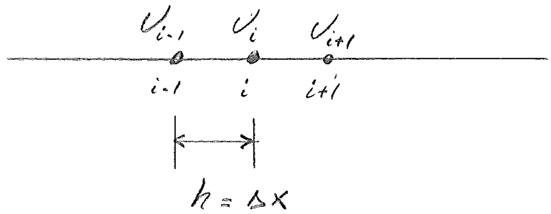
Diffusion Equation

$$\frac{\partial v}{\partial t} = \epsilon \frac{\partial^2 v}{\partial x^2} \qquad \text{PDE for } v(x,t)$$



$\Downarrow$ Finite differences (E2)

$$\frac{d}{dt} v_i = \underbrace{\epsilon \frac{(v_{i+1} - 2v_i + v_{i-1})}{h^2}}_{\equiv\ \left.\frac{\partial^2 v}{\partial x^2}\right|_i + \frac{(\Delta x)^2}{12} \left.\frac{\partial^4 v}{\partial x^4}\right|_i + \cdots}$$

$=$ system of ODEs for the $v_i(t)$

Periodic problem $\Leftrightarrow$ Modal analysis (Fourier modes)

Continuous problem: $v(x,t) = \sum_k A_k(t)\, e^{ikx}$

$$\boxed{\frac{dA_k}{dt} = -\epsilon k^2 A_k} \Longrightarrow \begin{cases} \lambda_k = -\epsilon k^2 & \text{real and negative} \\ A_k(t) = A_k(0) e^{-\epsilon k^2 t} \end{cases}$$

Discrete problem: $v_i(t) = \sum_k A_k(t)\, e^{ikx_i}$ (still continuous in time)

$$\frac{d}{dt} v_i = \sum_k e^{ikx_i} \frac{dA_k}{dt} = \sum_k \frac{\epsilon}{h^2} \left(e^{ikx_{i+1}} - 2e^{ikx_i} + e^{ikx_{i-1}}\right) A_k$$

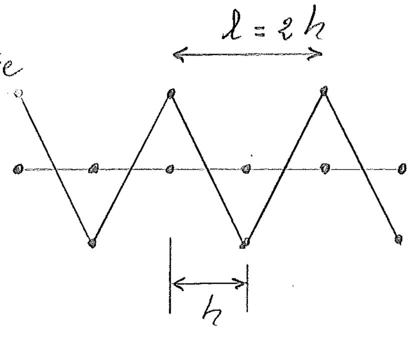
$$= \sum_k \frac{\epsilon}{h^2} e^{ikx_i} \underbrace{\left(e^{ikh} - 2 + e^{-ikh}\right)}_{\equiv\ 2\cos(kh) - 2\ \equiv\ -4\sin^2\left(\frac{kh}{2}\right)} A_k$$

"Von Neumann analysis"

$$\boxed{\frac{d}{dt} A_k = \underbrace{-4\frac{\epsilon}{h^2} \sin^2\left(\frac{kh}{2}\right)}_{\equiv\ \lambda_k \text{ real and negative}} A_k} \Rightarrow A_k(t) = A_k(0)\, e^{\lambda_k \cdot t}$$

- $|\lambda_k|_{max}$ if $\frac{kh}{2} = \frac{\pi}{2}$

  $kh = \pi \equiv$ "Flip-flop mode"

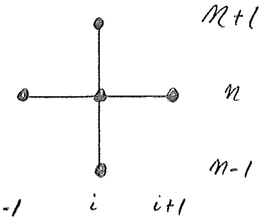


- $\lambda_k = \dfrac{-4\epsilon}{h^2}\sin^2\left(\dfrac{kh}{2}\right) = -\epsilon k^2 \left(\dfrac{\sin\left(\frac{kh}{2}\right)}{\left(\frac{kh}{2}\right)}\right)^2 = -\epsilon (k^2)^*$

  ↳ amplitude error

For kh small $\lambda_k = -\epsilon k^2\left(1 - \frac{1}{3}\left(\frac{kh}{2}\right)^2 + \frac{2}{45}\left(\frac{kh}{2}\right)^4 + \dots\right)$

- Leap-frog ? (Richardson 1910).



$$\frac{(v_i^{n+1} - v_i^{n-1})}{2\Delta t} = \frac{\epsilon}{h^2}\left(v_{i+1}^n - 2v_i^n + v_{i-1}^n\right)$$

$$v_i^{n+1} = v_i^{n-1} + 2\underbrace{\frac{\epsilon\Delta t}{h^2}}_{\equiv\,\eta}\left(v_{i+1}^n - 2v_i^n + v_{i-1}^n\right) \qquad \text{error: } O\left((\Delta t)^2, h^2\right)$$

Stability?

- Unstable as the $\lambda_k \Delta t$ cannot be put inside the stability curve of the leap-frog scheme whatever the value of η.

- Other way: $v_i^n = \sum_k (\rho_k)^n e^{ikx_i} A_k(0)$

$\equiv$ discrete space and time analysis

$$(\rho_k)^{n+1} e^{ikx_i} = (\rho_k)^{n-1} e^{ikx_i} + 2\eta\left(e^{ikh} - 2 + e^{-ikh}\right)(\rho_k)^n e^{ikx_i}$$

$$\hookrightarrow (\rho_k)^2 = 1 - \underbrace{8\eta\sin^2\left(\frac{kh}{2}\right)}_{\equiv\, 2K}\rho_k = 1 - 2K\rho_k$$

$2K$ real and positive

$$(\rho_k)^2 + 2K\rho_k - 1 = 0$$

$$\rho_k = -K \pm \sqrt{K^2+1}$$

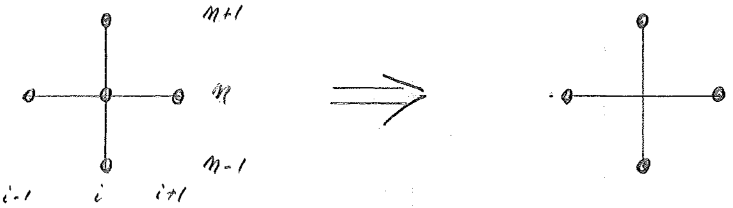
$$(\rho_k)_1 = -K + \sqrt{K^2+1} > 0$$

$$(\rho_k)_2 = -\left(K + \sqrt{K^2+1}\right) < 0$$

$|(\rho_k)_1| \leq 1$ but $|(\rho_k)_2| \geq 1 \Rightarrow$ unstable

Dufort - Frankel (1953)

