

# Computational Fluids Mechanics

Part 1: Numerical methods

Part 2: Turbulence models

Part 3: Practice of numerical simulation

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# Computational Fluid Mechanics

## Part1 : Numerical Methods

Objective :

**Numerical methods for fluids mechanics and their accuracy**

1. Introduction
2. Numerical methods for fluid mechanics (1) ~ Basic equations
3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

Summary

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# Computational Fluid Mechanics

## Part1 : Numerical Methods (3a)

1. Introduction
2. Numerical methods for fluid mechanics (1) ~ governing equations
3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
  - **Fundamentals for discretizing methods**
  - Schemes for convection and diffusion equation
  - Analysis of accuracy and instability
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

# Fundamentals for discretizing methods

## Generalized conservation eq.

$$\frac{\partial \phi}{\partial t} = -\mathbf{u} \cdot \nabla \phi - \nabla \cdot \mathbf{j} + S \quad \mathbf{j} = -\Gamma \nabla \phi$$

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$$\frac{\partial \phi}{\partial t} = -u_j \frac{\partial \phi}{\partial x_j} - \frac{\partial J_j}{\partial x_j} + S \quad J_j = -\Gamma \frac{\partial \phi}{\partial x_j}$$

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$$\frac{\partial \phi}{\partial t} = -\left( u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} + w \frac{\partial \phi}{\partial z} \right) - \left( \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right) + S$$

$$\mathbf{j}^t = \begin{bmatrix} J_x & J_y & J_z \end{bmatrix} = \begin{bmatrix} -\Gamma \frac{\partial \phi}{\partial x} & -\Gamma \frac{\partial \phi}{\partial y} & -\Gamma \frac{\partial \phi}{\partial z} \end{bmatrix}$$

# Fundamentals for discretizing methods

## Finite Different Method

Differential eq.

$$\frac{df}{dx} = g(x)$$



Polynomial eq.

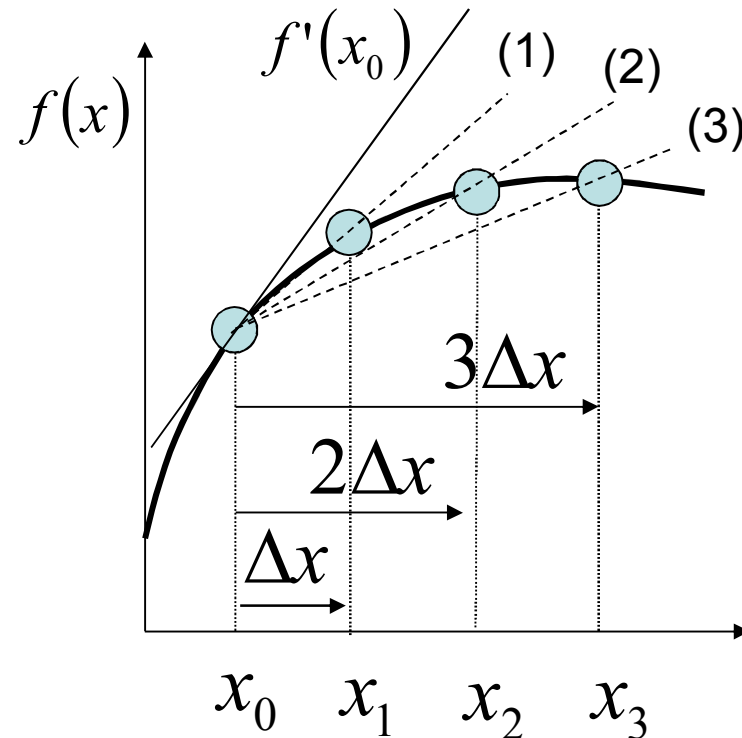
$$\frac{f(x_1) - f(x_0)}{x_1 - x_0} = g(x_0)$$

$$f'(x_0) \equiv \lim_{x \rightarrow x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

$$\approx \frac{f(x_1) - f(x_0)}{\Delta x} \quad (1)$$

$$\approx \frac{f(x_2) - f(x_0)}{2\Delta x} \quad (2)$$

$$\approx \frac{f(x_3) - f(x_0)}{3\Delta x} \quad (3)$$



# Taylor series expansion

## Taylor series expansion

$$f = \sum \frac{1}{k!} x^k \frac{\partial^k f}{\partial x^k} = f_i + x f'_i + \frac{1}{2} x^2 f''_i + \frac{1}{6} x^3 f'''_i + \frac{1}{24} x^4 f''''_i + \dots$$



$$f_{i\pm 1} = f_i \pm \delta x f'_i + \frac{1}{2} \delta x^2 f''_i \pm \frac{1}{6} \delta x^3 f'''_i + \frac{1}{24} \delta x^4 f''''_i + \dots$$



1<sup>st</sup> order forward scheme

truncation error


$\frac{f_{i+1} - f_i}{\delta x} \cong f'_i$	$+ \frac{1}{2} \delta x f''_i + \frac{1}{6} \delta x^2 f'''_i + \frac{1}{24} \delta x^3 f''''_i + \dots$
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1<sup>st</sup> order backward scheme

$\frac{f_i - f_{i-1}}{\delta x} \cong f'_i$	$- \frac{1}{2} \delta x f''_i + \frac{1}{6} \delta x^2 f'''_i - \frac{1}{24} \delta x^3 f''''_i + \dots$
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## 2nd order central scheme


$$\begin{array}{r}
 f_{i+1} = f_i + \cancel{\delta x f'_i} + \frac{1}{2} \cancel{\delta x^2 f''_i} + \frac{1}{6} \delta x^3 f'''_i + \frac{1}{24} \delta x^4 f''''_i + \dots \\
 - \left. \begin{array}{r}
 f_{i-1} = f_i - \cancel{\delta x f'_i} + \frac{1}{2} \cancel{\delta x^2 f''_i} - \frac{1}{6} \delta x^3 f'''_i + \frac{1}{24} \delta x^4 f''''_i + \dots
 \end{array} \right\} \\
 \hline
 f_{i+1} - f_{i-1} = 2\delta x f'_i + \frac{1}{3} \delta x^3 f'''_i + \dots
 \end{array}$$



$$\frac{f_{i+1} - f_{i-1}}{2\delta x} \cong f'_i$$
 1<sup>st</sup> derivative approx.

