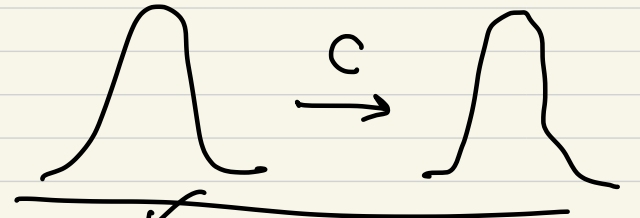


Modified wavenumber analysis

- ① calculate the modified wavenumber k' for spatial derivative.
- ② use results from ODE w/ λ replaced with the worst case for k' .

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



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

$$\rightarrow \frac{d\psi}{dt} = -i k c \psi$$

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

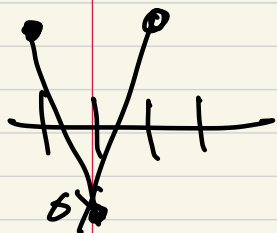
Assume $u_j = \psi(t) e^{ikx_j}$

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

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

k' : modified wavenumber
purely imaginary

$$K'_{OX} = \sin k_{OX} \quad \checkmark$$



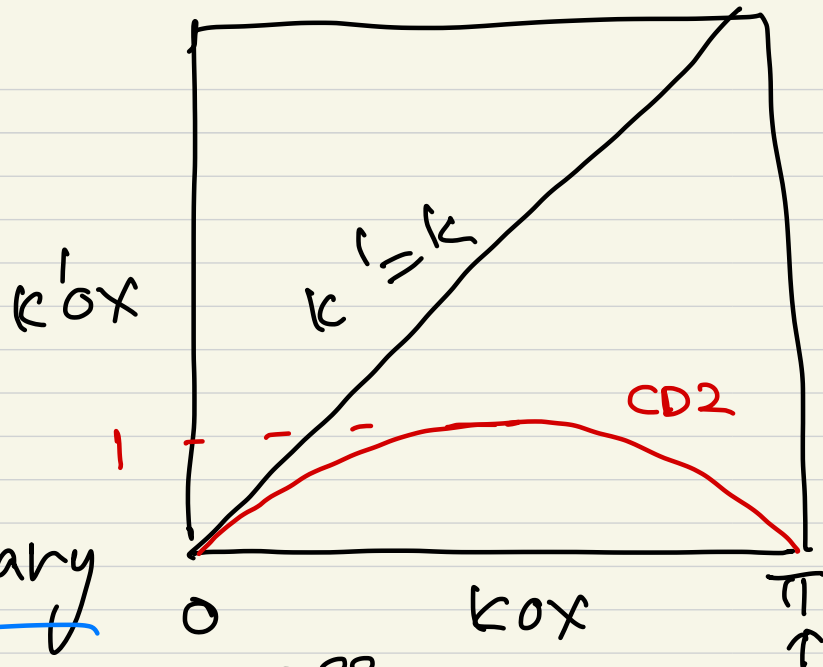
$$K(2\delta x) = 2\pi$$

$$K_{OX} = \pi$$

$$\rightarrow \frac{d\psi}{dt} = \omega \psi$$

$$\omega = -i \frac{\sin k_{OX}}{\delta x} c$$

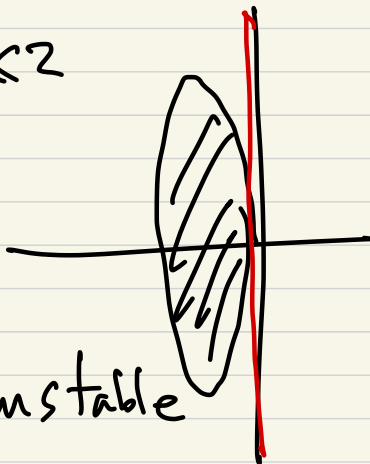
purely imaginary



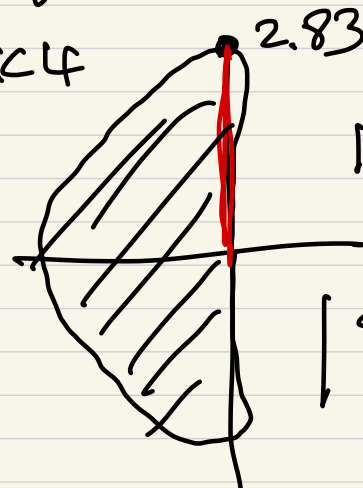
EE



RK2



RK4



