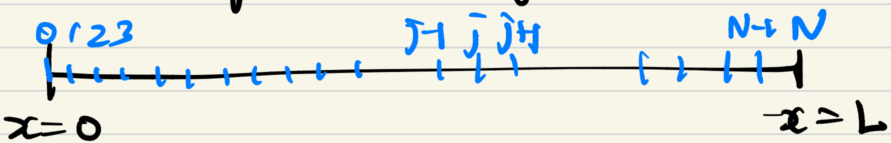
② Direct method

Approximate the derivatives in the diff'l eq. with finite difference. Also, incorporate the b.c.'s as required.

$$y''(x) + A(x)\, y'(x) + B(x)\, y(x) = C(x).$$



grids
$h = \Delta x$

CD2 : $$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} + A_j \frac{y_{j+1} - y_{j-1}}{2h} + B_j y_j = C_j, \quad j = 1, 2, \cdots, N-1$$

$$\rightarrow \underbrace{\left(\frac{1}{h^2} + \frac{A_j}{2h}\right)}_{\alpha_j} y_{j+1} + \underbrace{\left(B_j - \frac{2}{h^2}\right)}_{\beta_j} y_j + \underbrace{\left(\frac{1}{h^2} - \frac{A_j}{2h}\right)}_{\gamma_j} y_{j-1} = c_j$$

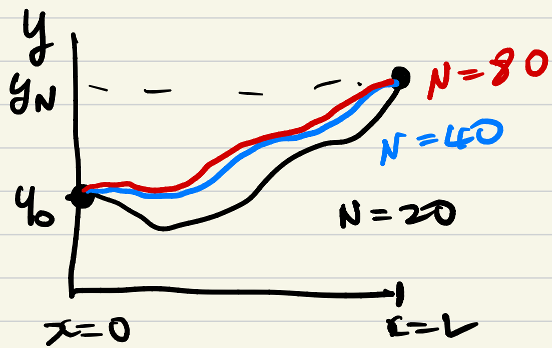
(a) $j=1$: $\alpha_1 y_2 + \beta_1 y_1 + \gamma_1 y_0 = c_1 \rightarrow \alpha_1 y_2 + \beta_1 y_1 = c_1 - \gamma_1 y_0$

(b) $j=N-1$: $\alpha_{N-1} y_N + \beta_{N-1} y_{N-1} + \gamma_{N-1} y_{N-2} = c_N$

$\rightarrow \beta_{N-1} y_{N-1} + \gamma_{N-1} y_{N-2} = c_N - \alpha_{N-1} y_N$

$$
\begin{pmatrix}
\beta_1 & \alpha_1 & & & 0 \\
\gamma_2 & \beta_2 & \alpha_2 & & \\
 & \ddots & \ddots & \ddots & \\
0 & & & \gamma_{N-1} & \beta_{N-1}
\end{pmatrix}
\begin{pmatrix}
y_1 \\ y_2 \\ \vdots \\ y_{N-2} \\ y_{N-1}
\end{pmatrix}
=
\begin{pmatrix}
c_1 - \gamma_1 y_0 \\ c_2 \\ \vdots \\ c_{N-2} \\ c_{N-1} - \alpha_{N-1} y_N
\end{pmatrix}
$$

TDMA



- $y'' + y^2 y' = 1$

CD2: $\dfrac{y_{j+1} - 2y_j + y_{j-1}}{h^2} + y_j^2 \dfrac{y_{j+1} - y_{j-1}}{2h} = 1$

nonlinear algebraic eq

↓

requires iterative approach.

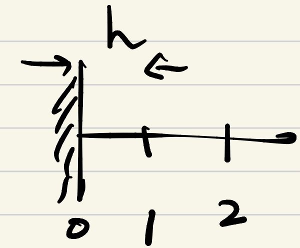
In some cases, shooting method may be better.