$$+ \frac{1}{6} \delta x^2 f'''_i + \dots$$
 truncation error

$$\begin{array}{r}
 f_{i+1} = f_i + \cancel{\delta x f'_i} + \frac{1}{2} \delta x^2 f''_i + \frac{1}{6} \cancel{\delta x^3 f'''_i} + \frac{1}{24} \delta x^4 f''''_i + \dots \\
 + \left. \begin{array}{r}
 f_{i-1} = f_i - \cancel{\delta x f'_i} + \frac{1}{2} \delta x^2 f''_i - \frac{1}{6} \cancel{\delta x^3 f'''_i} + \frac{1}{24} \delta x^4 f''''_i + \dots
 \end{array} \right\} \\
 \hline
 f_{i+1} + f_{i-1} = 2f_i + \delta x^2 f''_i + \frac{1}{12} \delta x^4 f''''_i + \dots
 \end{array}$$



$$\frac{f_{i+1} - 2f_i + f_{i-1}}{\delta x^2} \cong f''_i$$
 2nd derivative approx.

$$+ \frac{1}{12} \delta x^2 f''''_i + \dots$$
 truncation error

## Exercise

$$f'_i \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2\delta x}$$

Polynomial factors

$$\left\{ \begin{array}{l} \frac{3}{2\delta x} \times \\ -\frac{4}{2\delta x} \times \\ +\frac{1}{2\delta x} \times \end{array} \right.$$

$$\left. \begin{array}{l} f_i = f_i \\ f_{i-1} = f_i - \delta x f'_i + \frac{1}{2} \delta x^2 f''_i - \frac{1}{6} \delta x^3 f'''_i + \dots \\ f_{i-2} = f_i - (2\delta x) f'_i + \frac{1}{2} (2\delta x)^2 f''_i - \frac{1}{6} (2\delta x)^3 f'''_i + \dots \end{array} \right\} \text{Taylor series expansion}$$

Look here!

$$\frac{3f_i - 4f_{i-1} + f_{i-2}}{2\delta x} = \left( \frac{3}{2\delta x} - \frac{4}{2\delta x} + \frac{1}{2\delta x} \right) f_i = 0 \times f_i$$

$$+ \left( \frac{4}{2\delta x} \delta x - \frac{1}{2\delta x} (2\delta x) \right) f'_i = 1 \times f'_i \quad \Rightarrow \text{Approx.}$$

$$+ \left( -\frac{4}{2\delta x} \frac{(\delta x)^2}{2} + \frac{1}{2\delta x} \frac{(2\delta x)^2}{2} \right) f''_i = 0 \delta x \times f''_i \quad \Rightarrow \text{Truncation error}$$

$$+ \left( \frac{4}{2\delta x} \frac{(\delta x)^3}{6} - \frac{1}{2\delta x} \frac{(2\delta x)^3}{6} \right) f'''_i = -\frac{1}{3} \delta x^2 \times f'''_i \quad \Rightarrow \text{2nd order accuracy}$$



# Fundamentals for discretizing methods

## Numerical integration

(for Finite Element Method / Time marching scheme)

Differential eq.

$$\frac{df}{dx} = g(x, f(x))$$



Integral eq.

$$[f]_{x_0}^x \equiv f(x) - f(x_0) = \int_{x_0}^x g(x') dx'$$

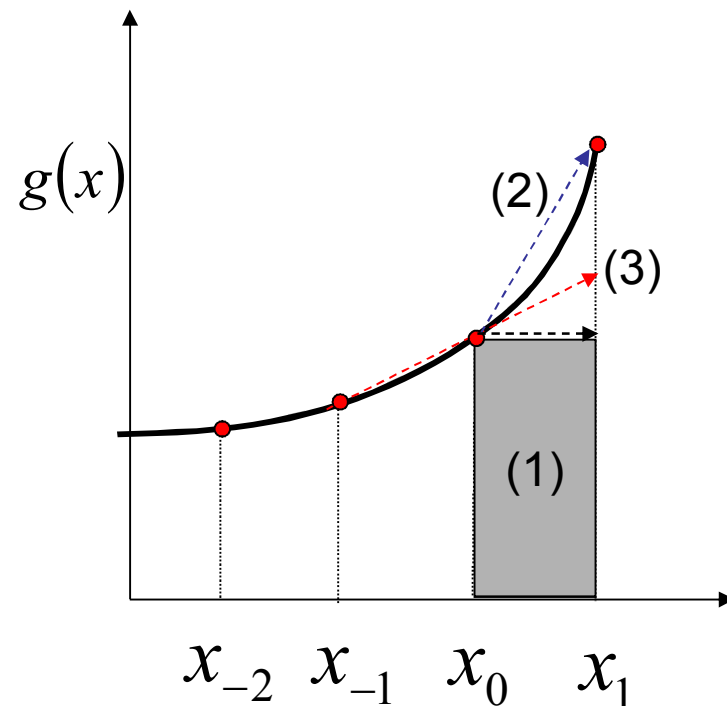
Numerical integration of (g)

$$f(x_1) - f(x_0)$$

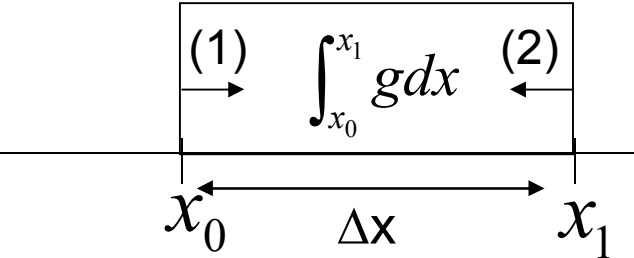
$$= \int_{x_0}^{x_1} g(x') dx' \cong g(x_0) \Delta x \quad (1)$$

$$\cong \frac{g(x_0) + g(x_1)}{2} (\Delta x) \quad (2)$$

$$\cong \frac{3g(x_0) - g(x_{-1})}{2} (\Delta x) \quad (3)$$



## Trapezoidal scheme

$$\int g dx \cong \int \left( g_i + xg'_i + \frac{1}{2}x^2g''_i + \frac{1}{6}x^3g'''_i + \dots \right) dx$$


1<sup>st</sup> order approx.

estimated error

$$\int_0^{\Delta x} g dx \cong g_0 \Delta x + g'_0 \frac{\Delta x^2}{2} + g''_0 \frac{\Delta x^3}{6} + \dots \quad (1) \times 1/2$$

$$\int_{-\Delta x}^0 g dx \cong g_1 \Delta x - g'_1 \frac{\Delta x^2}{2} + g''_1 \frac{\Delta x^3}{6} + \dots \quad (2) \times 1/2$$

$$+ \left( g_0 + g_1 \right) \frac{\Delta x}{2} + \frac{(g'_0 - g'_1) \Delta x^2}{2} + \frac{(g''_1 + g''_0) \Delta x^3}{6} \dots$$