$$|\lambda_{\text{inst}}| \leq 2.83$$

$$\left| \frac{\sin k_{OX}}{\delta x} c \delta t \right| \leq 2.83$$

worst case: $|\sin k_{OX}| = 1$

$$\rightarrow \frac{c \delta t}{\delta x} \lesssim \frac{2.83}{|\sin k_{OX}|}$$

$$(c > 0)$$

$$\rightarrow \frac{c \delta t}{\delta x} \leq 2.83$$

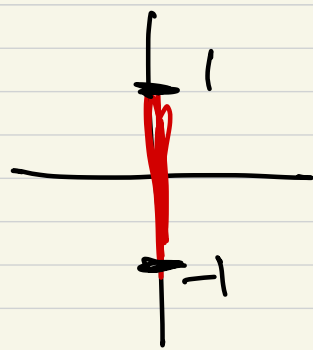
RK4

$$\delta t \sim \delta x$$

$\delta x \rightarrow \delta x/2$ CPU
 $\delta t \rightarrow \delta t/2$ times

$$\delta t \leq \frac{2.83 \delta x}{c}$$

leapfrog method



$$|\omega \Delta t| \leq 1$$

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

$$\text{worst case: } |\sin k \Delta x| = 1$$

$$\Delta t \leq \frac{\Delta x}{c}$$

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

leapfrog.

↑
much better
than diff.
eq.

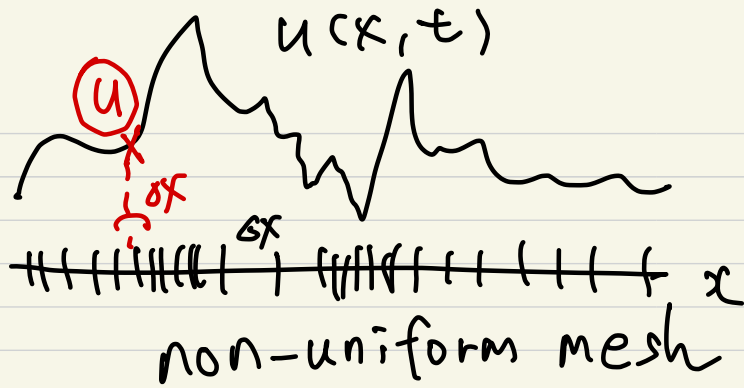
$\frac{c \Delta t}{\Delta x}$: non-dimensional variable

CFL (Courant, Friedrich & Levy) number

$$\left(\frac{\partial u}{\partial t} + \underbrace{c}_{\text{velocity}} \frac{\partial u}{\partial x} = 0 \right)$$

