

5.4 Implicit time advancement

노트 제목

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

- Crank - Nicolson method (CN) implicit method
very popular. trapezoidal method

$$CN: \frac{\phi^{n+1} - \phi^n}{\alpha t} = \frac{\alpha}{2} \left[\frac{\partial^2 \phi^{n+1}}{\partial x^2} + \frac{\partial^2 \phi^n}{\partial x^2} \right] + \Theta(\alpha t^2)$$

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

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

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

tri-diagonal system of eqs. \smile $j = 1, 2, \dots, N-1$

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

$$(y' = \lambda y \xrightarrow{\text{TR}} y_n = e^n y_0, \quad e = \frac{1 + \lambda \alpha t / 2}{1 - \lambda \alpha t / 2}) \quad \square$$

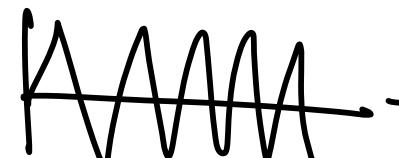
$$\frac{d\phi}{dt} = \alpha \frac{\partial^2 \phi}{\partial x^2} \xrightarrow{\text{CD 2}} \frac{dy}{dt} = -\alpha k'^2 y, \quad k'^2 = \frac{2(1 - \cos k \alpha x)}{\alpha x^2}$$

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

$\alpha x \rightarrow \alpha x / 2 \Rightarrow \alpha t \rightarrow \alpha t$ CPU time \rightarrow twice

for large αt , $\delta \rightarrow -1$, $\phi^\gamma = \phi^\circ \delta^\gamma$

(reduce αt ←
or apply IE .



unphysical but
never diverges.

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 CD2.

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

$$\frac{\hat{\phi}_j^{n+1} - \hat{\phi}_j^n}{\Delta t} = \alpha \frac{\hat{\phi}_{j+1}^n - 2\hat{\phi}_j^n + \hat{\phi}_{j-1}^n}{\Delta x^2}$$

$$L(\hat{\phi}_j^n) \equiv \frac{\hat{\phi}_j^{n+1} - \hat{\phi}_j^n}{\Delta t} - \alpha \frac{\hat{\phi}_{j+1}^n - 2\hat{\phi}_j^n + \hat{\phi}_{j-1}^n}{\Delta x^2} = 0$$

Taylor series expansion

$$\hat{\phi}_j^{n+1} = \hat{\phi}_j^n + \Delta t \frac{\partial \hat{\phi}_j}{\partial t} + \frac{1}{2} \Delta t^2 \frac{\partial^2 \hat{\phi}_j}{\partial t^2} + \dots \Rightarrow \frac{\hat{\phi}_j^{n+1} - \hat{\phi}_j^n}{\Delta t} = \frac{\partial \hat{\phi}_j}{\partial t} + \frac{1}{2} \Delta t \frac{\partial^2 \hat{\phi}_j}{\partial t^2}$$

$$\text{Similarly, } \frac{\hat{\phi}_{j+1}^n - 2\hat{\phi}_j^n + \hat{\phi}_{j-1}^n}{\Delta x^2} = \left. \frac{\partial^2 \hat{\phi}_j}{\partial x^2} \right|_j + \frac{\Delta x^2}{12} \left. \frac{\partial^4 \hat{\phi}_j}{\partial x^4} \right|_j + \dots$$

$$\Rightarrow L(\hat{\phi}_j^n) = \frac{\partial \hat{\phi}_j^n}{\partial t} + \frac{1}{2} \alpha t \frac{\partial^2 \hat{\phi}_j^n}{\partial t^2} - \alpha \frac{\partial^2 \hat{\phi}_j^n}{\partial x^2} \Big|_j - \alpha \frac{\alpha x^2}{12} \frac{\partial^4 \hat{\phi}_j^n}{\partial x^4} \Big|_j + \dots$$

remove n and j

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

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

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

EE + Φ2

$$\text{As } \alpha t \text{ & } \alpha x \rightarrow 0, \quad \frac{\partial \hat{\phi}}{\partial t} - \alpha \frac{\partial^2 \hat{\phi}}{\partial x^2} = 0$$

$$\text{error } \varepsilon = L(\hat{\phi}) = - \alpha \frac{\alpha x^2}{12} \frac{\partial^4 \hat{\phi}}{\partial x^4} + \frac{1}{2} \alpha t \frac{\partial^2 \hat{\phi}}{\partial t^2} + \dots$$

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

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

$= 0$ by choosing $\partial t = \partial x / 6\alpha$

then, we can increase accuracy.

stability limit for EE + CD2 : $\partial t \leq \frac{\partial x^2}{2\alpha}$

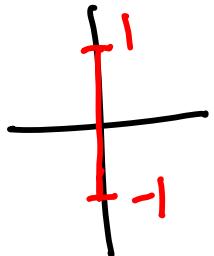
but $\partial t = \partial x / 6\alpha \rightarrow$ too restrictive.