Replace v_i^n by $\frac{1}{2}\left(v_i^{n+1} + v_i^{n-1}\right)$



$$v_i^{n+1} = v_i^{n-1} + 2r\left(v_{i+1}^n - \left(v_i^{n+1} + v_i^{n-1}\right) + v_{i-1}^n\right)$$

$$(1+2r)\, v_i^{n+1} = (1-2r)\, v_i^{n-1} + 2r\left(v_{i+1}^n + v_{i-1}^n\right)$$

↳ Unconditionally stable for all r (exercise). One obtains:

- $r \leq 1/2$: ρ_1 and ρ_2 are real
- $r > 1/2$: ρ_1 and ρ_2 are complex for modes with $\sin(kh) > \frac{1}{2r}$ $\equiv$ bad.

↳ Problem! In fact, what we do is:

$$\frac{\left(v_i^{n+1} - v_i^{n-1}\right)}{2\Delta t} = \frac{\epsilon}{h^2}\left(v_{i+1}^n - 2v_i^n + v_{i-1}^n\right) + \frac{\epsilon}{h^2}\left(2v_i^n - \left(v_i^{n+1} + v_i^{n-1}\right)\right)$$

$$\left(\frac{\partial v}{\partial t} + \frac{(\Delta t)^2}{6}\frac{\partial^3 v}{\partial t^3} + \dots\right) = \epsilon\left(\frac{\partial^2 v}{\partial x^2} + \frac{h^2}{12}\frac{\partial^4 v}{\partial x^4} + \dots\right)$$
$$- \epsilon\left(\frac{\Delta t}{h}\right)^2\left(\frac{\partial^2 v}{\partial t^2} + \frac{(\Delta t)^2}{12}\frac{\partial^4 v}{\partial t^4} + \dots\right)$$

$$\boxed{\frac{\partial v}{\partial t} = \epsilon\frac{\partial^2 v}{\partial x^2} - \epsilon\left(\frac{\Delta t}{h}\right)^2\frac{\partial^2 v}{\partial t^2} + \frac{\epsilon h^2}{12}\frac{\partial^4 v}{\partial x^4} - \frac{(\Delta t)^2}{6}\frac{\partial^3 v}{\partial t^3} + \dots}$$

$\equiv$ "Modified equation" = equation approximated by the scheme

1. The truncation error of DF is $O\left((\Delta t)^2, h^2, \underset{\sim}{\left(\frac{\Delta t}{h}\right)^2}\right)$

↳ DF is consistent if $\left(\frac{\Delta t}{h}\right) \to 0$ when $\Delta t \to 0$ and $h \to 0$

2. If $\frac{\Delta t}{h} = \underset{\substack{\text{|||}\\ \text{constant}}}{\frac{1}{c_0}}$ when $\Delta t \to 0$ and $h \to 0$, DF is inconsistent as it approximates:

$$\frac{\partial v}{\partial t} = \epsilon\underbrace{\left(\frac{\partial^2 v}{\partial x^2} - \frac{1}{c_0^2}\frac{\partial^2 v}{\partial t^2}\right)}$$

wave-like behavior! $\equiv$ not physical

3. Also: $\epsilon\left(\frac{\Delta t}{h}\right)^2 = \left(\frac{\epsilon \Delta t}{h^2}\right)\Delta t = r\Delta t$. Hence DF Modified equation

also is: $\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - r\,\Delta t\, \frac{\partial^2 u}{\partial t^2} + \frac{\epsilon h^2}{12}\frac{\partial^4 u}{\partial x^4} - \frac{(\Delta t)^2}{6}\frac{\partial^3 u}{\partial t^3} + \dots$

$\hookrightarrow$ DF scheme is consistent when $\Delta t \to 0$ and $h \to 0$ with r constant.

$\Delta t = r\frac{h^2}{\epsilon}$

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \frac{r^2 h^2}{\epsilon}\frac{\partial^2 u}{\partial t^2} + \frac{\epsilon h^2}{12}\frac{\partial^4 u}{\partial x^4} - \frac{r^2 h^4}{6\epsilon^2}\frac{\partial^3 u}{\partial t^3} + \dots$$

$$\hookrightarrow \frac{\partial^2 u}{\partial t^2} = \epsilon \frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial t}\right) - \dots = \epsilon^2 \frac{\partial^4 u}{\partial x^4} - \dots$$

$$\boxed{\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \epsilon\, h^2 \underbrace{\left(r^2 - \frac{1}{12}\right)}_{\text{changes sign when } r = \frac{1}{\sqrt{12}} \simeq 0.2887} \frac{\partial^4 u}{\partial x^4} + \dots}$$

$r = \frac{1}{\sqrt{12}} \Rightarrow$ hyper-diffusion term absent $\equiv$ optimum ?

$r > \frac{1}{\sqrt{12}} \Rightarrow$ hyper-diffusion of proper sign

$r < \frac{1}{\sqrt{12}} \Rightarrow$ hyper-diffusion of improper sign

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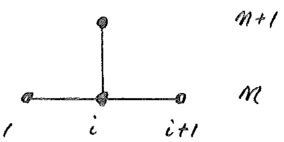
Euler explicit



$$\frac{(u_i^{n+1} - u_i^n)}{\Delta t} = \frac{\epsilon}{h^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) \qquad O(\Delta t, h^2)$$

$$u_i^{n+1} = u_i^n + r\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$$

$$u_i^{n+1} = r\,u_{i+1}^n + (1-2r)\,u_i^n + r\,u_{i-1}^n$$

simplified notation $\boxed{u_i^{n+1} = (I + r\delta^2)\,u_i^n}$

Stability:

- o.K. if all $\lambda_k \Delta t$ are within the stability region of the scheme:

$$-2 \le -\frac{4\epsilon\Delta t}{h^2}\sin^2\left(\frac{kh}{2}\right) \le 0 \quad \text{for all } kh$$

$\hookrightarrow$ $\boxed{r \le \frac{1}{2}}$

- Otherway $\quad v_i^n = \sum_k (\rho_k)^n e^{ikx_i} A_k(0)$

$$(\rho_k)^{n+1} e^{ikx_i} = r(\rho_k)^n e^{ik(x_i+h)} + (1-2r)(\rho_k)^n e^{ikx_i} + r(\rho_k)^n e^{ik(x_i-h)}$$

$$\rho_k = r\left(e^{ikh} + e^{-ikh}\right) + (1-2r)$$

$$= 2r\cos(kh) + (1-2r).$$

$$= 1 - 2r\left(1 - \cos(kh)\right)$$

$$\rho_k = 1 - 4r\sin^2\left(\frac{kh}{2}\right) \qquad \text{real}$$

Stable if $|\rho_k| \le 1$ for all kh..

$\iff -1 \le \rho_k \le 1 \quad$ (as ρ_k is real)

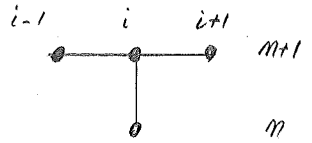
$$-1 \le 1 - 4r\sin^2\left(\frac{kh}{2}\right) \le 1$$

$\downarrow \qquad\qquad \hookrightarrow$ always true

$$r\sin^2\left(\frac{kh}{2}\right) \le \frac{1}{2}$$

$\boxed{r \le \frac{1}{2}}$ $\quad$ O.K. Same result

Euler implicit



$$\frac{\left(v_i^{n+1} - v_i^n\right)}{\Delta t} = \frac{\epsilon}{h^2}\left(v_{i+1}^{n+1} - 2v_i^{n+1} + v_{i-1}^{n+1}\right) \qquad O(\Delta t, h^2)$$

unconditionally stable

$$v_i^{n+1} - r\left(v_{i+1}^{n+1} - 2v_i^{n+1} + v_{i-1}^{n+1}\right) = v_i^n$$

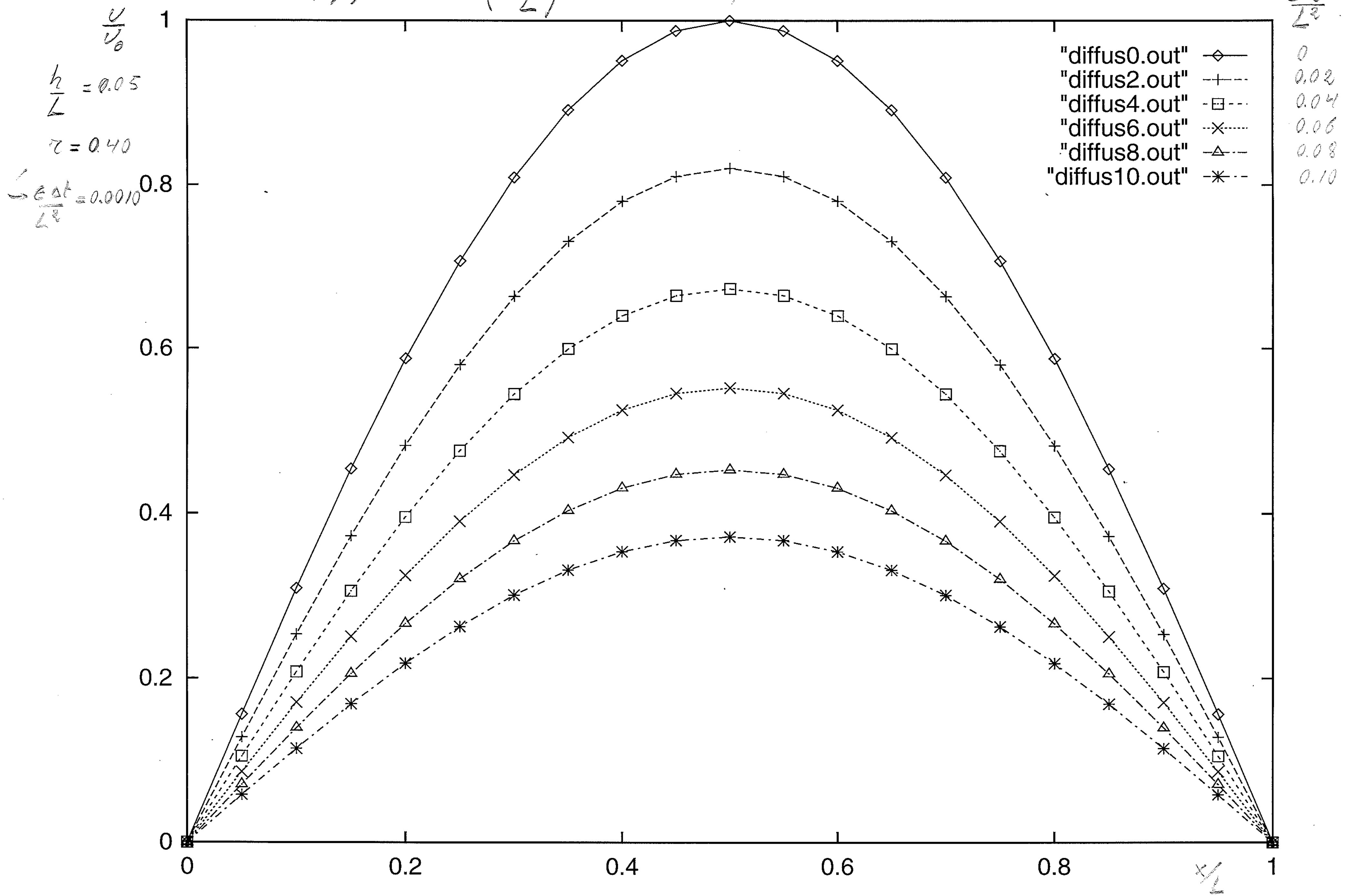
$$-r\,v_{i+1}^{n+1} + (1+2r)\,v_i^{n+1} - r\,v_{i-1}^{n+1} = v_i^n$$

