- Nov. 8th (Wed) 6pm – 9pm 301–118 (Midterm)
- Nov. 13th (Mon) those who go for military practise can watch lecture later. (Video will be loaded)
- there is class on Nov. 8th

5.4 Implicit time advancement

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

too restrictive → implicit method

- Crank–Nicolson method (CN) = trapezoidal method
  very popular

$$\boxed{y' = \lambda y \qquad \frac{y^{n+1} - y^n}{\Delta t} = \frac{1}{2}\lambda(y^{n+1} + y^n)}$$

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

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

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

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

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

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

tri-diagonal system of eqs.

Solve this sys. of eqs. to get ϕ_j^{n+1} with $O(N)$ operations.

($y'=\lambda y \xrightarrow{TR} y^n=\sigma^n y^0 \rightarrow \sigma = \dfrac{1+\lambda\Delta t/2}{1-\lambda\Delta t/2}$)

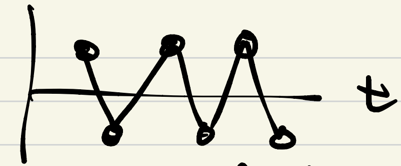
$$\frac{\partial\phi}{\partial t}=\alpha\frac{\partial^2\phi}{\partial x^2} \xrightarrow{CD2} \frac{d\psi}{dt}=-\alpha k'^2\psi \qquad k'^2=\frac{2(1-\cos k\Delta x)}{\Delta x^2}$$

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

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

For large Δt, $\sigma \to -1$

$$\phi^1 = \sigma^n \phi^0 = (-1)^n \phi^0$$



unphysical but never diverges.

dangerous

① reduce Δt

② apply different numerical method like IE.

6.5 Accuracy via modified partial differential eq.

Since the numerical sol. is an approximation of the exact solution, 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 CD2.

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

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

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

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

Taylor series expansion

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

Similarly, $$\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} = \frac{\partial^2 \phi_j^n}{\partial x^2} + \frac{1}{12}\Delta x^2 \frac{\partial^4 \phi_j^n}{\partial x^4} + \cdots$$

$$\Rightarrow L(\phi_j^n) = \frac{\partial \phi_j^n}{\partial t} + \frac{1}{2}\Delta t \frac{\partial^2 \phi_j^n}{\partial t^2} - \alpha \frac{\partial^2 \phi_j^n}{\partial x^2} - \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi_j^n}{\partial x^4} + \cdots = 0$$

remove n and j

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

Thus, the numerical sol. actually satisfies the following $\boxed{\text{modified PDE}}$:

$$\boxed{\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} - \frac{1}{2}\Delta t \frac{\partial^2 \phi}{\partial t^2} + \cdots}$$

EE + CD2

As Δt & $\Delta x \to 0$, $\frac{\partial \tilde{\phi}}{\partial t} - \alpha \frac{\partial^2 \tilde{\phi}}{\partial x^2} = 0$

error $\varepsilon = L(\tilde{\phi}) = -\alpha \frac{\Delta x^2}{12} \frac{\partial^4 \tilde{\phi}}{\partial x^4} + \frac{1}{2}\Delta t \frac{\partial^2 \tilde{\phi}}{\partial t^2} + \cdots$

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

$$= \alpha \frac{\partial^2}{\partial x^2}\left(\alpha \frac{\partial^2 \tilde{\phi}}{\partial x^2}\right) = \alpha^2 \frac{\partial^4 \tilde{\phi}}{\partial x^4}$$

too restrictive

$\Delta t = \frac{\Delta x^2}{6\alpha}$ ← 0 to increase accuracy

stability limit for EE & CD2 : $\Delta t \le \frac{\Delta x^2}{2\alpha}$

$$= \left(-\alpha \frac{\Delta x^2}{12} + \alpha^2 \frac{\Delta t}{2}\right) \frac{\partial^4 \tilde{\phi}}{\partial x^4} + \cdots$$

- Dufort-Frankel method : an inconsistent numerical method

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

$$\left(\begin{array}{c} y' = \lambda y \\ \dfrac{y^{n+1} - y^{n-1}}{2\Delta t} = \lambda y^n \end{array} \right)$$

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

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

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

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

Stability analysis ($\phi_j^n = \sigma^n e^{ikx_j}$) → unconditionally stable!

(no matrix inversion is required
2nd-order accuracy → too good to be true.