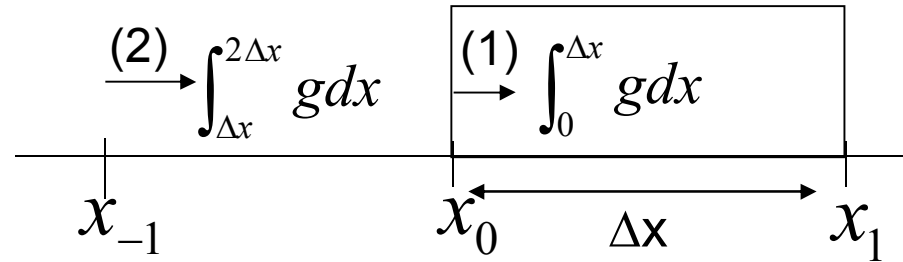
2<sup>nd</sup> order approx.

$$= -\bar{g}'' \frac{\Delta x^3}{4} \cong \bar{g}'' \frac{\Delta x^3}{6} \Rightarrow \boxed{-\bar{g}'' \frac{\Delta x^3}{12}} \text{ estimated error}$$

$$\bar{g} = \frac{1}{\Delta x} \int_{x_0}^{x_1} g dx \cong \frac{g_0 + g_1}{2} \Rightarrow -\bar{g}'' \frac{\Delta x^2}{12} \text{ Error for averaged value}$$

## Exercise

### Adams–Bashforth scheme



$$\begin{aligned}
 \int_0^{\Delta x} g dx &\cong g_0 \Delta x + g'_0 \frac{\Delta x^2}{2} + g''_0 \frac{\Delta x^3}{6} + \dots && (1) \times (3/2) \\
 + \int_{\Delta x}^{2\Delta x} g dx &\cong g_{-1} \Delta x + g'_{-1} \frac{3\Delta x^2}{2} + g''_{-1} \frac{8\Delta x^3}{6} + \dots && (2) \times (-1/2)
 \end{aligned}$$

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$$\left( \frac{3}{2} g_0 - \frac{1}{2} g_{-1} \right) \Delta x + \frac{3(g'_0 - g'_{-1})}{4} \Delta x^2 + \frac{(3g''_0 - 8g''_{-1})}{12} \Delta x^3 \dots$$

$$\cong \bar{g}'' \frac{3\Delta x^3}{4} \qquad \cong -\bar{g}'' \frac{5\Delta x^3}{12} \qquad \Rightarrow \bar{g}'' \frac{\Delta x^3}{3} \text{ Estimated error}$$

# Fundamentals for discretizing methods

## Finite Volume Method

Flux type differential eq

$$\frac{d}{dx} J(\phi(x)) = g(\phi(x))$$



Integral eq.

$$J(x_+) - J(x_-) = \int_{x_-}^{x_+} g(x') dx'$$

$$\begin{aligned} J(x_0^-) &\cong J(\phi(x_0)) \\ J(x_1^-) &\equiv J(x_0^+) \cong J(\phi(x_1)) \\ J(x_2^-) &\equiv J(x_1^+) \cong J(\phi(x_2)) \\ &\vdots \end{aligned}$$

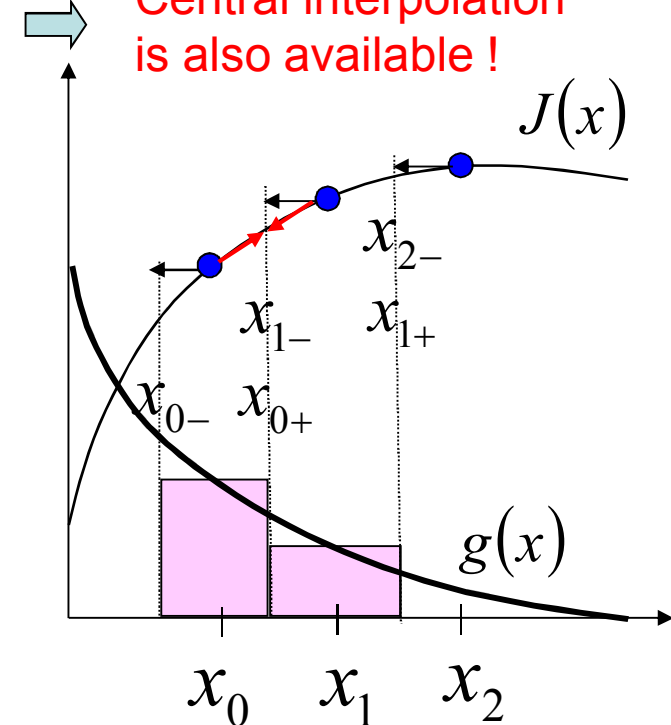


$$\begin{aligned} J(x_{0+}) - J(x_{0-}) &\cong g(\phi(x_0)) \Delta x \\ J(x_{1+}) - J(x_{1-}) &\cong g(\phi(x_1)) \Delta x \\ &\vdots \end{aligned}$$

Backward approximation

Midway-rule integration

Central interpolation is also available !



# Finite Volume Method for generalized conservation eq.

Differential form

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot [\mathbf{u}\phi + \mathbf{j}] + S \quad \Rightarrow \quad \nabla \cdot \mathbf{J}(\phi(\mathbf{x})) = g(\phi(\mathbf{x}))$$

$$\mathbf{J}(\phi(\mathbf{x})) \Rightarrow \mathbf{u}\phi + \mathbf{j}(\phi)$$

$$g(\phi(\mathbf{x})) \Rightarrow S(\phi) - \frac{\partial \phi}{\partial t}$$

Integration form

$$\int_{\Omega} \frac{\partial \phi}{\partial t} dv = \int_{\Sigma} [\mathbf{u}\phi + \mathbf{j}] \cdot d\mathbf{n} + \int_{\Omega} S dv \quad \Rightarrow \quad J(x_+) - J(x_-) = \int_{x_-}^{x_+} g(x') dx'$$

(1D case)

$$\frac{\partial \phi}{\partial t} = -\frac{\partial}{\partial x} [u_x \phi + j_x(\phi)] + S(\phi) \quad \Rightarrow \quad \frac{\partial}{\partial x} J(x, \phi(x)) = g(x, \phi(x))$$

$$J(x, \phi(x)) \Rightarrow u_x \phi + j_x(\phi)$$

$$g(x, \phi(x)) \Rightarrow S(\phi) - \frac{\partial \phi}{\partial t}$$

backward  
approximation scheme

	$f_0 = f_+$	$-\left(\frac{\delta x}{2}\right) f'_+ + \frac{1}{2} \left(\frac{\delta x}{2}\right)^2 f''_+ + \dots$	x1/2
+	$f_1 = f_+$	$+\left(\frac{\delta x}{2}\right) f'_+ + \frac{1}{2} \left(\frac{\delta x}{2}\right)^2 f''_+ + \dots$	x1/2
	$\frac{f_0 + f_1}{2} = f_+$	$+\frac{1}{4} \delta x^2 f'' \dots$	...2 <sup>nd</sup> order accuracy
	central interpolation scheme	Estimated error	