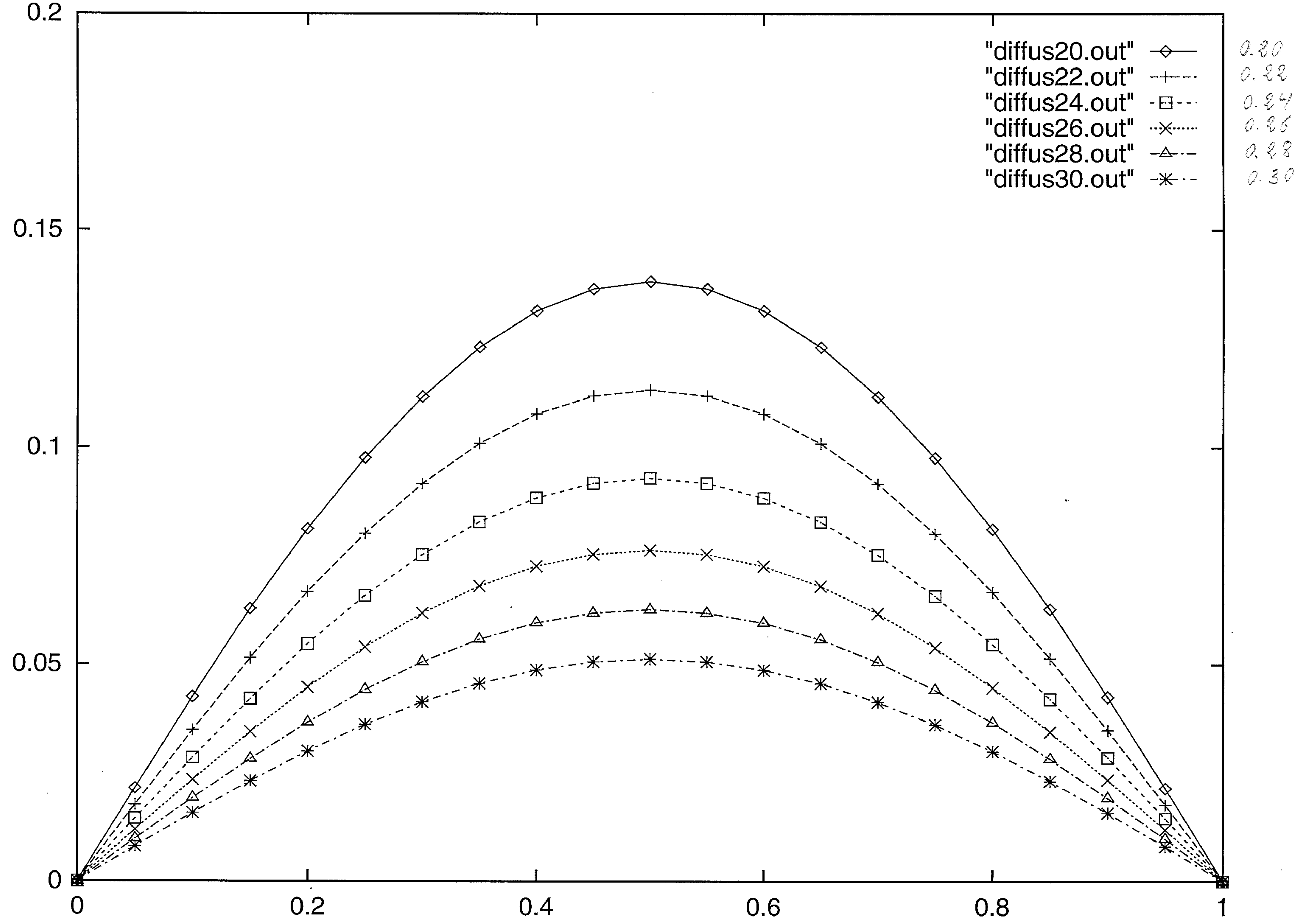
notation

$\boxed{(I - r\delta^2)\, v_i^{n+1} = v_i^n}$

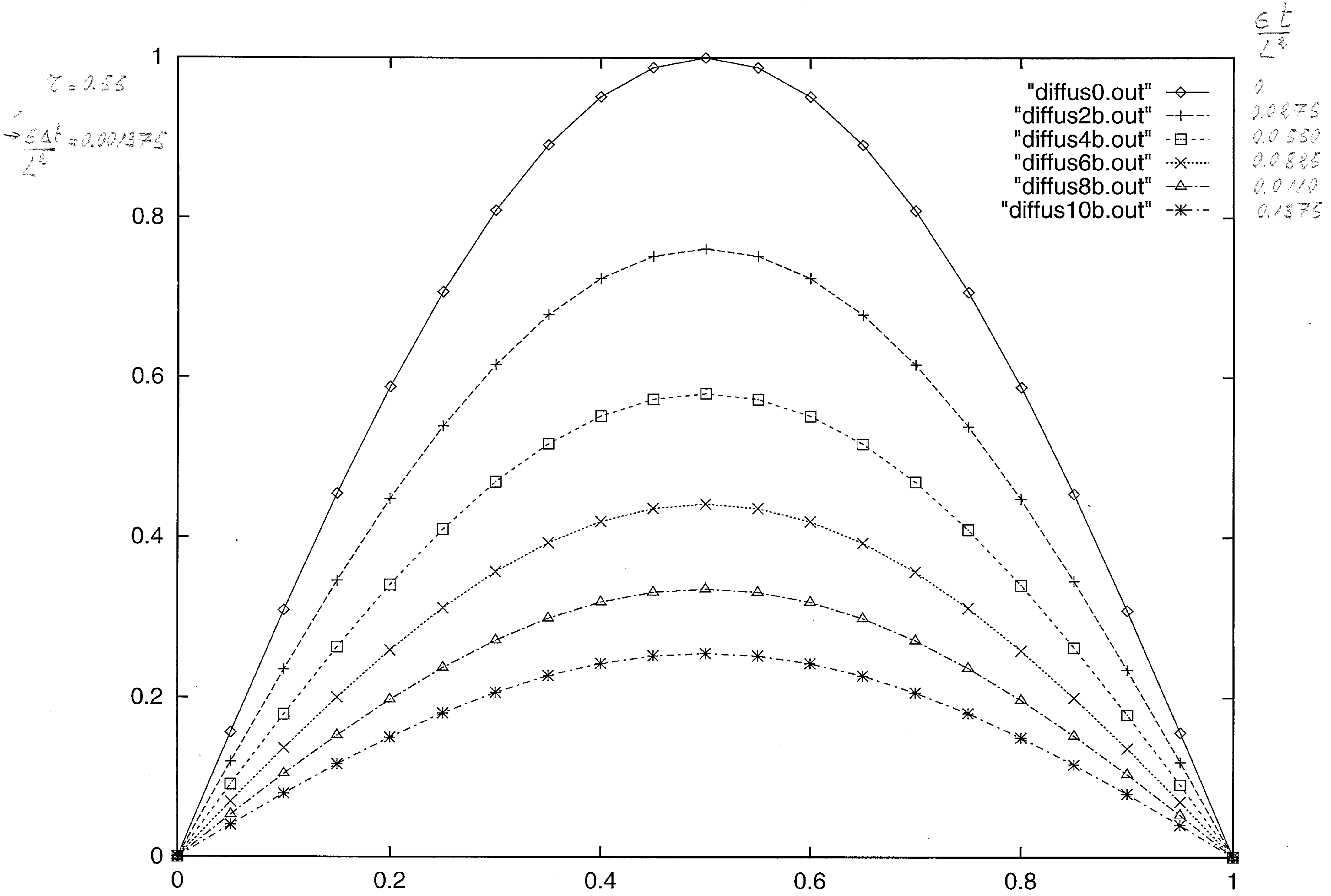
$\longrightarrow$ Need to solve a tridiagonal system