RK4 : CFL ≤ 2.83

Leapfrog : CFL ≤ 1




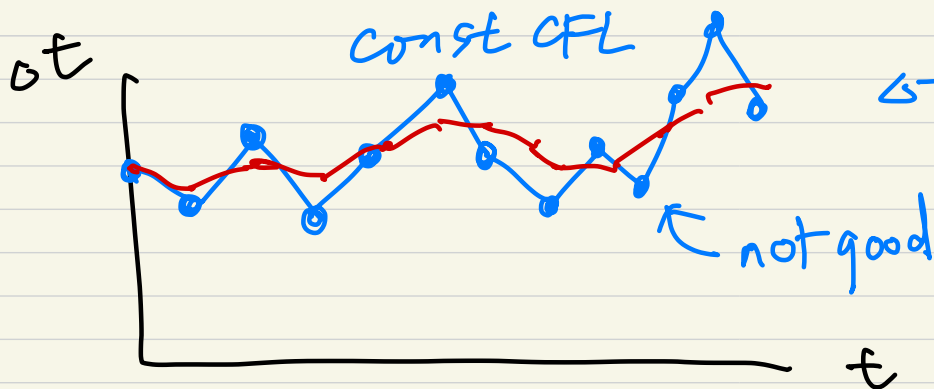
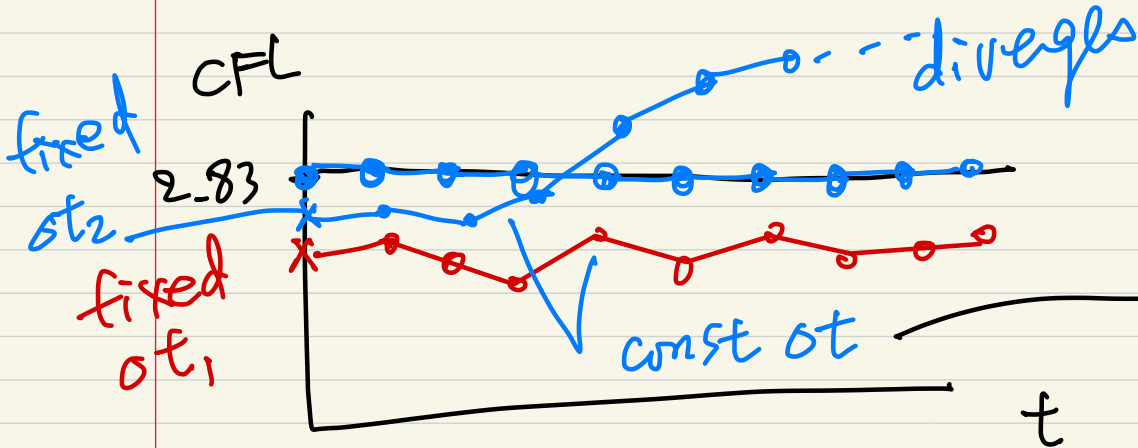
$$CFL = \left| \frac{u \Delta t}{\Delta x} \right| = \left| \frac{u(x, t) \Delta t}{\Delta x(x)} \right| \leq 2.83 \text{ for RK4}$$

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

worst case : $\Delta x/|u|$ minimum

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

is required for FFT. 



$$\Delta t = \alpha \Delta t_{\text{new}} + (1 - \alpha) \Delta t_{\text{old}} \quad (0 \leq \alpha \leq 1)$$

5.4 Implicit time advancement

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \xrightarrow[\text{CD2}]{\text{EE}} \Delta t \leq \frac{\Delta x^2}{2\alpha} \quad \text{too restrictive}$$

↓
implicit method

- Crank-Nicolson method (CN) — trapezoidal method
very popular

$$\text{C-N: } \frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{\alpha}{2} \left[\frac{\partial^2 \phi^{n+1}}{\partial x^2} + \frac{\partial^2 \phi^n}{\partial x^2} \right] + \mathcal{O}(\Delta t^2) \quad \left(\begin{array}{l} y' = \lambda y \\ \frac{y^{n+1} - y^n}{\Delta t} = \frac{1}{2} \lambda (y^{n+1} + y^n) \end{array} \right)$$

$$\text{CD2: } \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \frac{\alpha}{2} \left[\frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\Delta x^2} + \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} \right] + \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2)$$

$$(\beta \equiv \alpha \Delta t / \Delta x^2)$$

$$\rightarrow -\beta \phi_{j+1}^{n+1} + (1+2\beta) \phi_j^{n+1} - \beta \phi_{j-1}^{n+1} = \beta \phi_{j+1}^n + (1-2\beta) \phi_j^n + \beta \phi_{j-1}^n$$

$j=1, 2, \dots, N-1$

tri-diagonal system of eqs. 😊

Solve this sys. of eqs. to get ϕ_j^{n+1} w/ $\mathcal{O}(N)$ operations,

$$\left(y' = \lambda y \xrightarrow{TR} y_n = \sigma^n y_0, \quad \sigma = \frac{1 + \lambda \Delta t/2}{1 - \lambda \Delta t/2} \right)$$