	$f_0 = f_+$	$-\left(\frac{\delta x}{2}\right) f'_+ + \frac{1}{2} \left(\frac{\delta x}{2}\right)^2 f''_+ + \dots$	x3/2
+	$f_{-1} = f_+$	$-\left(\frac{3\delta x}{2}\right) f'_+ + \frac{1}{2} \left(\frac{3\delta x}{2}\right)^2 f''_+ + \dots$	x-1/2
	$\frac{3f_0 - f_{-1}}{2} = f_+$	$+\frac{3}{4} \delta x^2 f'' + \dots$	...2 <sup>nd</sup> order accuracy
	extrapolation scheme	Estimated error	

## Exercise

### Estimation of accuracy for Finite Volume Method

Central interpolation  $J_+ - J_- \cong \frac{1}{2}(J_0 + J_1) - \frac{1}{2}(J_{-1} + J_0) + \frac{\Delta x^2}{4}(J''_+ - J''_-) + \dots$

Midway rule integration  $\int_{-\Delta x/2}^{\Delta x/2} g dx \cong g(f(x_0))\Delta x + g''_0 \frac{\Delta x^3}{24} + \dots$

$$\frac{1}{2}(J_0 + J_1) - \frac{1}{2}(J_{-1} + J_0) \cong g(f(x_0))\Delta x$$

Discretized eq.

$$-\frac{\Delta x^3}{4} J''' + \frac{\Delta x^3}{24} g''$$

Truncation error

For averaged value of volume  $\Delta x$  estimated error in order of  $(\Delta x)^2$  !!

$$\frac{1}{\Delta x} \int g(\phi(\mathbf{x})) dx \equiv \overline{g(\phi(\mathbf{x}))} = \overline{S(\phi)} - \frac{\partial \phi}{\partial t}$$

# Computational Fluid Mechanics

## Part1 : Numerical Methods (3b)

1. Introduction
2. Numerical methods for fluid mechanics (1) ~ governing equations
3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
  - Fundamentals for discretizing methods
  - **Schemes for convection and diffusion equation**
  - Analysis of accuracy and instability
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation



# Schemes for convection and diffusion equation

## Finite Difference Method

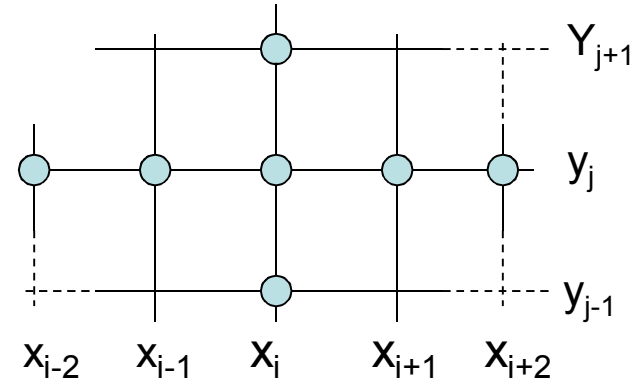
$$\frac{\partial \phi}{\partial t} = - \boxed{\mathbf{u} \cdot \nabla \phi} - \nabla \cdot \mathbf{j} + S$$

- Convection term

$$u \frac{\partial \phi}{\partial x} \cong \begin{cases} u_i \frac{\phi_i - \phi_{i-1}}{\delta x} & (u_i \geq 0) \\ u_i \frac{\phi_{i+1} - \phi_i}{\delta x} & (u_i < 0) \end{cases}$$

$$u \frac{\partial \phi}{\partial x} \cong u_i \frac{\phi_{i+1} - \phi_{i-1}}{2\delta x}$$

$$u \frac{\partial \phi}{\partial x} \cong \begin{cases} u_i \frac{3\phi_i - 4\phi_{i-1} + \phi_{i-2}}{2\delta x} & (u_i \geq 0) \\ u_i \frac{-\phi_{i+1} + 4\phi_i - 3\phi_{i-1}}{2\delta x} & (u_i < 0) \end{cases}$$



1<sup>st</sup> order **UPWIND** difference scheme

$$v \frac{\partial \phi}{\partial y} \cong v_j \frac{\phi_j - \phi_{j-1}}{\delta y} \quad (v_j \geq 0)$$

2<sup>nd</sup> order central difference scheme

$$v \frac{\partial \phi}{\partial y} \cong v_j \frac{\phi_{j+1} - \phi_{j-1}}{2\delta y}$$

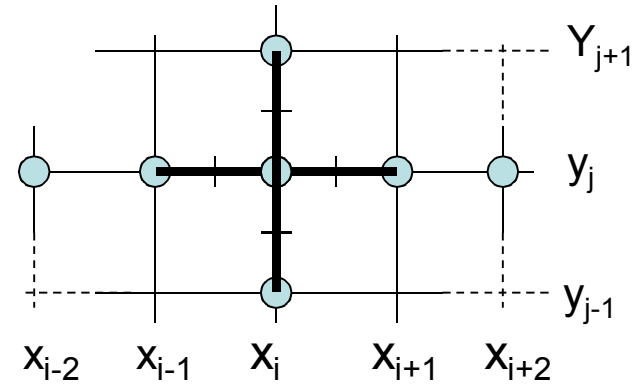
2<sup>nd</sup> order **UPWIND** difference scheme

# Schemes for convection and diffusion equation

## Finite Difference Method (continued)

$$\frac{\partial \phi}{\partial t} = -\mathbf{u} \cdot \nabla \phi - \boxed{\nabla \cdot \mathbf{j}} + S$$

$$\mathbf{j} = -\Gamma \nabla \phi$$



- Diffusion term

$$\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} \cong \frac{J_{i+} - J_{i-}}{\delta x} + \frac{J_{j+} - J_{j-}}{\delta y} \quad \leftarrow \quad J_{i+} \cong -\Gamma \frac{\phi_{i+1} - \phi_i}{\delta x}, \quad J_{i-} \cong -\Gamma \frac{\phi_i - \phi_{i-1}}{\delta x}$$

$$\cong \Gamma \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\delta x^2} + \Gamma \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\delta y^2} \quad \text{2nd order central difference scheme}$$