- Types of boundary conditions

Dirichlet b.c. : $y(0) = y_0, \; y(L) = y_L$

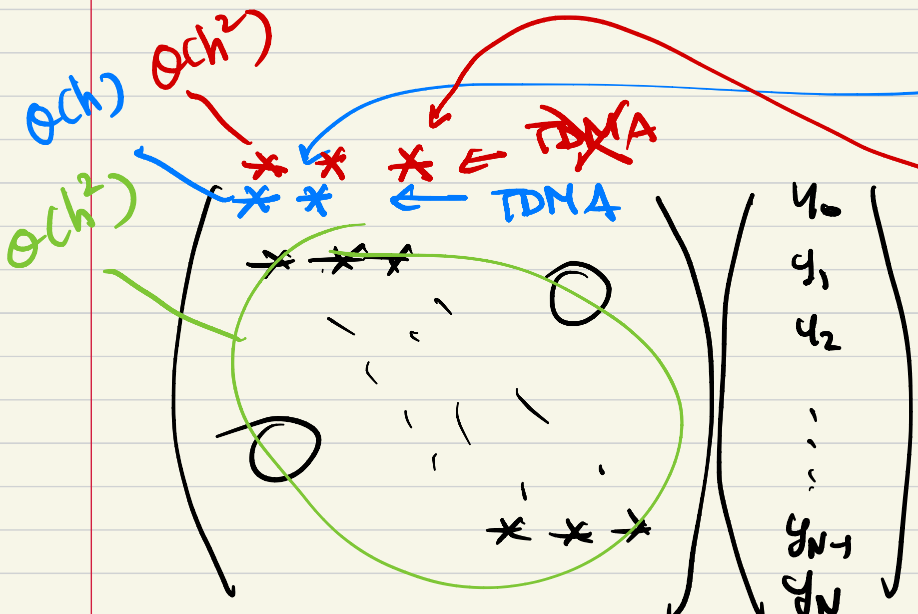
Neumann b.c. : $\frac{dy}{dx}(0) = 0$

mixed b.c. : $\beta y(0) + \alpha \frac{dy}{dx}(0) = g$



$$= \frac{y_1 - y_0}{h} + O(h)$$

$$= \frac{-3y_0 + 4y_1 - y_2}{2h} + O(h^2)$$



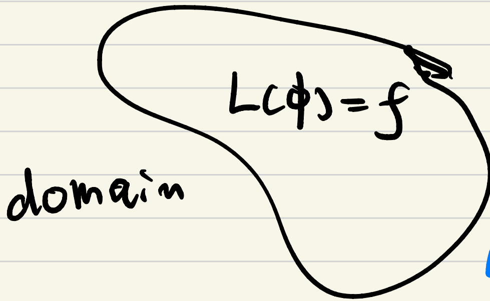
Difficulty near boundaries when higher-order FD is used at (or near) the boundary.

Ch. 5 Numerical Solution of Partial diff'l eq. (PDE)

> No class on Wed.
> physical video lecture instead

* Physical classification

① Equilibrium problems — steady state probs.



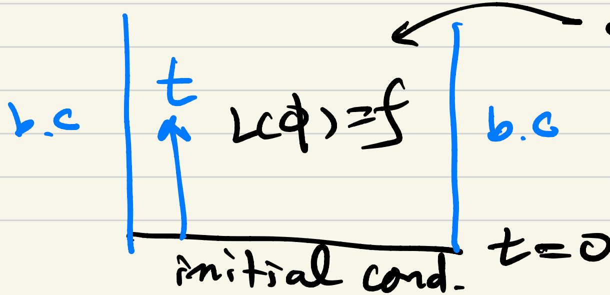
L: diff'l operator

← closed boundary : specify something about ϕ on the boundary.

Elliptic PDE

② Propagation problems — transient nature

initial value probs.