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \xrightarrow{CD2} \frac{d\psi}{dt} = -\alpha |k|^2 \psi \quad k^2 = \frac{2(1 - \cos k\Delta x)}{\Delta x^2}$$

$$\text{Then, } \sigma = \frac{1 - \alpha \frac{\Delta t}{\Delta x^2} (1 - \cos k\Delta x)}{1 + \alpha \frac{\Delta t}{\Delta x^2} (1 - \cos k\Delta x)} \Rightarrow |\sigma| \leq 1$$

unconditionally stable

$\Delta x \rightarrow \frac{\Delta x}{2}$, $\Delta t \Rightarrow \Delta t$ CPU time twice

For large Δt , $\sigma \rightarrow -1$. $\phi^n = \sigma^n \phi^0 = (-1)^n \phi^0$



unphysical but never diverges.

① reduce Δt dangerous

② apply different method like IE.

5.5 Accuracy via modified equation

Since the numerical sol. is an approx. of the exact sol., it does not satisfy the continuous PDE at hand, but satisfies a modified PDE.

Let $\tilde{\phi}$ be the exact sol. and ϕ be the numerical sol. obtained from EE and CP2.

$$\frac{\partial^2 \tilde{\phi}}{\partial t} = \alpha \frac{\partial^2 \tilde{\phi}}{\partial x^2}$$

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

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

Taylor series expansion

$$\phi_j^{n+1} = \phi_j^n + \Delta t \frac{\partial \phi_j^n}{\partial t} + \frac{1}{2} \Delta t^2 \frac{\partial^2 \phi_j^n}{\partial t^2} + \dots = \frac{\partial \phi_j^n}{\partial t} + \frac{1}{2} \Delta t \frac{\partial^2 \phi_j^n}{\partial t^2} + \dots$$

Similarly,
$$\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} = \frac{\partial^2 \phi}{\partial x^2} \Big|_j + \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} \Big|_j + \dots$$

$$\Rightarrow L(\phi_j^n) = \frac{\partial \phi_j^n}{\partial t} + \frac{1}{2} \Delta t \frac{\partial^2 \phi_j^n}{\partial t^2} - \alpha \frac{\partial^2 \phi_j^n}{\partial x^2} - \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi_j^n}{\partial x^4} + \dots$$

remove n and j .

$$L(\phi) = \frac{\partial \phi}{\partial t} + \frac{1}{2} \Delta t \frac{\partial^2 \phi}{\partial t^2} - \alpha \frac{\partial^2 \phi}{\partial x^2} - \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} + \dots = 0$$

Thus, the numerical sol. actually satisfies the following modified PDE.

$$\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} - \frac{1}{2} \Delta t \frac{\partial^2 \phi}{\partial t^2} + \dots$$
 EE
+CD2

As $\Delta t \Delta x \rightarrow 0$,
$$\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0$$

error $\epsilon = L(\phi^n) = -\alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi^n}{\partial x^4} + \frac{1}{2} \Delta t \frac{\partial^2 \phi^n}{\partial t^2} + \dots$ $\alpha \frac{\partial^4 \phi^n}{\partial x^4}$

$$\frac{\partial}{\partial t} \left(\frac{\partial \phi^n}{\partial t} \right) = \frac{\partial}{\partial t} \left(\alpha \frac{\partial^2 \phi^n}{\partial x^2} \right) = \frac{\partial^2}{\partial x^2} \left(\alpha \frac{\partial \phi^n}{\partial t} \right)$$

$$\rightarrow \epsilon = \left(-\alpha \frac{\Delta x^2}{12} + \alpha^2 \frac{\Delta t}{2} \right) \frac{\partial^2 \phi}{\partial x^2} + \dots$$

$= 0$ by choosing $\Delta t = \Delta x^2 / 6\alpha$

Then, we can increase accuracy.

Stability limit for EE + CP2: $\Delta t \leq \frac{\Delta x^2}{2\alpha}$

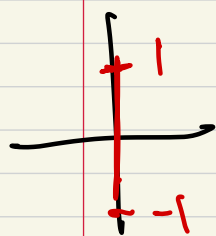
but $\Delta t = \Delta x^2 / 6\alpha \rightarrow$ too restrictive (3 times!)

- DuFort-Frankel method: an inconsistent numerical method.