What is the modified PDE for Dufort-Frankel method?

$$\begin{cases} \phi_j^{n+1} = \phi_j^n + \Delta t \dfrac{\partial \phi_j^n}{\partial t} + \cdots \\ \phi_{j+1}^n = \phi_j^n + \Delta t \dfrac{\partial \phi_j^n}{\partial x} + \cdots \end{cases}$$

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

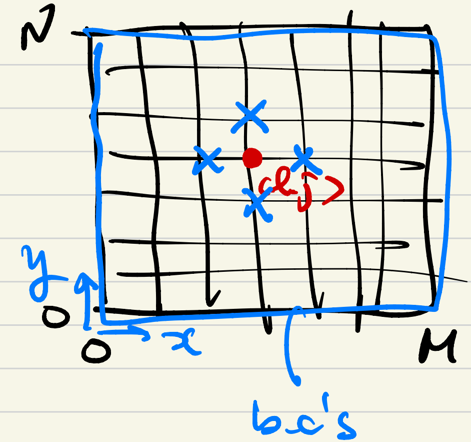
For a given Δt, $\Delta x \downarrow \rightarrow \dfrac{\Delta t^2}{\Delta x^2} \uparrow$

Thus, one cannot increase accuracy by arbitrarly letting $\Delta x \to 0$ and $\Delta t \to 0$.

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

This method is an example of <u>inconsistent numerical method</u>.

5.7 Higher dimensions



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

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

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

start from initial cond $\phi_{l,j}^{0}$, and march in time using b.c's.

Stability CD2 : modified wavenumbers k_1' & k_2' (k_x') (k_y')

$$\phi(x,y,t) = \psi(t)\, e^{ik_1 x_l}\, e^{ik_2 y_j}$$

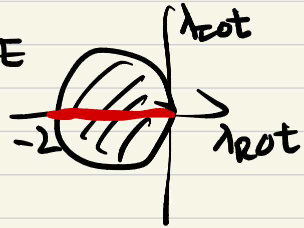
$$\rightarrow \frac{d\psi}{dt} = \boxed{\alpha\left(-k_1'^2 - k_2'^2\right)}\psi \quad \text{where} \quad k_1'^2 = \frac{2(1-\cos k_1 \Delta x)}{\Delta x^2}$$

CD2

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

λ : real and negative

EE



$$|\lambda_{Rot}| \le 2$$

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

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

$$\Rightarrow \boxed{\Delta t \le \frac{1}{2\alpha\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)}}$$

EE + CD2 for 2D diff. eq.

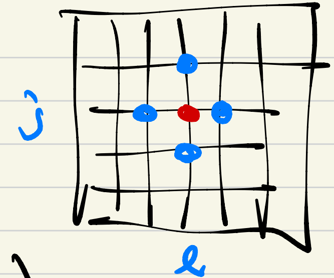
if $\Delta x = \Delta y$, $\Delta t \le \frac{\Delta x^2}{4\alpha}$ (2D) $\qquad \Delta t \le \frac{\Delta x^2}{2\alpha}$ (1D)

$\Delta t \le \frac{\Delta x^2}{6\alpha}$ (3D) $\Rightarrow$ too restrictive

$\Downarrow$

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)

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

$\Delta x = \Delta y = h$

CD2 :
$$\frac{\phi^{n+1}_{l,j} - \phi^{n}_{l,j}}{\Delta t} = \frac{\alpha}{2h^2}\left(\phi^{n+1}_{l+1,j} - 2\phi^{n+1}_{l,j} + \phi^{n+1}_{l-1,j}\right)$$
$$+ \;''\; \left(\phi^{n+1}_{l,j+1} - 2\phi^{n+1}_{l,j} + \phi^{n+1}_{l,j-1}\right)$$
$$+ \;''\; \left(\phi^{n}_{l+1,j} - 2\phi^{n}_{l,j} + \phi^{n}_{l-1,j}\right)$$
$$+ \;''\; \left(\phi^{n}_{l,j+1} - 2\phi^{n}_{l,j} + \phi^{n}_{l,j-1}\right)$$

CD2 + CN

$$\beta = \frac{\alpha \Delta t}{2h^2}$$

$$\Rightarrow \boxed{-\beta \phi^{n+1}_{l+1,j} + (1+4\beta)\phi^{n+1}_{l,j} - \beta \phi^{n+1}_{l-1,j} - \beta \phi^{n+1}_{l,j+1} - \beta \phi^{n+1}_{l,j-1} = F^{n}_{l,j}}$$

$\ell = 1, 2, \cdots, M-1$; $j = 1, 2, \cdots, N-1$

$\ell = 1, j = 1$: — — —

$\ell = 1, j = 2$: — — —

$\cdots$

$\ell = M-1, j = N-1$: — — . .