← open boundary

parabolic PDE

Hyperbolic PDE

* Mathematical classification

Quasi-linear 2nd-order PDE

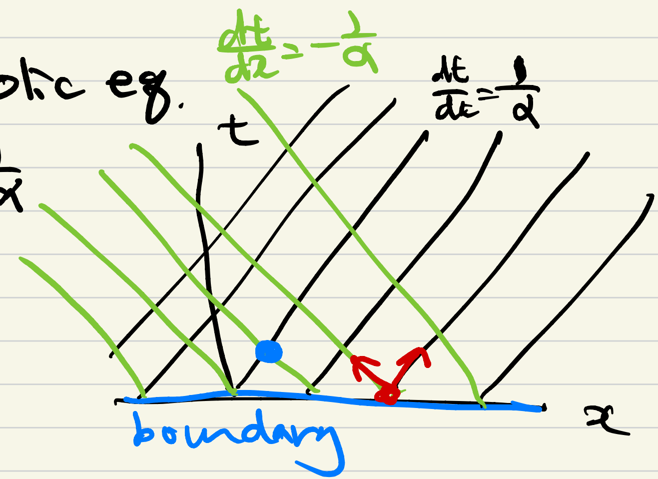
$$u_{xx} = \frac{\partial^2 u}{\partial x^2}$$

$$\boxed{a u_{xx} + b u_{xy} + c u_{yy} = f} \qquad a, b, c \sim f(x, y, u, u_x, u_y)$$

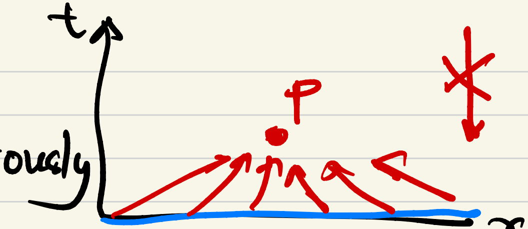
$$\begin{cases} \text{hyperbolic PDE if } b^2 - 4ac > 0 \rightarrow \text{two real characteristics} \\ \text{parabolic PDE if } b^2 - 4ac = 0 \rightarrow \text{one} \quad \text{"} \quad \text{"} \\ \text{elliptic PDE if } b^2 - 4ac < 0 \rightarrow \text{no} \quad \text{"} \quad \text{"} \end{cases}$$

ex) $\frac{\partial^2 u}{\partial t^2} - \alpha^2 \frac{\partial^2 u}{\partial x^2} = f \rightarrow$ hyperbolic eq.

two char. lines : $\frac{dt}{dx} = \pm \frac{1}{\alpha}$



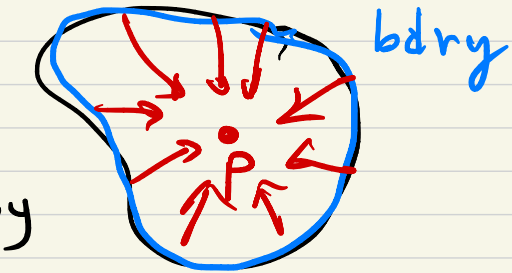
$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \rightarrow \text{parabolic eq.}$$



"P" knows what has happened previously along the entire x-axis.

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \rightarrow \text{elliptic eq.}$$

no char. line



At any P, the sol. is influenced by all other pts.

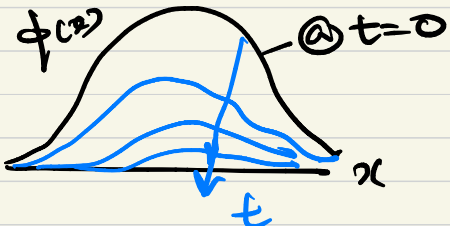
5.1 Semi-discretization (SD) : PDE $\longrightarrow$ system of ODEs

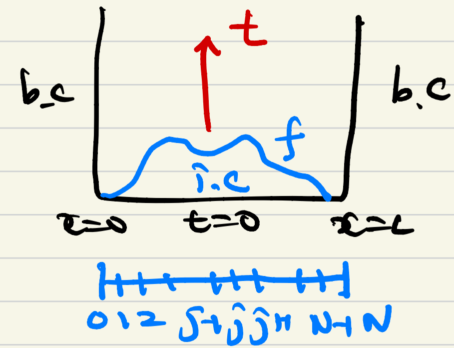
$$\boxed{\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}}$$ diffusion eq.