- Dufort - Frankel method: an inconsistent numerical method

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

Leapfrog method + CD2



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

is unconditionally unstable for real & negative λ .

$$\phi_j^n = \frac{1}{2} (\phi_j^{n+1} + \phi_j^{n-1}) + O(\Delta t^2)$$

$$\rightarrow \phi_j^{n+1} - \phi_j^{n-1} = \frac{2\Delta t}{\Delta x^2} (\phi_{j+1}^n - \phi_j^n - \phi_j^{n-1} + \phi_{j-1}^n)$$

$$\rightarrow (1 + 2\beta) \phi_j^{n+1} = (1 - 2\beta) \phi_j^{n-1} + 2\beta \phi_{j+1}^n + 2\beta \phi_{j-1}^n$$

Dufort - Frankel method.

stability analysis ($\phi_j^n = \sigma^n e^{ikx_j}$) \rightarrow unconditionally stable.

no matrix inversion is required.
 2nd-order order accurate \Rightarrow too good to be true!

What is the modified PDE for DuFort-Frankel method?

$$\phi_j^{n+1} = \phi_j^n + \Delta t \frac{\partial \phi^n}{\partial t_j} + \dots$$

$$\phi_{j+1}^n = \phi_j^n + \Delta x \frac{\partial \phi^n}{\partial x} \Big|_j + \dots$$

$$\Rightarrow \frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = -\frac{\Delta t^2}{6} \frac{\partial^3 \phi}{\partial t^3} + \alpha \frac{\Delta x^2}{12} \frac{\partial^3 \phi}{\partial x^3} - \alpha \frac{\Delta t^2}{\Delta x^2} \frac{\partial^2 \phi}{\partial t^2} - \alpha \frac{\Delta t^4}{12 \Delta x^2} \frac{\partial^4 \phi}{\partial x^4} + \dots$$

For a given Δt , the error actually increases when we refine Δx .

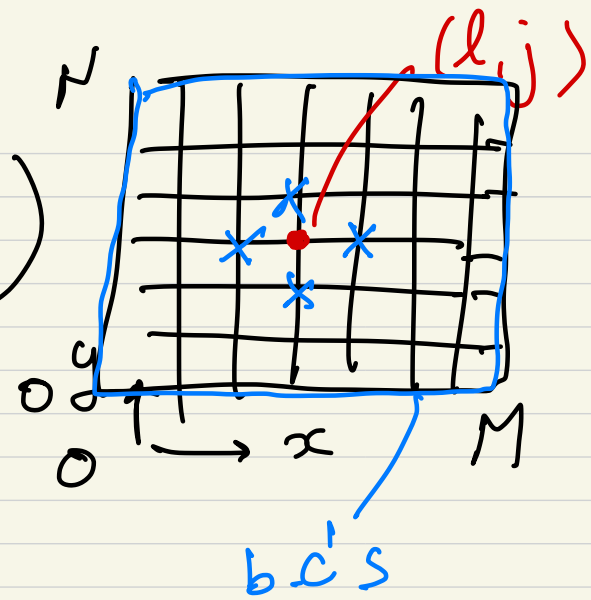
Thus, one cannot increase the accuracy of numerical sol. by arbitrarily letting $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$.

The third term on RHS approaches zero only if $\Delta t \rightarrow 0$ faster than $\Delta x \rightarrow 0$.

This is an example of inconsistent numerical method.

5.7 Higher dimensions

2D diffusion eq. $\frac{\partial \phi}{\partial t} = \alpha \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right)$



CD2: $\frac{\partial \phi_{l,j}}{\partial t} = \alpha \left(\frac{\phi_{l+1,j} - 2\phi_{l,j} + \phi_{l-1,j}}{\Delta x^2} + \frac{\phi_{l,j+1} - 2\phi_{l,j} + \phi_{l,j-1}}{\Delta y^2} \right)$

EE: $\frac{\phi_{l,j}^{n+1} - \phi_{l,j}^n}{\Delta t} = \alpha \left(\frac{\phi_{l+1,j}^n - 2\phi_{l,j}^n + \phi_{l-1,j}^n}{\Delta x^2} + \frac{\phi_{l,j+1}^n - 2\phi_{l,j}^n + \phi_{l,j-1}^n}{\Delta y^2} \right)$

$l = 1, 2, \dots, M-1 ; j = 1, 2, \dots, N-1$

start from initial condition $\phi_{l,j}^0$

and then march in time using b.c.'s.