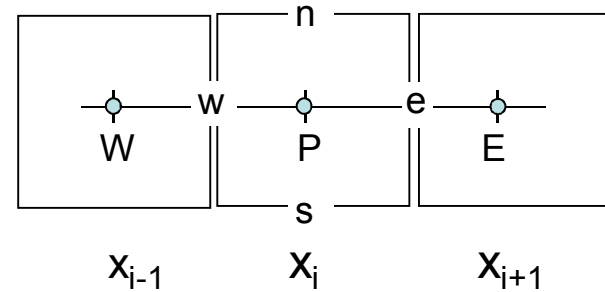
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$$\Gamma \nabla^2 \phi \equiv \Gamma \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \cong \Gamma \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\delta x^2} + \Gamma \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\delta y^2}$$

# Schemes for convection and diffusion equation

## Finite Volume (control volume) Method

$$\int \left( \frac{\partial \phi}{\partial t} - S \right) dV = - \int_w (\mathbf{u}\phi + \mathbf{j}) \cdot \mathbf{n} dA$$



$$\bar{\phi} \delta x \delta y \equiv \iint \phi dx dy \quad \bar{J}_w \delta y \equiv \int_w J_x dy$$

$$\left( \frac{\partial \bar{\phi}}{\partial t} - \bar{S} \right) \delta x \delta y = - \left\{ (u_e \bar{\phi}_e + \bar{J}_e) - (u_w \bar{\phi}_w + \bar{J}_w) \right\} \delta y - \left\{ (u_n \bar{\phi}_n + \bar{J}_n) - (u_s \bar{\phi}_s + \bar{J}_s) \right\} \delta x$$

$$\bar{J}_w \cong -\Gamma \frac{\bar{\phi}_{i+1} - \bar{\phi}_i}{\delta x}$$

Diffusion term ~ 2<sup>nd</sup> order accuracy

$$\Rightarrow (\bar{J}_e - \bar{J}_w) dy + (\bar{J}_n - \bar{J}_s) dx \cong \Gamma \frac{\bar{\phi}_{i+1} - 2\bar{\phi}_i + \bar{\phi}_{i-1}}{\delta x^2} + \Gamma \frac{\bar{\phi}_{j+1} - 2\bar{\phi}_j + \bar{\phi}_{j-1}}{\delta y^2}$$

$$\frac{\partial \bar{\phi}}{\partial t} \delta x \delta y \equiv \iint \left( \frac{\partial \phi}{\partial t} \right) dx dy = \frac{\partial \bar{\phi}}{\partial t} \delta x \delta y$$

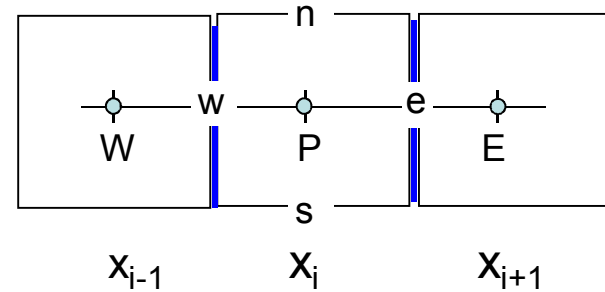
$$\bar{S} \equiv \iint S(\phi) dx dy \cong \bar{S}(\bar{\phi})$$

Source term ~ 2<sup>nd</sup> order accuracy

# Schemes for convection and diffusion equation

## Finite Volume (control volume) Method

$$\int \left( \frac{\partial \phi}{\partial t} - S \right) dV = - \int_w (\mathbf{u}\phi + \mathbf{j}) \cdot \mathbf{n} dA$$



$$\bar{\phi} \delta x \delta y \equiv \iint \phi dx dy \quad J_w \equiv \frac{1}{\delta y} \int_w J_x dy$$

$$\left( \frac{\partial \bar{\phi}}{\partial t} - \bar{S} \right) \delta x \delta y = - \{ (u_e \phi_e + J_e) - (u_w \phi_w + J_w) \} \delta y - \{ (u_n \phi_n + J_n) - (u_s \phi_s + J_s) \} \delta x$$

$$\phi_w \cong \begin{cases} \bar{\phi}_{i-1} & (u_i \geq 0) \\ \bar{\phi}_i & (u_i < 0) \end{cases} \quad \text{1<sup>st</sup> Upwind scheme}$$

Convection term

$$\phi_w = \frac{1}{2} (\bar{\phi}_i + \bar{\phi}_{i-1}) + \left[ -\frac{1}{8} \delta x^2 \frac{\partial^2 \phi}{\partial x^2} + 0(\delta x^4) \right] \quad \text{2<sup>nd</sup> Central scheme}$$

$$\phi_w = \frac{1}{8} (3\bar{\phi}_i + 6\bar{\phi}_{i-1} - \bar{\phi}_{i-2}) + \left[ \frac{1}{24} \delta x^2 \frac{\partial^2 u}{\partial x^2} + 0(\delta x^3) \right] \quad \text{QUICK scheme}$$

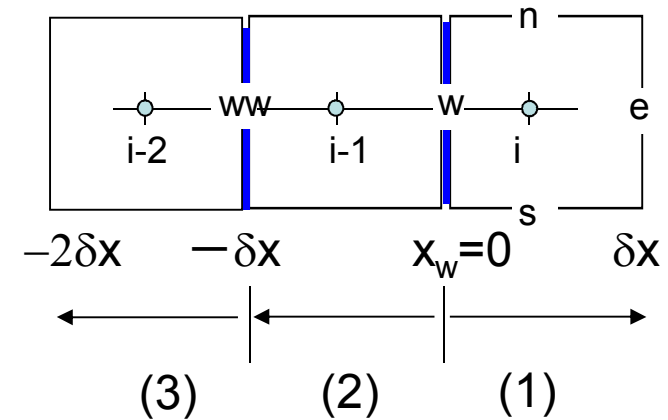
**Exercise** Analyze the accuracy of FVM schemes by following way

$$\phi = f_w - x f'_w + \frac{x^2}{2} f''_w \dots$$

$$(1) \quad \bar{\phi}_i \delta x = \int_0^{\delta x} \phi dx = \delta x \phi_w + \frac{\delta x^2}{2} \phi'_w + \frac{\delta x^3}{6} \phi''_w \dots$$

$$(2) \quad \bar{\phi}_{i-1} \delta x = \int_{-\delta x}^0 \phi dx = \delta x \phi_w - \frac{\delta x^2}{2} \phi'_w + \frac{\delta x^3}{6} \phi''_w \dots$$

$$(3) \quad \bar{\phi}_{i-2} \delta x = \int_{-2\delta x}^{-\delta x} \phi dx = \delta x \phi_w - \frac{3\delta x^2}{2} \phi'_w + \frac{7\delta x^3}{6} \phi''_w \dots$$