$\phi(0,t)=0$

$\phi(L,t)=0$

$\phi(x,0)=f$





CD2 : @ j, $\quad \dfrac{\partial \phi_j}{\partial t} = \alpha \dfrac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2}$, $\quad j = 1, 2, \cdots, N-1$

$\downarrow$

$$\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N-1} \end{pmatrix} \qquad \frac{\partial \phi}{\partial t} = A\phi \qquad A = \frac{\alpha}{\Delta x^2}\begin{pmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ 0 & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

$$\text{PDE} \xrightarrow{\text{SD}} \text{system of ODEs.}$$

$$A = \frac{\alpha}{\Delta x^2} B[1, -2, 1] \qquad (N-1)\times(N-1)$$

$$\left(\begin{aligned} A &= B[a, b, c] \\ \lambda_j &= b + 2\sqrt{ac}\cos\alpha_j \\ \alpha_j &= j\pi/(m+1) \\ j &= 1, 2, \cdots, m \end{aligned} \right)$$

$$\lambda_j = \frac{\alpha}{\Delta x^2}\left(-2 + 2\cos\frac{j\pi}{N}\right), \quad j = 1, 2, \cdots, N-1$$

$$\lambda_1 = \frac{\alpha}{\Delta x^2}\left(-2 + 2\cos\frac{\pi}{N}\right) = -\frac{\alpha}{\Delta x^2}\left(\frac{\pi}{N}\right)^2 + \cdots$$

$$\left(\text{for large } N,\ \cos\frac{\pi}{N} = 1 - \frac{1}{2!}\left(\frac{\pi}{N}\right)^2 + \cdots\right)$$

$$\lambda_{N-1} = \frac{\alpha}{\Delta x^2}\left(-2 + 2\cos\frac{(N-1)\pi}{N}\right) \simeq -\frac{4\alpha}{\Delta x^2}$$

$$\left|\frac{\lambda_{N-1}}{\lambda_1}\right| \simeq \frac{+\frac{4\alpha}{\Delta x^2}}{\frac{\alpha}{\Delta x^2}\left(\frac{\pi}{N}\right)^2} = 4\frac{N^2}{\pi^2}$$

: large for large N

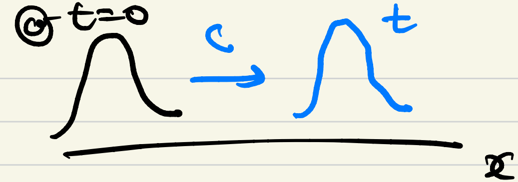
→ system is stiff.

eigenvalues are real & negative $\left(\frac{dy}{dt} = \lambda y\right)$

→ sol. decays in time

• $\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$: convection eq.

c: convection velocity



SD : CD2 → $\frac{\partial u_j}{\partial t} + c\,\frac{u_{j+1} - u_{j-1}}{2\Delta x} = 0$ $j = 1, 2, \cdots, N-1$

$$u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{pmatrix} \rightarrow \frac{du}{dt} = -\frac{c}{2\Delta x} B[\underset{j-1}{\underset{\uparrow}{-1}}, \underset{j}{\underset{\uparrow}{0}}, \underset{j+1}{\underset{\uparrow}{1}}]u$$

$$\lambda_j = -\frac{c}{2\Delta x} \cdot 2i\cos\frac{j\pi}{N} = -i\,\frac{c}{\Delta x}\cos\frac{j\pi}{N}$$

purely imaginary

↓

wave-like behavior

- Matrix stability analysis

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \xrightarrow[\text{CD2}]{\text{SD}} \frac{d\phi}{dt} = \frac{\alpha}{\Delta x^2} B[1,-2,1]\phi$$

$$\text{EE}: \quad \frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{\alpha}{\Delta x^2} B[1,-2,1]\phi^n$$

$$\rightarrow \phi^{n+1} = \left(I + \Delta t \frac{\alpha}{\Delta x^2} B\right)\phi^n \rightarrow \phi^n = \left(I + \Delta t \frac{\alpha}{\Delta x^2} B\right)^n \phi^0$$