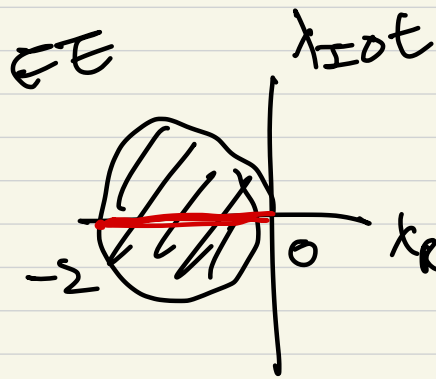
Δt ?

Stability CD2: modified wavenumber k'_x & k'_y

$$\phi(x, y, t) = \psi(t) e^{i k_1 x} e^{i k_2 y}$$

$$\rightarrow \frac{d\psi}{dt} = \alpha (-k_1'^2 - k_2'^2) \psi \quad \text{where } k_1'^2 = \frac{2(1 - \cos k_1 \Delta x)}{\Delta x^2}$$

$$k_2'^2 = \frac{2(1 - \cos k_2 \Delta y)}{\Delta y^2}$$



λ : real & negative

$$|\lambda \Delta t| \leq 2 \quad \text{for stability}$$

$$\Delta t \leq \frac{2}{|\lambda|} = \frac{2}{\alpha \left[\frac{2(1 - \cos k_1 \Delta x)}{\Delta x^2} + \frac{2(1 - \cos k_2 \Delta y)}{\Delta y^2} \right]}$$

worst case: $\cos k_1 \Delta x = \cos k_2 \Delta y = -1$

$$\Rightarrow \Delta t \leq \frac{1}{2\alpha \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)} \quad \text{EE + CD2 for 2D diff. eq.}$$

if $\Delta x = \Delta y$, $\Delta t \leq \frac{\Delta x^2}{4\alpha}$ (2D) $\Delta t \leq \frac{\Delta x^2}{2\alpha}$ (1D)

$\Delta t \leq \frac{\Delta x^2}{6\alpha}$ (3D) \Rightarrow too restrictive \Rightarrow use implicit methods!

5.8

Implicit methods in high dimensions

$$\frac{\partial \phi}{\partial t} = \alpha \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right)$$

Crank-Nicolson method (CN)

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{\alpha}{2} \left(\frac{\partial^2 \phi^{n+1}}{\partial x^2} + \frac{\partial^2 \phi^n}{\partial x^2} + \frac{\partial^2 \phi^{n+1}}{\partial y^2} + \frac{\partial^2 \phi^n}{\partial y^2} \right)$$

$$\Delta x = \Delta y = h$$

$$\begin{aligned} \text{CD2: } \phi_{l,j}^{n+1} - \phi_{l,j}^n &= \frac{\alpha \Delta t}{2h^2} \left(\phi_{l+1,j}^{n+1} - 2\phi_{l,j}^{n+1} + \phi_{l-1,j}^{n+1} \right) \\ &+ \text{" } \left(\phi_{l+1,j}^n - 2\phi_{l,j}^n + \phi_{l-1,j}^n \right) \\ &+ \text{" } \left(\phi_{l,j+1}^{n+1} - 2\phi_{l,j}^{n+1} + \phi_{l,j-1}^{n+1} \right) \\ &+ \text{" } \left(\phi_{l,j+1}^n - 2\phi_{l,j}^n + \phi_{l,j-1}^n \right) \end{aligned}$$

$$\Rightarrow -\beta \phi_{l+1,j}^{n+1} + (1+4\beta) \phi_{l,j}^{n+1} - \beta \phi_{l-1,j}^{n+1} - \beta \phi_{l,j+1}^{n+1} - \beta \phi_{l,j-1}^{n+1} = \tau_{l,j}^n$$