Dufort - Frankel method : an inconsistent numerical method.

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

Leapfrog method
+ CD 2

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



is unconditionally
unstable for
real & negative λ .

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

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

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

Dufort
-Frankel
method

stability analysis ($\phi_j^n = \sigma^n e^{ikx_j}$) \rightarrow unconditionally stable
no matrix inversion is required

2nd-order accurate.

⇒ too good to be true!

What is the modified PDE for DuFort-Frankel method?

$$\phi_j^{n+1} = \phi_j^n + \alpha t \frac{\partial \phi}{\partial t}_j + \dots$$

$$\phi_j^n = \phi_j^1 + \alpha x \frac{\partial \phi}{\partial x}_j + \dots$$

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

For a given αt , when we refine αx , the error actually increases.

thus, one cannot increase the accuracy of numerical

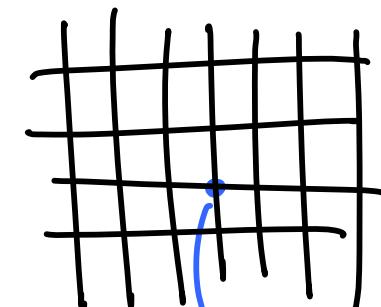
Sol. by arbitrarily letting $\alpha x \rightarrow 0$ and $\alpha t \rightarrow 0$.

The third term approaches zero only if $\alpha t \rightarrow 0$ faster than αx .

This is an example of inconsistent numerical method.

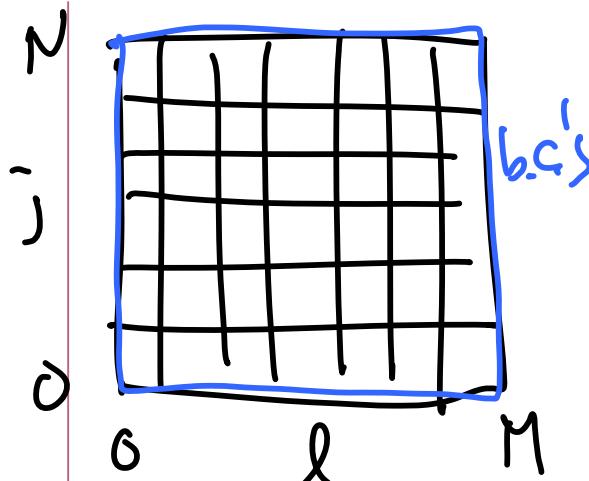
5.7 Higher dimensions

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

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



$\ell = 1, 2, \dots, M-1 ; j = 1, 2, \dots, N-1$
 start from initial condition $\phi_{\ell,j}^*$
 and then march in time using b.c.'s.

stability

CD2: modified wave numbers k'_1 & k'_2

(x) (y)

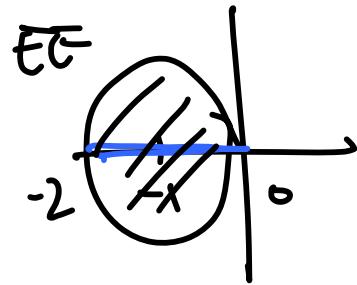
$$\phi(x,y,t) = \psi(t) e^{ik_1' x} e^{ik_2' y}$$

$$\rightarrow \frac{d\psi}{dt} = \alpha (-k_1'^2 - k_2'^2) \psi$$

where $k_1'^2 = \frac{2(1-\cos k_1 \alpha x)}{\Delta x^2}$

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

λ : real & negative



$|\lambda_{\text{rot}}| \leq 2$ for stability

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

worst case : $\cos k_1 \alpha = \cos k_2 \alpha = -1$

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

EE + CD2 for 2D diff. eq.

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

$$\Delta t \leq \frac{\alpha x^2}{6\alpha} \quad (3D) \quad \rightarrow \text{too restrictive}$$

\rightarrow use implicit methods!