For stability, $\left|1 + \Delta t \frac{\alpha}{\Delta x^2}\lambda_j\right| \le 1$ $\quad \left(\lambda_j = -2 + 2\cos\frac{j\pi}{N}\right)$

real & negative

$$\rightarrow -1 \le 1 + \Delta t \frac{\alpha}{\Delta x^2}\lambda_j \le 1$$

$$\rightarrow \Delta t \le \frac{2}{\frac{\alpha}{\Delta x^2}|\lambda_j|}$$

worst case $|\lambda_{max}| = 4$

$$\rightarrow \boxed{\Delta t \le \frac{\Delta x^2}{2\alpha}} \qquad \Delta t_{max} = \frac{\Delta x^2}{2\alpha}$$

very restrictive

more accuracy in x

$\Delta x \downarrow$ (or $N\uparrow$) $\rightarrow \Delta t \propto \Delta x^2$

$N \rightarrow 2N \quad \Delta t \rightarrow \frac{1}{4}\Delta t$

total CPU time $\rightarrow$ 8 times!

① Von Neumann stability analysis

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \xrightarrow[CD2]{SD} \frac{\partial \phi_j}{\partial t} = \alpha \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2}$$

"full" discretization (using EE)

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \alpha \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}, \quad j = 1, 2, \cdots, N-1$$

Assume sol. of the form $\boxed{\phi_j^n = \sigma^n e^{ikx_j}}$ ← assume spatial periodicity

$$\rightarrow \frac{\sigma^{n+1} e^{ikx_j} - \sigma^n e^{ikx_j}}{\Delta t} = \alpha \frac{\sigma^n e^{ikx_{j+1}} - 2\sigma^n e^{ikx_j} + \sigma^n e^{ikx_{j-1}}}{\Delta x^2}$$

$e^{ikx_{j+1}} = e^{ik(x_j + \Delta x_j)}$

$e^{ikx_{j-1}} = e^{ik(x_j - \Delta x_j)}$

$$\rightarrow \sigma = 1 + \frac{\alpha \Delta t}{\Delta x^2}(-2 + 2\cos k\Delta x)$$ real & negative

for stability, $|\sigma| \leq 1$

$$\rightarrow -1 \leq 1 + \frac{\alpha \Delta t}{\Delta x^2}(-2 + 2\cos k\Delta x) \leq 1$$

$$\rightarrow \Delta t \le \frac{2}{\frac{\alpha}{\Delta x^2}(2-2\cos k\Delta x)} = \frac{\Delta x^2}{\alpha(1-\cos k\Delta x)}$$ worst case @ $\cos k\Delta x = -1$

$$\rightarrow \boxed{\Delta t \le \frac{\Delta x^2}{2\alpha}}$$ same as that by matrix stability analysis

* Von Neumann stability analysis assumes periodic boundary condition (or periodicity).
In many cases, numerical stability comes from full discretization of PDE and NOT from the b.c.'s.

⑥ Modified wavenumber analysis

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \qquad \text{Assume } \phi(x,t) = \psi(t)\, e^{ikx}$$

$$\rightarrow \frac{d\psi}{dt} \cancel{e^{ikx}} = \alpha(-k^2)\psi \cancel{e^{ikx}}$$

$$\rightarrow \boxed{\frac{d\psi}{dt} = -\alpha k^2 \psi} \qquad \frac{dy}{dt} = \lambda y$$