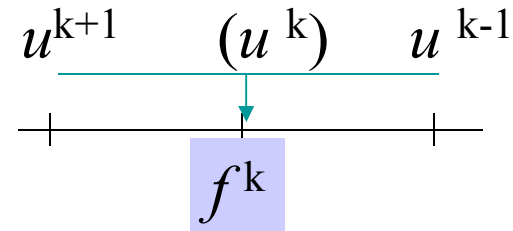


# Time marching schemes

$$\frac{\partial u}{\partial t} = f \quad \Rightarrow \quad \begin{cases} f \Rightarrow f^k & \text{(explicit scheme)} \\ f \Rightarrow f^{k+1} & \text{(implicit scheme)} \end{cases}$$

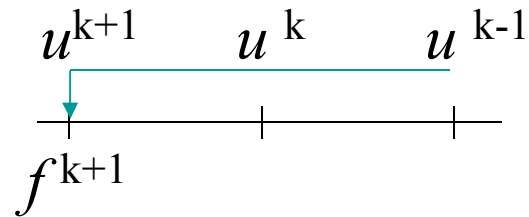
- (2<sup>nd</sup> order) leap-frog

$$\frac{u^{k+1} - u^{k-1}}{2\delta t} = f^k$$



- 2<sup>nd</sup> order backward scheme

$$\frac{3u^{k+1} - 4u^k + u^{k-1}}{2\delta t} = f^{k+1}$$



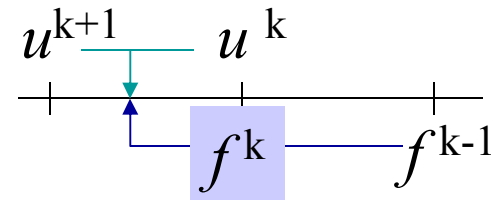
# Time marching schemes

$$\frac{\partial u}{\partial t} = f \quad \Rightarrow \quad \frac{u^{k+1} - u^k}{\delta t} = \bar{f}$$

• mid-point rule

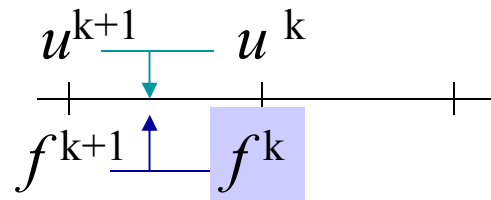
- 2<sup>nd</sup> order Adams-Bashforth

$$\frac{u^{k+1} - u^k}{\delta t} = \frac{1}{2} (3f^k - f^{k-1})$$



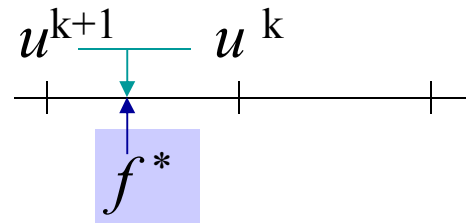
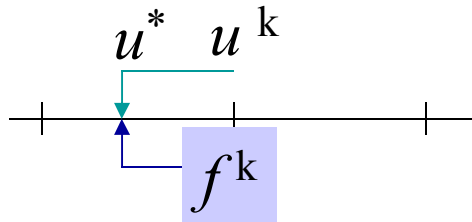
- (2<sup>nd</sup> order) Crank-Nicolson

$$\frac{u^{k+1} - u^k}{\delta t} = \frac{1}{2} (f^{k+1} + f^k)$$



- predictor (Euler) -corrector (Crank-Nicolson)

$$\frac{u^* - u^k}{\delta t} = f(u^k) \Rightarrow \frac{u^{k+1} - u^k}{\delta t} = \hat{f}(u^*)$$



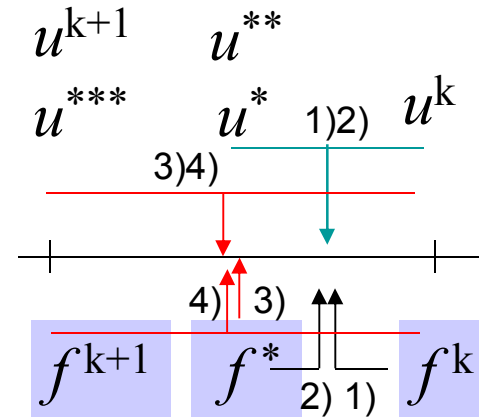
- 4<sup>th</sup> order Runge-Kutta

$$1) u^* = u^k + \frac{\delta t}{2} f(u^k)$$

$$2) u^{**} = u^k + \frac{\delta t}{2} f^*(u^*)$$

$$3) u^{***} = u^k + \delta t \cdot f^*(u^{**})$$

$$4) u^{k+1} = u^k + \frac{\delta t}{6} \{ f^k(u^k) + 2f^*(u^*) + 2f^*(u^{**}) + f^{k+1}(u^{***}) \}$$





# Computational Fluid Mechanics

## Part1 : Numerical Methods (3c)

1. Introduction
2. Numerical methods for fluid mechanics (1) ~ governing equations
3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
  - Fundamentals for discretizing methods
  - Schemes for convection and diffusion equation
  - **Analysis of accuracy and instability**
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

# Numerical accuracy

- Steady C-D problem

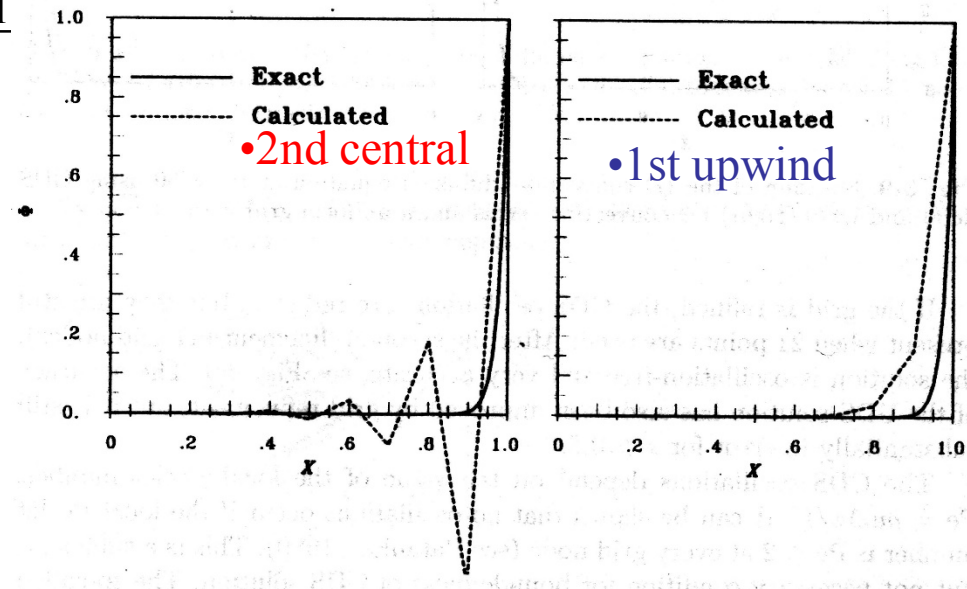
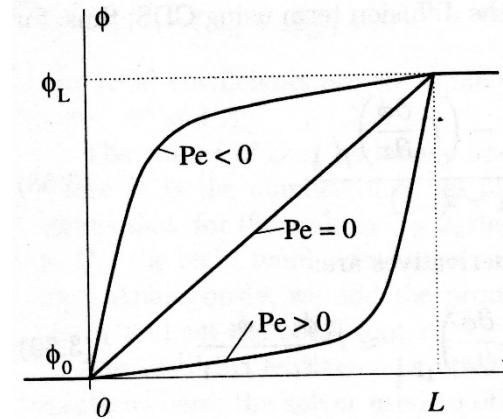
$$c \frac{\partial u}{\partial x} = \Gamma \frac{\partial^2 u}{\partial x^2} \quad Pe = \frac{c\delta x}{\Gamma}$$