5.9 Alternating directional implicit (ADI) method
and approximate factorization

$$\frac{\partial \phi}{\partial t} = \alpha \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right)$$

$$\frac{\phi_{i,j}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i,j}^{n+1}}{\Delta x^2}$$

$$\text{CN} + \text{CDZ} : \frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{\alpha}{2} \left(A_x \phi^{n+1} + A_x \phi^n + A_y \phi^{n+1} + A_y \phi^n \right) + \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta y^2)$$

vector

A_x, A_y : difference operators having 2nd-order accuracy representing derivatives in x and y directions.

$$\rightarrow \left[I - \frac{\alpha \Delta t}{2} A_x - \frac{\alpha \Delta t}{2} A_y \right] \phi^{n+1} = \left[I + \frac{\alpha \Delta t}{2} A_x + \frac{\alpha \Delta t}{2} A_y \right] \phi^n + \Delta t \left(\mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta y^2) \right)$$

$$\left(I - \frac{\alpha \Delta t}{2} A_x \right) \left(I - \frac{\alpha \Delta t}{2} A_y \right) - \frac{\alpha^2 \Delta t^2}{4} A_x A_y \quad \left(I + \frac{\alpha \Delta t}{2} A_x \right) \left(I + \frac{\alpha \Delta t}{2} A_y \right) - \frac{\alpha^2 \Delta t^2}{4} A_x A_y$$

$$\rightarrow \left(\mathbf{I} - \frac{\Delta t}{2} A_x \right) \left(\mathbf{I} - \frac{\Delta t}{2} A_y \right) \phi^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} A_x \right) \left(\mathbf{I} + \frac{\Delta t}{2} A_y \right) \phi^n$$

$$+ \frac{\Delta t^2}{4} A_x A_y (\phi^{n+1} - \phi^n) + \Delta t \left(\mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta y^2) \right)$$

Δt^3 $\mathcal{O}(\Delta t^3)$ $= \Delta t \frac{\partial \phi}{\partial t} + \dots$ \therefore neglect \square term w/o losing accuracy

approximate factorization (AF)

$$\Rightarrow \underbrace{\left(\mathbf{I} - \frac{\Delta t}{2} A_x \right) \left(\mathbf{I} - \frac{\Delta t}{2} A_y \right)}_Z \phi^{n+1} = \underbrace{\left(\mathbf{I} + \frac{\Delta t}{2} A_x \right) \left(\mathbf{I} + \frac{\Delta t}{2} A_y \right)}_{CN + CD2 + AF} \phi^n = F$$

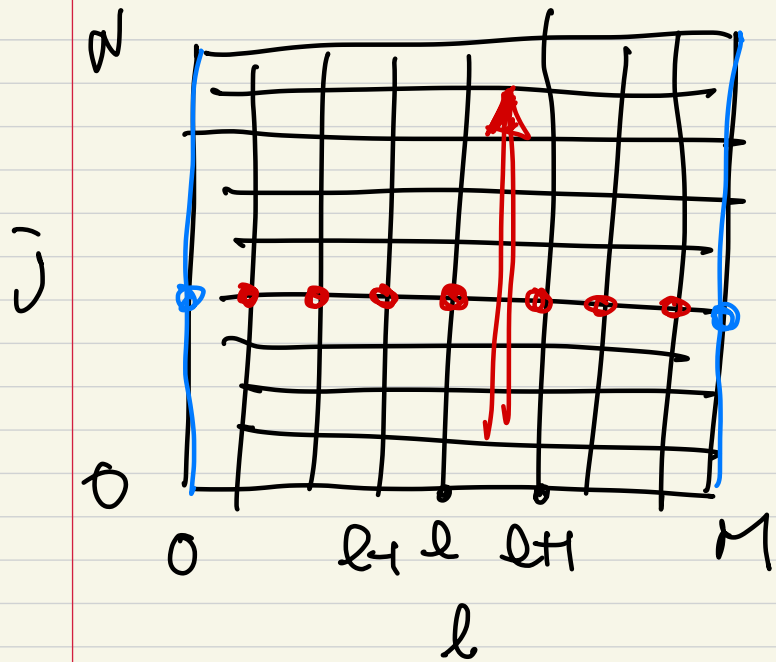
$$\left(\mathbf{I} - \frac{\Delta t}{2} A_x \right) z = F$$

$$\rightarrow z_{l,j} - \frac{\Delta t}{2} \frac{z_{l+1,j} - 2z_{l,j} + z_{l-1,j}}{\Delta x^2} = F_{l,j} \quad \begin{matrix} l=1, 2, \dots, M-1 \\ j=1, 2, \dots, N-1 \end{matrix}$$

tri-diagonal matrix for l

*

For each j , solve a tri-diagonal matrix for $z_{l,j}$.