$\downarrow$ SD (CD2)

$$\frac{\partial \phi_j}{\partial t} = \alpha \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2}$$

$$\boxed{\text{Assume } \phi_j = \psi(t)\, e^{ikx_j}}$$

$$\rightarrow \frac{d\psi}{dt} \cancel{e^{ikx_j}} = \alpha \frac{1}{\Delta x^2}\left(\psi e^{ikx_{j+1}} - 2\psi e^{ikx_j} + \psi e^{ikx_{j-1}}\right)$$

$$= \frac{\alpha}{\Delta x^2}(-2 + 2\cos k\Delta x)\, \psi \cancel{e^{ikx_j}}$$

$$\rightarrow \boxed{\frac{d\psi}{dt} = -\alpha \underbrace{\boxed{\frac{2}{\Delta x^2}(1 - \cos k\Delta x)}}_{= k'^2} \psi}$$

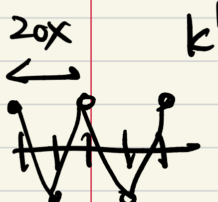
k' : modified wavenumber

$$\rightarrow (k'\Delta x)^2 = 2(1-\cos k\Delta x) = 2\cdot 2\sin^2\frac{k\Delta x}{2}$$

$$\rightarrow k'\Delta x = 2\sin\frac{k\Delta x}{2} \rightarrow \boxed{k' = 2\,\frac{\sin k\Delta x/2}{\Delta x}}\quad \text{CD2}$$

$$\rightarrow \boxed{\frac{d\psi}{dt} = -\alpha k'^2\psi} \text{ — } (*)$$

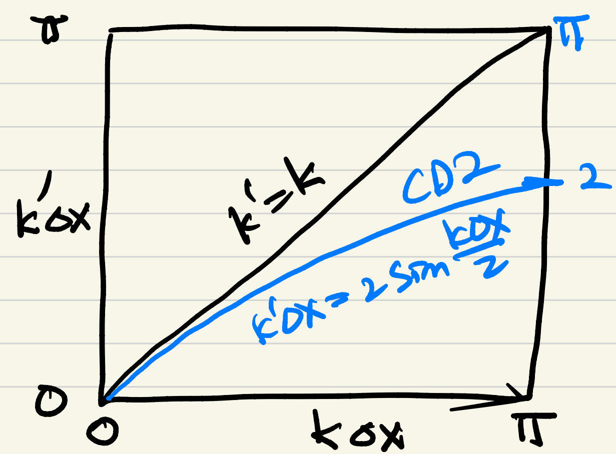
Application of any other FD schemes instead of CD2 used here would have also led to the same form as (*) but with different modified wavenumbers.



$$k'\Delta x = 2\sin\frac{k\Delta x}{2} \quad (\text{CD2})$$

$$K\cdot 2\Delta x = 2\pi$$

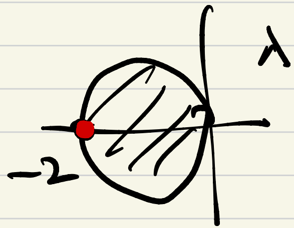
$$K\Delta x = \pi$$



not bad!

$$\frac{d\psi}{dt} = -\alpha k'^2 \psi = \lambda \psi \qquad \lambda = -\alpha k'^2$$ real & negative

EE



$|\lambda_R \Delta t| \le 2$ CD2

$$\rightarrow \Delta t \le \frac{2}{|\lambda_R|} = \frac{2}{|\alpha k'^2|} = \frac{2}{\alpha \frac{2}{\Delta x^2}(1-\cos k\Delta x)}$$

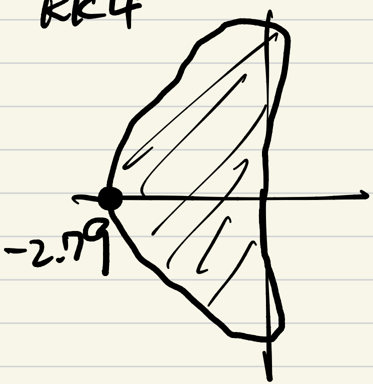
worst case @ $\cos k\Delta x = -1$

$$\rightarrow \boxed{\Delta t \le \frac{\Delta x^2}{2\alpha}}$$

same as those by matrix stability analysis

and von Neumann " "

RK4



$|\lambda_R \Delta t| \le 2.79$

$$\rightarrow \Delta t \le \frac{2.79\,\Delta x^2}{4\alpha}$$

Modified wavenumber analysis

① calculate the modified wavenumber k' for spatial derivative.