$v(x,0) = v_0 \sin(\pi \frac{x}{L})$ Euler explicit scheme



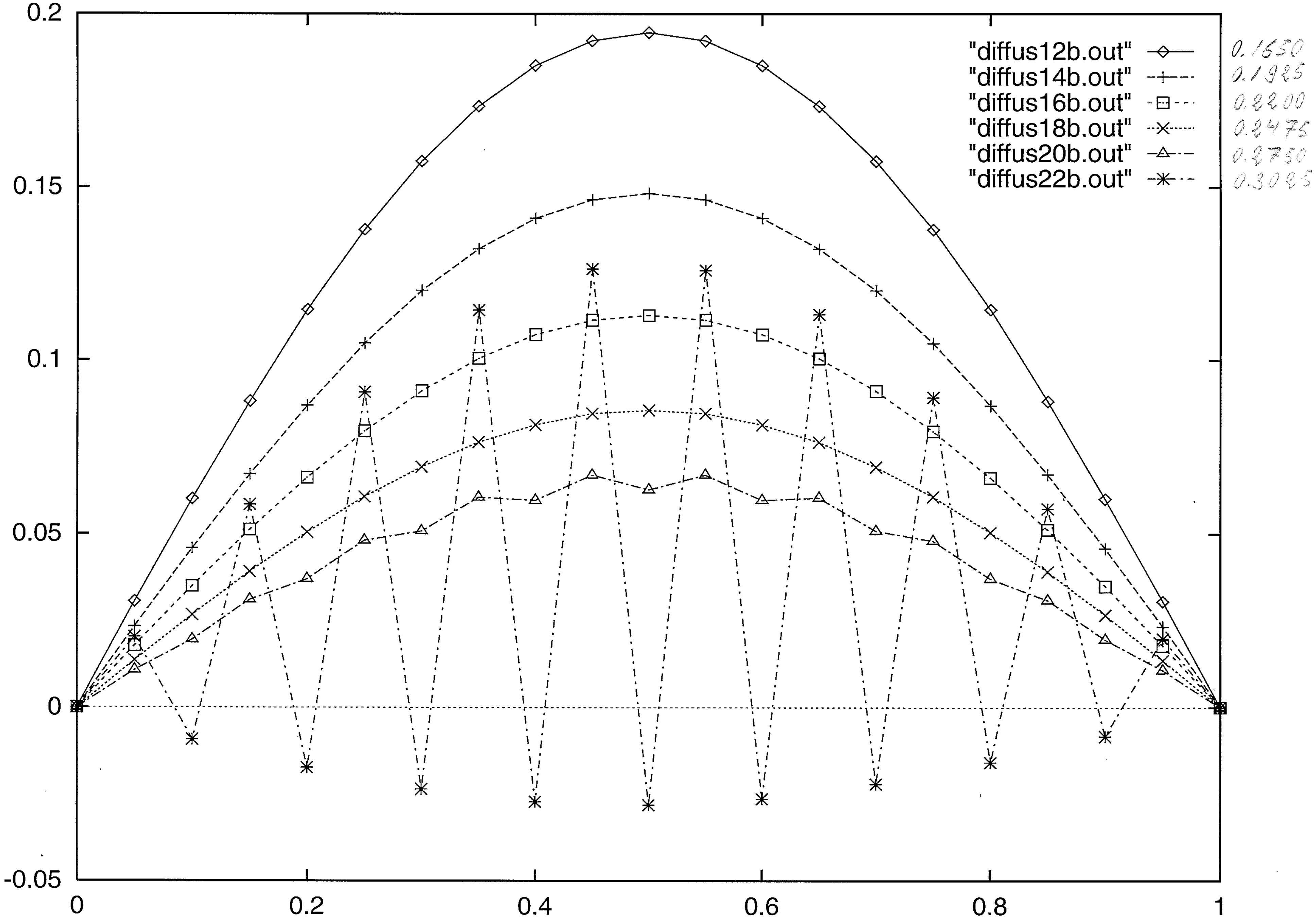


0.2
0.15
0.1
0.05
0
0
0.2
0.4
0.6
0.8
1
"diffus20.out"
"diffus22.out"
"diffus24.out"
"diffus26.out"
"diffus28.out"
"diffus30.out"
0.20
0.22
0.24
0.26
0.28
0.30