$\Rightarrow$ sys. of eqs

tri-diagonal matrices

$$\underbrace{\begin{bmatrix} B & C & & O \\ A & B & C & \\ & A & B & C \\ O & & \ddots & \ddots \\ & & A & B \end{bmatrix}}_{(M-1)(N-1) \times (M-1)(N-1)} \begin{bmatrix} \phi_{11} \\ \phi_{21} \\ \vdots \\ \phi_{\ell j} \\ \vdots \\ \phi_{M-1\,N-1} \end{bmatrix} = \begin{bmatrix} F_{11} \\ F_{21} \\ \vdots \\ F_{\ell j} \\ \vdots \\ F_{M-1\,N-1} \end{bmatrix}$$

Block-tridiagonal matrix

$M = N = 100$: # of elts in the matrix $= 10^8$

$\rightarrow$ direct inversion requires $\Theta(M^3N^3)$ operations.

too expensive!

too difficult to solve

→ may have to introduce an iterative method.

→ but actually NOT! → use ADI method!

5.9 Alternating directional implicit (ADI) method and approximate factorization

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

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

$$=$$

CN + CD2 : $\dfrac{\phi^{n+1} - \phi^n}{\Delta t} = \dfrac{\alpha}{2} \left(A_x \phi^{n+1} + A_x \phi^n + A_y \phi^{n+1} + A_y \phi^n \right)$

$$+ O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2)$$

$$\frac{\phi_{l,j+1}^{n+1} - 2\phi_{l,j}^{n+1} + \phi_{l,j-1}^{n+1}}{\Delta y^2}$$

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

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

$$+ \Delta t \left[O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2) \right]$$

$$\underbrace{\left[I - \frac{\alpha\Delta t}{2}A_x - \frac{\alpha\Delta t}{2}A_y\right]}_{\left(I - \frac{\alpha\Delta t}{2}A_x\right)\left(I - \frac{\alpha\Delta t}{2}A_y\right) - \frac{\alpha^2\Delta t^2}{4}A_xA_y}\phi^{n+1} = \underbrace{\left[I + \frac{\alpha\Delta t}{2}A_x + \frac{\alpha\Delta t}{2}A_y\right]}_{\left(I + \frac{\alpha\Delta t}{2}A_x\right)\left(I + \frac{\alpha\Delta t}{2}A_y\right) - \frac{\alpha^2\Delta t^2}{4}A_xA_y}\phi^n + \Delta t\left[O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2)\right]$$

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

$$+ \boxed{\frac{\alpha^2\Delta t^2}{4}A_xA_y\underbrace{(\phi^{n+1} - \phi^n)}_{= O(\Delta t)}} + \underbrace{\Delta t\left[O(\Delta t^2)\right.}_{\simeq O(\Delta t^3)}\left. + O(\Delta x^2) + O(\Delta y^2)\right]$$

neglect this term w/o losing accuracy

approximate factorization (AF)

$$\Rightarrow \boxed{\left(I - \frac{\alpha\Delta t}{2}A_x\right)\underbrace{\left(I - \frac{\alpha\Delta t}{2}A_y\right)\phi^{n+1}}_{z} = \underbrace{\left(I + \frac{\alpha\Delta t}{2}A_x\right)\left(I + \frac{\alpha\Delta t}{2}A_y\right)\phi^n}_{F}}$$

CD2 + CN + AF

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

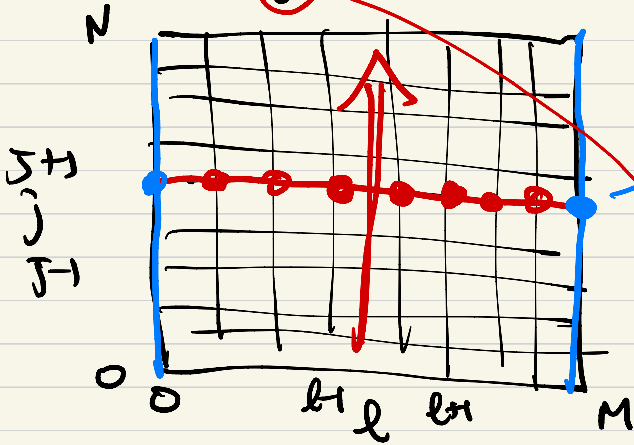
$$\rightarrow z_{l,j} - \frac{\alpha\Delta t}{2}\,\frac{z_{l+1,j} - 2z_{l,j} + z_{l-1,j}}{\Delta x^2} = F_{l,j} \quad (*)$$

$l = 1, 2, \cdots, M-1$

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

→ tri-diagonal matrix for ℓ

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



$$* z_{\ell+1,j} - * z_{\ell,j} + * z_{\ell-1,j} = F_{\ell,j}$$

we need b.c's for $z_{0,j}$ & $z_{M,j}$.

