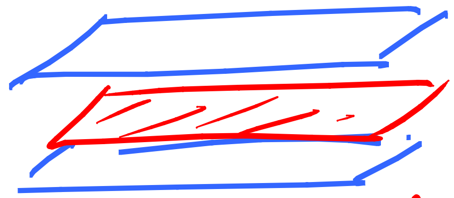


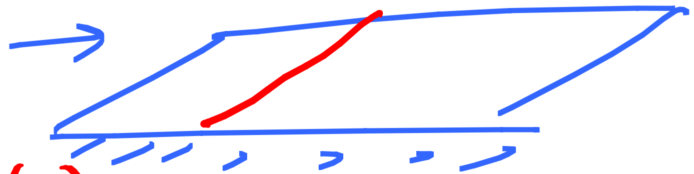
$$(C_s \bar{\Delta})^2 = -\frac{1}{2} \frac{\langle L_{ij} M_{ij} \rangle_h}{\langle M_{ij} M_{ij} \rangle_h}$$



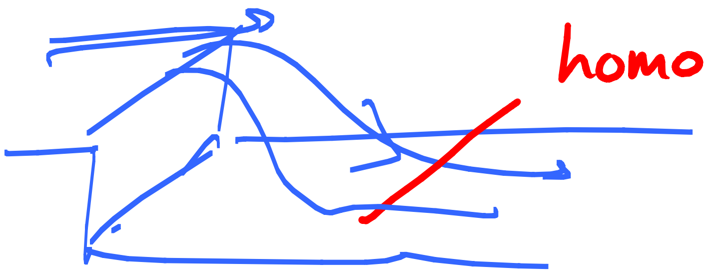
↳ numerical stability

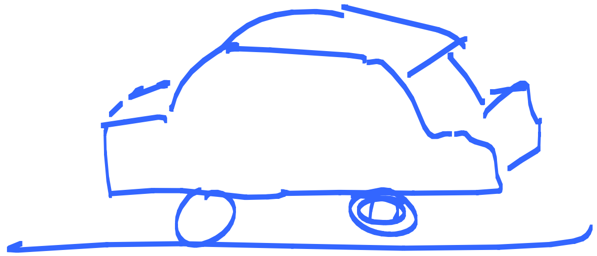






homo. direction(s)





no homo. direction

↳ dynamic Smag. model ✗

- Vreman model (2004, PoF)

$$\nu_T = C_v \sqrt{\frac{\Pi_\beta}{\bar{\alpha}_{ij}\bar{\alpha}_{ij}}}, \quad \bar{\alpha}_{ij} = \frac{\partial \bar{u}_j}{\partial x_i},$$

Vreman coefficient

$\boxed{C_v = 0.07}$ isotropic flow

$$\Pi_\beta = \beta_{11}\beta_{22} - \beta_{12}^2 + \beta_{11}\beta_{33} - \beta_{13}^2 + \beta_{22}\beta_{33} - \beta_{23}^2,$$

$$\beta_{ij} = \sum_{m=1}^{3} \bar{\Delta}_m^2 \, \bar{\alpha}_{mi} \, \bar{\alpha}_{mj}$$

$$\nu_T = 2(C_s\bar{\Delta})^2|\bar{S}_{ij}|$$

$|\bar{S}_{ij}| \neq 0$

Park, Lee & Choi (2006, PoF)

Lee, Choi & Park (2010, PoF)

Dynamic global model to determine C_v

Germano identity $L_{ij} = T_{ij} - \widehat{\tau_{ij}} = \widehat{\overline{u_i}\,\overline{u_j}} - \widehat{\overline{u}_i}\,\widehat{\overline{u}_j}$

$$\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = \overline{u_i u_j} - \overline{u}_i\,\overline{u}_j = -2C_v\sqrt{\frac{\overline{\Pi_\beta}}{\overline{\alpha_{ij}}\,\overline{\alpha_{ij}}}}\,\overline{S}_{ij}$$

$$T_{ij} - \frac{1}{3}\delta_{ij}T_{kk} = \widehat{\overline{u_i u_j}} - \widehat{\overline{u}_i}\,\widehat{\overline{u}_j} = -2C_v\sqrt{\frac{\widehat{\Pi_\beta}}{\widehat{\alpha_{ij}}\,\widehat{\alpha_{ij}}}}\,\widehat{\overline{S}}_{ij}$$

and

introduce least square error minimization to get C_v

$$\Rightarrow \boxed{C_v(t) = -\frac{1}{2}\frac{\langle L_{ij}M_{ij}\rangle_V}{\langle M_{ij}M_{ij}\rangle_V}}$$

volume averaging

$$L_{ij} = \widehat{\bar{u}_i \bar{u}_j} - \widehat{\bar{u}}_i \widehat{\bar{u}}_j \,, \quad M_{ij} = \sqrt{\frac{\widehat{\Pi_\beta}}{\widehat{\alpha_{ij}}\widehat{\alpha_{ij}}}}\,\widehat{\bar{S}_{ij}} - \sqrt{\frac{\Pi_\beta}{\bar{\alpha}_{ij}\bar{\alpha}_{ij}}}\,\bar{S}_{ij}$$

- C_r is constant in space but varies in time
- No clipping
- No homo. direction required

$\longrightarrow$ Can be applied to complex geometry.

Ch. 10. Compressible flow — skip

Ch. 11. Efficiency and accuracy improvement

- errors
  - modeling errors : turbulence
    combustion
    multi-phase flow
  - discretization errors
  - iteration errors ← $A\underline{x} = b$ 10^{-12} $\underline{10}^{-5}$ $\underline{10}^{-6}$
  - programming and user errors X

- estimating errors — validation and uncertainty quantification

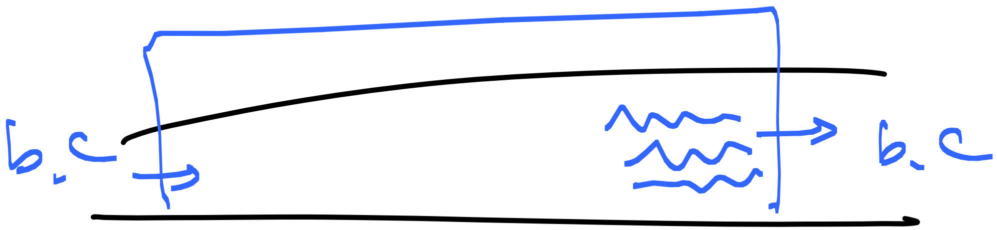
- grid quality and optimization
- multigrid methods for flow calculation
- adaptive grid methods and local grid refinement
- parallel computing in CFD

Ch. 12 Special Topics

1. Heat and mass transfer

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \frac{1}{Pr\,Re} \nabla^2 \theta$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{1}{Re} \nabla^2 u_i - \nabla p$$



2. Flows w/ variable fluid properties

$$\frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j}\right) \qquad \mu = \mu_0 + (\mu - \mu_0)$$

$$\mu \downarrow \mu(\underline{x}, t)$$

3. Moving grids
4. Free-surface flows
5. Meteorological and oceanographic applications
6. Multiphase flows
7. Combustion