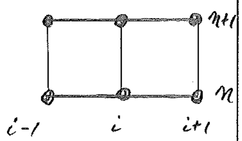
$\tau = 0.55$
$\frac{\epsilon \Delta t}{L^2} = 0.001375$
$\frac{\epsilon t}{L^2}$
"diffus0.out" 0
"diffus2b.out" 0.0275
"diffus4b.out" 0.0550
"diffus6b.out" 0.0825
"diffus8b.out" 0.0110
"diffus10b.out" 0.1375
0
0.2
0.4
0.6
0.8
1

5d


"diffus12b.out"
"diffus14b.out"
"diffus16b.out"
"diffus18b.out"
"diffus20b.out"
"diffus22b.out"
0.1650
0.1925
0.2200
0.2475
0.2750
0.3025
0.2
0.15
0.1
0.05
0
-0.05
0
0.2
0.4
0.6
0.8
1

Crank-Nicolson Generalized

$$\frac{\left(U_i^{n+1} - U_i^{n}\right)}{\Delta t} = \frac{\epsilon}{h^2}\left(\theta\left(U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}\right) + (1-\theta)\left(U_{i+1}^{n} - 2U_i^{n} + U_{i-1}^{n}\right)\right)$$

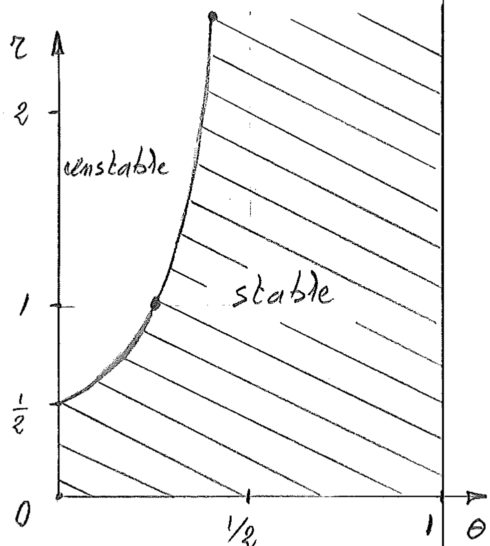


$$-\theta r\, U_{i+1}^{n+1} + (1+2\theta r)U_i^{n+1} - \theta r\, U_{i-1}^{n+1} = r(1-\theta)\, U_{i+1}^{n} + \left(1-2r(1-\theta)\right)U_i^{n} + r(1-\theta)U_{i-1}^{n}$$

$\theta = 1$: Euler implicit, $O(\Delta t, h^2)$

$\theta = 0$: Euler explicit, $O(\Delta t, h^2)$

$\theta = \frac{1}{2}$: $\begin{cases}\text{Crank Nicolson}, & O((\Delta t)^2, h^2)\\ \text{Trapezoid rule}\end{cases}$



<u>θ general:</u> (exercise)

$$\begin{cases} 0 \le \theta < \frac{1}{2} & \text{stable if } r \le \frac{1}{2(1-2\theta)} \\ \frac{1}{2} \le \theta \le 1 & \text{uncond. stable} \end{cases}$$

notation.

$$\boxed{\left(I - \theta r\,\delta^2\right) U_i^{n+1} = \left(I + (1-\theta) r\,\delta^2\right) U_i^{n}}$$

<u>Other schemes?</u> OK as long as all the $(\lambda_k \Delta t)$ are within the stability region of the scheme used:

<u>RK2</u> $\quad r \le \frac{1}{2}$

<u>RK3</u> $\quad r \le \frac{5}{8}$

<u>AB2</u> $\quad r \le \frac{1}{4}$

<u>AM3</u> $\quad r \le \frac{3}{2}$ $\quad$ etc.

Scheme of Douglas

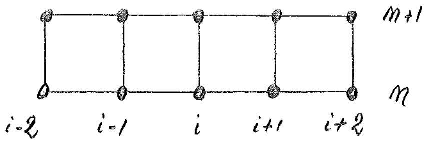
$$\left(\frac{v_i^{n+1}-v_i^n}{\Delta t}\right) = \epsilon\,\frac{1}{2}\left(\frac{\partial^2 v}{\partial x^2}\Big|_i^{n+1} + \frac{\partial^2 v}{\partial x^2}\Big|_i^{n}\right) \quad O((\Delta t)^2)$$

$$= \frac{\epsilon}{2h^2}\,\delta^2\left(I-\frac{\delta^2}{12}+\frac{\delta^4}{90}\dots\right)(v_i^{n+1}+v_i^n)$$

$$(v_i^{n+1}-v_i^n) = \frac{r}{2}\,\delta^2\left(I-\frac{\delta^2}{12}+\frac{\delta^4}{90}\dots\right)(v_i^{n+1}+v_i^n)$$

- If we only use δ^2, we obtain the Crank-Nicolson scheme $\Rightarrow O(h^2)$
- How to obtain $O(h^4)$?

(1) use $\delta^2\left(I-\frac{\delta^2}{12}\right)(v_i^{n+1}+v_i^n) \Rightarrow$ Wider stencil!
↳ Need to solve a pentadiagonal system



(2) Idea: operate on both sides using $\left(I+\frac{\delta^2}{12}\right)$:

$$\left(I+\frac{\delta^2}{12}\right)(v_i^{n+1}-v_i^n) = \frac{r}{2}\left(I+\frac{\delta^2}{12}\right)\delta^2\left(I-\frac{\delta^2}{12}+\frac{\delta^4}{90}\dots\right)(v_i^{n+1}+v_i^n)$$

$$= \frac{r}{2}\,\delta^2\left(I-\cancel{\frac{\delta^2}{12}}+\frac{\delta^4}{90}+\cancel{\frac{\delta^2}{12}}-\frac{\delta^4}{144}\dots\right)(v_i^{n+1}+v_i^n)$$

$$= \frac{r}{2}\,\delta^2\left(I+\left(\frac{1}{90}-\frac{1}{144}\right)\delta^4\dots\right)(v_i^{n+1}+v_i^n)$$