$O(M)$ operations

$O(MN)$ operations

$$\left(I - \frac{\alpha \Delta t}{2} A_y\right)\phi^{n+1} = z \rightarrow \phi^{n+1}_{\ell,j} - \frac{\alpha\Delta t}{2}\,\frac{\phi^{n+1}_{\ell,j+1} - 2\phi^{n+1}_{\ell,j} + \phi^{n+1}_{\ell,j-1}}{\Delta y^2} = z_{\ell,j}$$

for $\ell = 1, 2, \cdots, M-1$

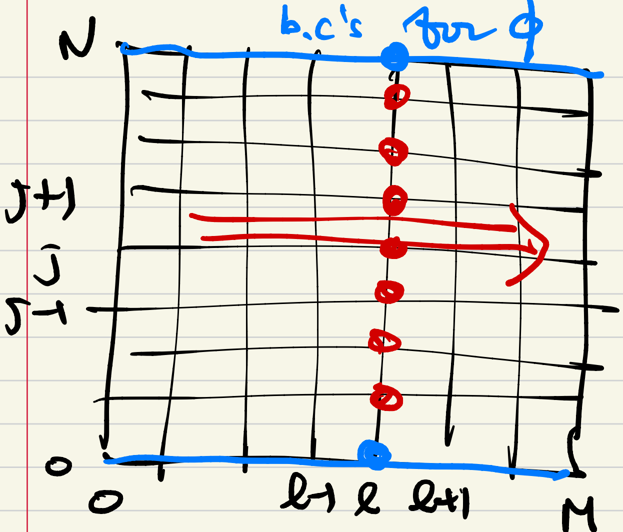
$j = 1, 2, \cdots, N-1$

(**)

for each ℓ, solve a tri-diagonal matrix for $\phi^{n+1}_{\ell,j}$.

$O(N)$ operations

$O(MN)$ operations.



$\therefore$ total $O(2MN)$ operations are required to get ϕ^{n+1}.

Alternation directional implicit (ADI) method !

$\circledast$ eq. requires b.c's for $z_{0,j}$ and $z_{M,j}$ for $j=1,2,\cdots,N-1$.

$\circledast\circledast$ eq: @ $l=0$: $$z_{0,j} = \phi_{0,j}^{n+1} - \frac{\alpha \Delta t}{2} \frac{\phi_{0,j+1}^{n+1} - 2\phi_{0,j}^{n+1} + \phi_{0,j-1}^{n+1}}{\Delta y^2}$$

@ $l=M$: $$z_{M,j} = \underbrace{\phi_{M,j}^{n+1} - \frac{\alpha \Delta t}{2} \frac{\phi_{M,j+1}^{n+1} - 2\phi_{M,j}^{n+1} + \phi_{M,j-1}^{n+1}}{\Delta y^2}}_{\text{obtain from b.c's for } \phi}$$

$\Rightarrow$ ADI method w/ approximate factorization

no iteration required $\Rightarrow$ Great!

implicit method

$$\text{ADI}: \left(I - \frac{\alpha \Delta t}{2} A_x\right)\left(I - \frac{\alpha \Delta t}{2} A_y\right)\phi^{n+1} = \left(I + \frac{\alpha \Delta t}{2} A_x\right)\left(I + \frac{\alpha \Delta t}{2} A_y\right)\phi^{n}$$

stability? $\phi^n = \sigma^n \phi^0$

$$A_x : k_1'^2 = \frac{2(1-\cos k_1 \Delta x)}{\Delta x^2} \qquad \text{CD2}$$

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

$$|\sigma| = \frac{\left(1 + \frac{\alpha \Delta t}{2}(-k_1'^2)\right)\left(1 + \frac{\alpha \Delta t}{2}(-k_2'^2)\right)}{\left(1 - \frac{\alpha \Delta t}{2}(-k_1'^2)\right)\left(1 - \frac{\alpha \Delta t}{2}(-k_2'^2)\right)}$$

$$= \frac{\left(1 - \frac{\alpha \Delta t}{2\Delta x^2}(1-\cos k_1 \Delta x)\right)\left(1 - \frac{\alpha \Delta t}{2\Delta y^2}(1-\cos k_2 \Delta y)\right)}{\left(1 + \quad '' \quad\right)\left(1 + \quad '' \quad\right)} \leq 1$$

$\therefore$ unconditionally stable!