- 2nd central

$$c \frac{u_{i+1} - u_{i-1}}{2\delta x} = \Gamma \frac{u_{i+1} - 2u_i + u_{i-1}}{\delta x^2}$$

- 1st upwind

$$c \frac{u_i - u_{i-1}}{\delta x} = \Gamma \frac{u_{i+1} - 2u_i + u_{i-1}}{\delta x^2}$$



# Numerical accuracy

- Comparison between 1<sup>st</sup> Upwind and 2<sup>nd</sup> central schemes

$$\frac{\partial u}{\partial x} = \frac{1}{\delta x} (u_i - u_{i-1}) + \left[ \frac{\delta x}{2} \frac{\partial^2 u}{\partial x^2} + O(\delta x^2) \right]$$

1st upwind

$$= \frac{1}{\delta x} (u_i - u_{i-1}) + \frac{1}{2\delta x} (u_{i+1} - 2u_i + u_{i-1}) + O(\delta x^2)$$

2<sup>nd</sup> central

$$\therefore \frac{\partial u}{\partial t} = (\text{1<sup>st</sup> upwind}) - \boxed{\left| u \right| \frac{\delta x}{2} \frac{\partial^2 u}{\partial x^2}}$$

=  $\Gamma_{\text{eff}}$

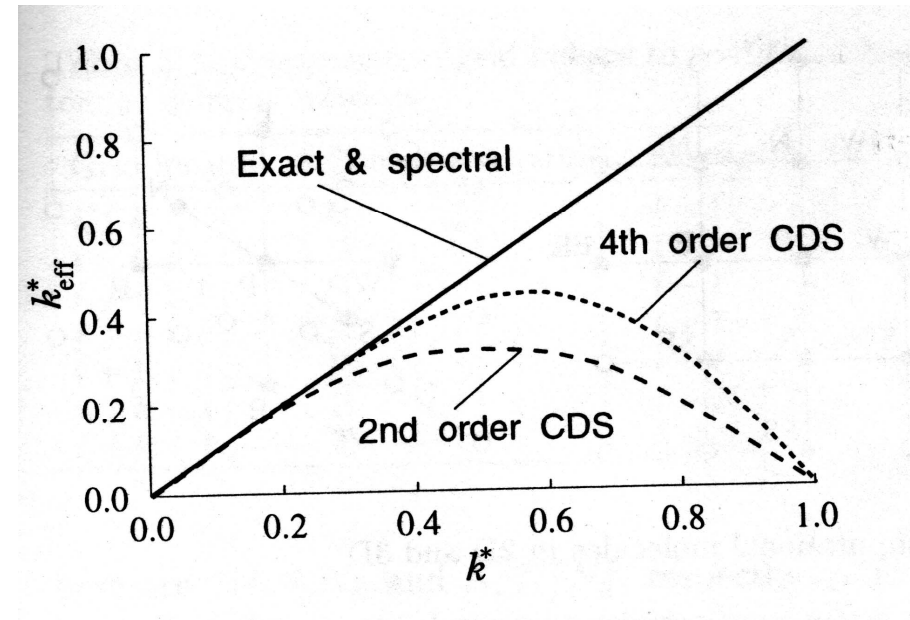
Upwind = Numerical diffusion

# Numerical accuracy

- Fourier expansion

$$u = \sum a_k e^{ikx}$$

$$\Rightarrow \frac{\partial u}{\partial x} = \sum a_k \frac{\partial e^{ikx}}{\partial x} = \sum a_k i k e^{ikx}$$



- effective wave number

$$\frac{\partial e^{ikx}}{\partial x} \approx \frac{e^{ik(x+\delta x)} - e^{ik(x-\delta x)}}{2\delta x} = i \frac{\sin(k\delta x)}{\delta x} e^{ikx}$$

$$\equiv k_{eff} \approx k - \frac{k^3 \delta x^2}{6}$$

# Numerical instability

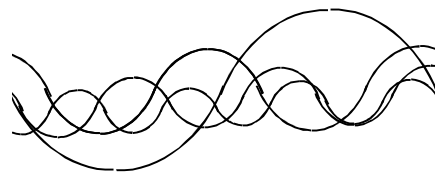
- von Neuman's condition

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} \quad (\text{i.c. } u_{(t_n)} = e^{ikx})$$

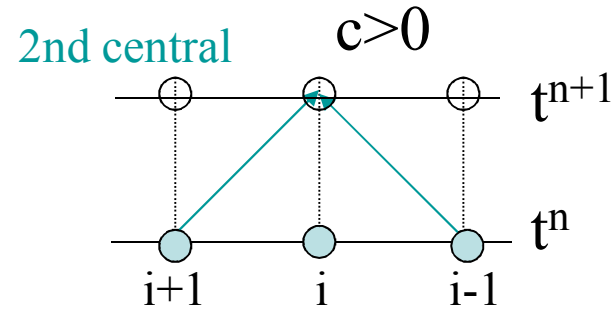
$$\frac{u_i^{n+1} - u_i^n}{\delta t} = -c \frac{u_{i+1}^n - u_{i-1}^n}{2\delta x}$$

$$u_i^{n+1} = \left\{ 1 - i \frac{c\delta t}{\delta x} \sin(k\delta x) \right\} u_i^n$$