② use results from ODE with λ replaced with the worst case for k'.

- $\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$ convection eq.

$$u(x,t) = \psi(t) e^{ikx} \rightarrow \frac{d\psi}{dt}\cancel{e^{ikx}} + cik\psi\cancel{e^{ikx}} = 0$$

$$\rightarrow \boxed{\frac{d\psi}{dt} = -ikc\psi}$$

SD (CD2): $\frac{\partial u_j}{\partial t} + c\frac{u_{j+1} - u_{j-1}}{2\Delta x} = 0$

Assume $u_j = \psi(t) e^{ikx_j} \rightarrow \frac{d\psi}{dt} e^{ikx_j} + c\frac{\psi e^{ikx_{j+1}} - \psi e^{ikx_{j-1}}}{2\Delta x} = 0$

$$\rightarrow \boxed{\frac{d\psi}{dt} = -i\frac{\sin k\Delta x}{\Delta x}c\psi}$$

CD2

k' : modified wavenumber

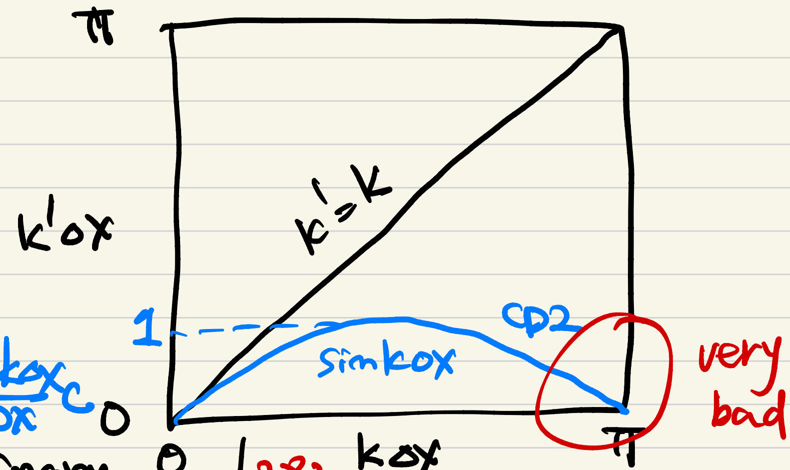
$\rightarrow$ purely imaginary λ

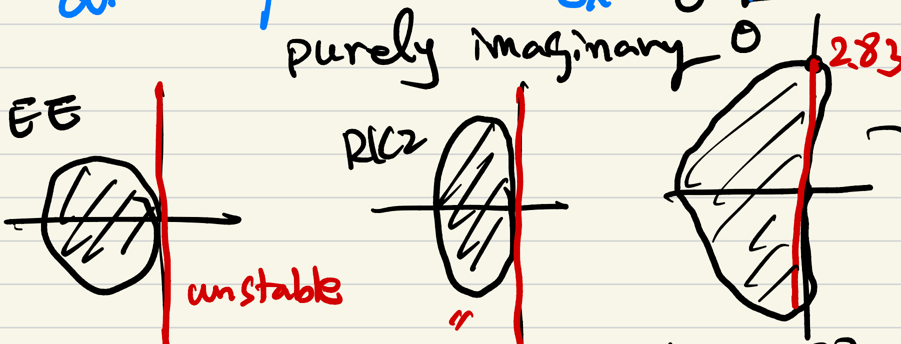
$k'\Delta x = \sin k\Delta x \leftarrow$ CD2

$k \cdot 2\Delta x = 2\pi$

$k\Delta x = \pi$

$\Rightarrow \frac{d\psi}{dt} = \omega\psi \quad \omega = -i\frac{\sin k\Delta x}{\Delta x}c$