b.c.'s
for z

N $O(M)$

$O(MN)$ operations

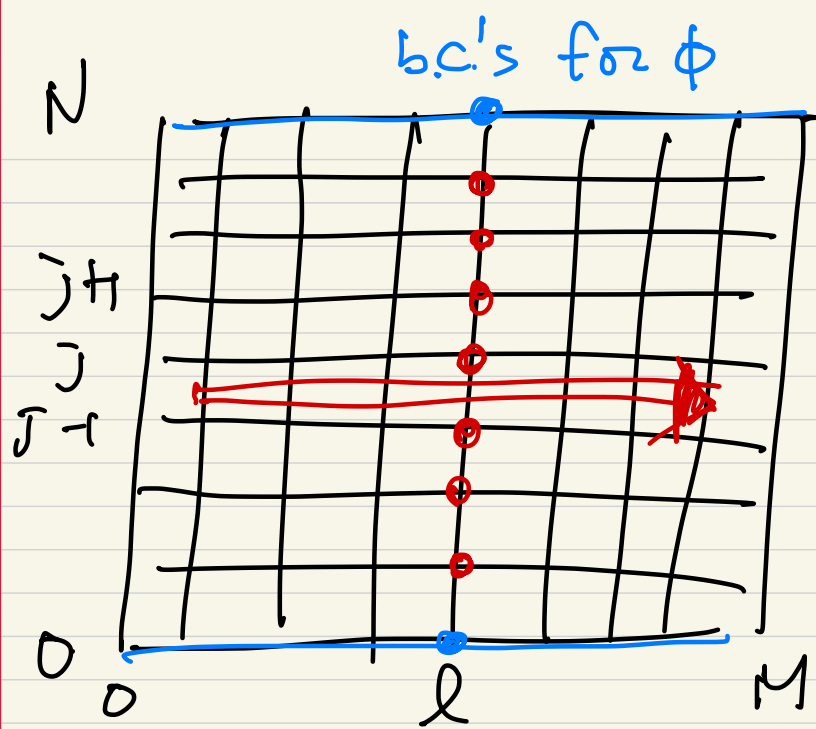
Having solved for $z_{l,j}$, $(I - \frac{\alpha \Delta t}{2} A_y) \phi^{n+1} = z$.

$$\rightarrow \phi_{l,j}^{n+1} - \frac{\alpha \Delta t}{2} \frac{\phi_{l,j+1}^{n+1} - 2\phi_{l,j}^{n+1} + \phi_{l,j-1}^{n+1}}{\Delta y^2} = z_{l,j} \quad \text{--- } \otimes$$

for each l , solve a tri-diagonal matrix for $\phi_{l,j}$.

M $O(N)$

$O(MN)$ operations



\therefore total $\mathcal{O}(2MN)$ operations are required.

Alternating directional implicit (ADI) method!

(*) eq. requires b.c.'s for $z_{0,\bar{j}}$ & $z_{M,\bar{j}}$ for $\bar{j}=1, 2, \dots, N-1$.

(**) eq. @ $l=0$: $z_{0,\bar{j}} = \phi_{0,\bar{j}}^{n+1} - \frac{\alpha \tau}{2} \frac{\phi_{0,\bar{j}+1}^{n+1} - 2\phi_{0,\bar{j}}^{n+1} + \phi_{0,\bar{j}-1}^{n+1}}{\Delta y^2}$

@ $l=M$: $z_{M,\bar{j}} = \dots$

obtain from b.c.'s for ϕ

\Rightarrow ADI method w/ approximate factorization
 no iteration required \Rightarrow Great!
 implicit method