$$|\dots| = \sqrt{1 + c^2 \lambda^2 \sin^2(k\delta x)}$$



$$u_{(t_n)} = e^{ikx}$$

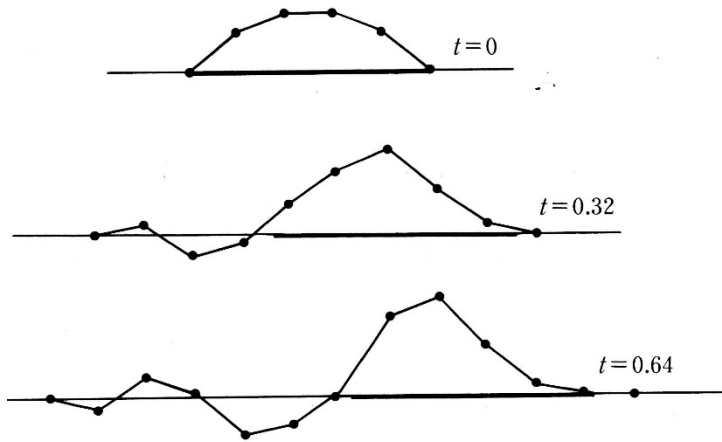


$$\max|\dots| = \sqrt{1 + c^2 \lambda^2} > 1$$

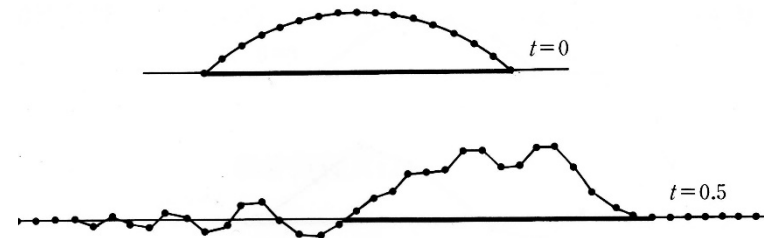
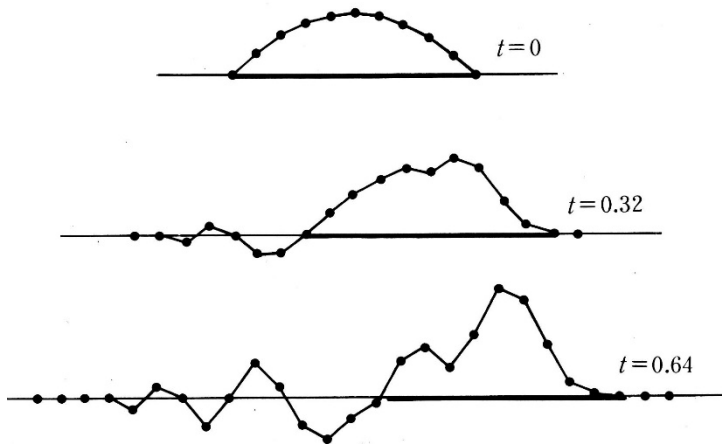
$$\left( \text{if } \frac{\delta t}{\delta x} = \lambda \text{ (const.)} \right)$$

$$\max|\dots| = \sqrt{1 + c^2 \rho \delta t} \leq 1 + \frac{c^2 \rho}{2} \delta t$$

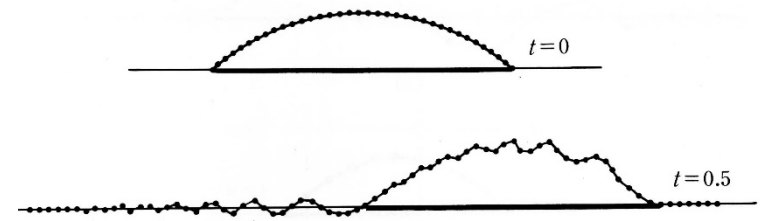
$$\left( \text{if } \frac{\delta t}{\delta x^2} = \rho \text{ (const.)} \right)$$



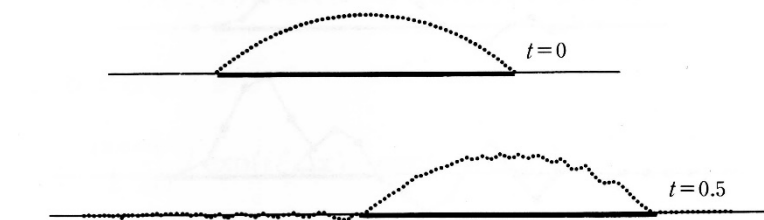
(a)



(a)



(b)



(c)

# Numerical instability

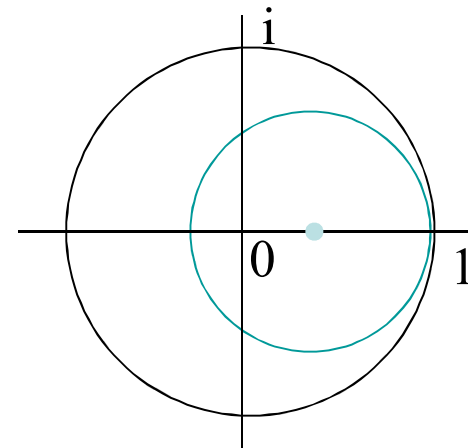
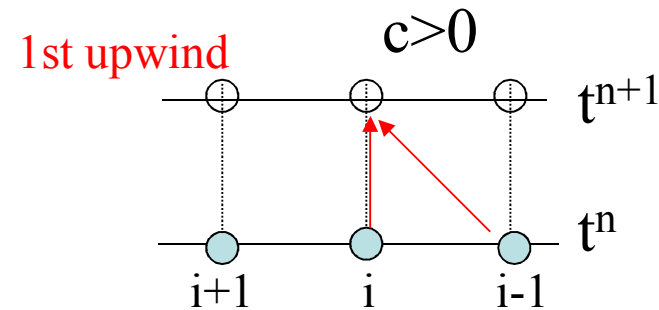
- von Neuman's condition

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} \quad (\text{i.c. } u(t_n) = e^{ikx})$$

$$\frac{u_i^{n+1} - u_i^n}{\delta t} = -c \frac{u_i^n - u_{i-1}^n}{\delta x}$$

$$u_i^{n+1} = \left\{ \left( 1 - \frac{c\delta t}{\delta x} \right) - \frac{c\delta t}{\delta x} e^{-ik\delta x} \right\} u^n$$

CFL condition  $c \frac{\delta t}{\delta x} \leq 1$



## Exercise

### Neumann's condition of diffusion step

$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \quad \Rightarrow \quad \phi = \phi_n \exp\left(inx - \frac{t}{\Gamma}\right)$$

- Euler (1<sup>st</sup> explicit)

$$\frac{u_i^{n+1} - u_i^n}{\delta t} = \Gamma \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\delta x^2} \quad \dots \text{stable ?}$$

- Crank-Ncolsin (2<sup>nd</sup> implicit)

$$\frac{u_i^{n+1} - u_i^n}{\delta t} = \Gamma \frac{\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right) + \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)}{2\delta x^2} \quad ?$$