$\to |\lambda_I \Delta t| \le 2.83$

$\left|\frac{\sin k\Delta x}{\Delta x}\cdot c\cdot\Delta t\right| \le 2.83$

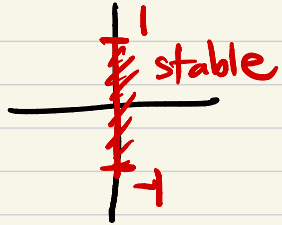
worst case @ $\sin k\Delta x = \pm 1$

$\to \frac{c\Delta t}{\Delta x} \le \frac{2.83}{|\sin k\Delta x|} \to \boxed{\frac{c\Delta t}{\Delta x} \le 2.83}$ RK4

$\Delta t \sim \Delta x$ cf. $\Delta t \sim \Delta x^2$ diff.eq. $\to$ CPU 8 times

$\Delta x \to \Delta x/2$, $\Delta t \to \Delta t/2 \Rightarrow$ CPU 4 times $\Leftarrow$ not bad.

leapfrog method



$$|\omega \Delta t| \le 1$$

$$\Delta t \le \frac{1}{|\omega|} = \frac{\Delta x}{c\,|\sin k\Delta x|}$$

worst case @ $|\sin k\Delta x| = 1$

$$\rightarrow \Delta t \le \frac{\Delta x}{c}$$

$$\boxed{\frac{c\Delta t}{\Delta x} \le 1}$$

leapfrog method

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

$$[c] \sim \frac{x}{t}$$

$\boxed{\dfrac{c\Delta t}{\Delta x}}$: non-dimensional variable

CFL (Courant, Friedrich & Lewy) number

RK4 : CFL ≤ 2.83

Leapfrog : CFL ≤ 1

$$CFL = \left|\frac{u\Delta t}{\Delta x}\right| = \left|\frac{u(x,t)\,\Delta t}{\Delta x}\right| \le 2.83 \text{ from RK4}$$

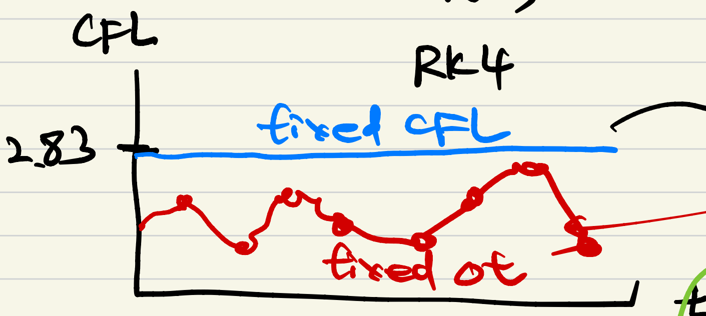
$$\rightarrow \Delta t(t) \le \frac{2.83\,\Delta x(x)}{|u(x,t)|}$$

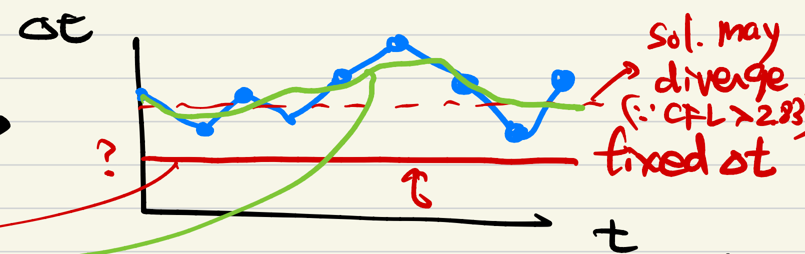
non-uniform grids

$\Delta x \sim f(x)$

worst case occurs when $\frac{\Delta x}{|u|}$ is minimum.

$$\Delta t_{max}^{(t)} = 2.83 \left.\frac{\Delta x}{|u|}\right|_{min}$$





fixed Δt may be required for example for FT in time.

$$\Delta t = \alpha\,\Delta t_{new} + (1-\alpha)\,\Delta t_{old} \quad (0 < \alpha \le 1)$$

for smooth change of Δt in time.