⇓ scheme

$$\left(I+\frac{\delta^2}{12}\right)(v_i^{n+1}-v_i^n) = \frac{r}{2}\,\delta^2(v_i^{n+1}+v_i^n)$$

$$\boxed{\left(I-\frac{1}{2}\left(r-\frac{1}{6}\right)\delta^2\right)v_i^{n+1} = \left(I+\frac{1}{2}\left(r+\frac{1}{6}\right)\delta^2\right)v_i^n}$$

$$12\,v_i^{n+1}-(6r-1)\,\delta^2 v_i^{n+1} = 12\,v_i^n+(6r+1)\,\delta^2 v_i^n$$

$$(1-6r)\, v_{i+1}^{n+1} + (10+12r)\, v_i^{n+1} + (1-6r)\, v_{i-1}^{n+1}$$

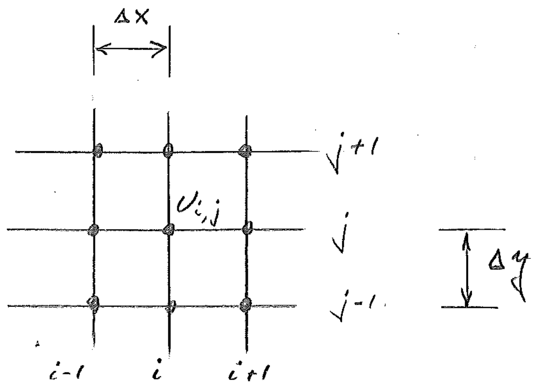
$$= (1+6r)\, v_{i+1}^{n} + (10-12r)\, v_i^{n} + (1+6r)\, v_{i-1}^{n}$$

Error is $O\left((\Delta t)^2, h^4, (\Delta t) h^2\right)$
and we still have a tridiagonal system

Diffusion equation in 2-D

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

$\Downarrow$ Finite differences (E2)



$$\frac{d}{dt} u_{i,j} = \epsilon\left(\frac{(u_{i+1,j} - 2u_{i,j} + u_{i-1,j})}{(\Delta x)^2} + \frac{(u_{i,j+1} - 2u_{i,j} + u_{i,j-1})}{(\Delta y)^2}\right)$$

$$\overset{\text{notation}}{=} \epsilon\left(\frac{\delta_x^2}{(\Delta x)^2} + \frac{\delta_y^2}{(\Delta y)^2}\right) u_{i,j} \qquad \text{error } O((\Delta x)^2, (\Delta y)^2)$$

$\equiv$ system of ODEs for the $u_{ij}(t)$

Periodic problem $\Longleftrightarrow$ modal analysis

Continuous problem: $u(x,y,t) = \sum_{k,l} A_{kl}(t)\, e^{i(kx+ly)}$

$$\boxed{\frac{d}{dt} A_{kl} = \underbrace{-\epsilon(k^2+l^2)}_{\lambda_{k,l}} A_{kl}} \Longrightarrow A_{kl}(t) = A_{kl}(0)\, e^{-\epsilon(k^2+l^2)t}$$

Discrete problem (still continuous in time)

$$u_{ij}(t) = \sum_{k,l} A_{kl}(t)\, e^{i(kx_i + l y_j)}$$

$$\frac{d}{dt} A_{kl}(t) = \underbrace{-4\epsilon\left(\frac{\sin^2\left(\frac{k\Delta x}{2}\right)}{(\Delta x)^2} + \frac{\sin^2\left(\frac{l\Delta y}{2}\right)}{(\Delta y)^2}\right)}_{\lambda_{kl} \text{ real and negative}} A_{kl}(t)$$

$$\lambda_{kl} = \lambda_k + \lambda_l$$

- $|\lambda_{kl}|_{max}$ if $\frac{k\Delta x}{2} = \frac{l\Delta y}{2} = \frac{\pi}{2}$

$$\hookrightarrow \lambda_{crit} = -4\epsilon\left(\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}\right)$$

$$\lambda_{crit}\cdot\Delta t = -4\epsilon\left(\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}\right)\Delta t = -4(\eta_x + \eta_y)$$

$$\begin{cases} \eta_x = \dfrac{\epsilon\Delta t}{(\Delta x)^2} \\ \eta_y = \dfrac{\epsilon\Delta t}{(\Delta y)^2} \end{cases}$$ notation

Example : Euler explicit :

$$4(\eta_x + \eta_y) \leq 2$$

$$\boxed{\eta_x + \eta_y \leq \frac{1}{2}}$$

Case $\Delta x = \Delta y = h \Rightarrow \eta_x = \eta_y = \eta \Rightarrow$ need $\boxed{\eta \leq \frac{1}{4}}$

$$v_{ij}^{n+1} = v_{ij}^n + \epsilon\Delta t\left(\frac{\delta_x^2}{(\Delta x)^2} + \frac{\delta_y^2}{(\Delta y)^2}\right)v_{ij}^n$$

$$v_{ij}^{n+1} = v_{ij}^n + \frac{\epsilon\Delta t}{(\Delta x)^2}\delta_x^2 v_{ij}^n + \frac{\epsilon\Delta t}{(\Delta y)^2}\delta_y^2 v_{ij}^n$$

$$v_{ij}^{n+1} = \left(I + (\eta_x\delta_x^2 + \eta_y\delta_y^2)\right)v_{ij}^n$$

Another simplification of notation

$$\boxed{v^{n+1} = \left(I + (\eta_x\delta_x^2 + \eta_y\delta_y^2)\right)v^n}$$

Generalized Crank Nicolson (Implicit)

$$\frac{U^{n+1}-U^n}{\Delta t} = \epsilon\left(\frac{\delta_x^2}{(\Delta x)^2}+\frac{\delta_y^2}{(\Delta y)^2}\right)\left(\theta U^{n+1}+(1-\theta)U^n\right)$$

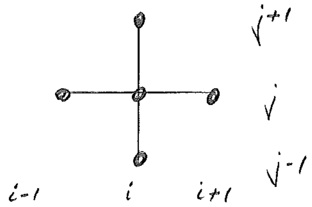
$$U^{n+1} = U^n + (\eta_x\delta_x^2+\eta_y\delta_y^2)\left(\theta U^{n+1}+(1-\theta)U^n\right)$$

$$\boxed{\left(I-\theta(\eta_x\delta_x^2+\eta_y\delta_y^2)\right)U^{n+1} = \left(I+(1-\theta)(\eta_x\delta_x^2+\eta_y\delta_y^2)\right)U^n}$$

$O((\Delta t)^2)$ if $\theta = 1/2$ (= Crank Nicolson)

$$\boxed{\underbrace{\left(I-\tfrac{1}{2}(\eta_x\delta_x^2+\eta_y\delta_y^2)\right)}_{}U^{n+1} = \left(I+\tfrac{1}{2}(\eta_x\delta_x^2+\eta_y\delta_y^2)\right)U^n}$$

coupling of U_{ij}^{n+1} with the 4 neighbors



But the $U_{i,j}$ matrix is stored in the computer as a vector! Hence it is not convenient to solve the above numerically.

↳ We need to seek alternatives

↳ "Operator splitting" methods

ADI methods ("Alternate Direction Implicit")

Peaceman - Rachford (1955), Douglas (1955)

Step 1:

$$\frac{(U^*-U^n)}{\Delta t/2} = \epsilon\left(\frac{\delta_x^2}{(\Delta x)^2}U^* + \frac{\delta_y^2}{(\Delta y)^2}U^n\right)$$

one tridiagonal system to solve for each j

implicit in x

explicit in y

U^* is essentially an approximation of $U^{n+1/2}$

Step 2:

$$\frac{(v^{n+1}-v^{*})}{\Delta t/2} = \epsilon\left(\frac{\delta_x^2}{(\Delta x)^2}\, v^{*} + \frac{\delta_y^2}{(\Delta y)^2}\, v^{n+1}\right)$$

explicit in x

implicit in y

↳ one tridiagonal systems to solve for each i

Using the simplified notation:

$$\boxed{\begin{aligned}\left(I-\tfrac{1}{2}\, r_x \delta_x^2\right) v^{*} &= \left(I+\tfrac{1}{2}\, r_y \delta_y^2\right) v^{n} \quad (1)\\ \left(I-\tfrac{1}{2}\, r_y \delta_y^2\right) v^{n+1} &= \left(I+\tfrac{1}{2}\, r_x \delta_x^2\right) v^{*} \quad (2)\end{aligned}}$$

Composite form of the scheme

$$\left(I-\tfrac{1}{2} r_x \delta_x^2\right)\left(I-\tfrac{1}{2} r_y \delta_y^2\right) v^{n+1} = \left(I-\tfrac{1}{2} r_x \delta_x^2\right)\left(I+\tfrac{1}{2} r_x \delta_x^2\right) v^{*}$$

δ_x^2 commutes with itself

$$= \left(I+\tfrac{1}{2} r_x \delta_x^2\right)\underbrace{\left(I-\tfrac{1}{2} r_x \delta_x^2\right) v^{*}}_{\parallel}$$

$$= \left(I+\tfrac{1}{2} r_x \delta_x^2\right)\left(I+\tfrac{1}{2} r_y \delta_y^2\right) v^{n}$$

$$\hookrightarrow \left(I-\tfrac{1}{2}\left(r_x \delta_x^2 + r_y \delta_y^2\right) + \tfrac{1}{4} r_x r_y \delta_x^2 \delta_y^2\right) v^{n+1} = \left(I+\tfrac{1}{2}\left(r_x \delta_x^2 + r_y \delta_y^2\right) + \tfrac{1}{4} r_x r_y \delta_x^2 \delta_y^2\right) v^{n}$$

This is basically the Crank-Nicolson scheme, with a higher order error term:

$$\tfrac{1}{4} r_x r_y \delta_x^2 \delta_y^2 \left(v^{n+1}-v^{n}\right) \simeq \tfrac{1}{4} r_x r_y \Delta t\, \delta_x^2 \delta_y^2 \left(\frac{\partial v}{\partial t}\right)^{n+1/2}$$

↳ scheme is $O((\Delta t)^2)$ still.

Stability

$$v_{ij}^{n} = \rho^{n} e^{i(k x_i + l y_j)} A(0)$$

≡ simplified notation ... it stands for ρ_{kl} and $A_{kl}(0)$ and there should also be $\sum_{k,l} \dots$

$$v_{ij}^{*} = \xi_1 \cdot \rho^n \, e^{i(k x_i + l y_j)} A(0) \text{ after step 1}$$

$$v_{ij}^{n+1} = \underbrace{\underbrace{\xi_2 \cdot \xi_1}_{\rho} \cdot \rho^n}_{\rho^{n+1}} \, e^{i(k x_i + l y_j)} A(0) \text{ after step 2}$$

One obtains (exercise):

$$\xi_1 = \frac{\left(1 - 2\eta_y \sin^2\left(\frac{l \Delta y}{2}\right)\right)}{\left(1 + 2\eta_x \sin^2\left(\frac{k \Delta x}{2}\right)\right)} = \frac{\left(1 - \frac{1}{2} a_y\right)}{\left(1 + \frac{1}{2} a_x\right)} = \frac{\left(1 + \frac{1}{2} \lambda_y \Delta t\right)}{\left(1 - \frac{1}{2} \lambda_x \Delta t\right)}$$

notation
$$\begin{cases} a_x \triangleq 4\eta_x \sin^2\left(\frac{k \Delta x}{2}\right) \triangleq -\lambda_x \Delta t \\ a_y \triangleq 4\eta_y \sin^2\left(\frac{l \Delta y}{2}\right) \triangleq -\lambda_y \Delta t \end{cases}$$

and

$$\xi_2 = \frac{\left(1 - 2\eta_x \sin^2\left(\frac{k \Delta x}{2}\right)\right)}{\left(1 + 2\eta_y \sin^2\left(\frac{l \Delta y}{2}\right)\right)} = \frac{\left(1 - \frac{1}{2} a_x\right)}{\left(1 + \frac{1}{2} a_y\right)} = \frac{\left(1 + \frac{1}{2} \lambda_x \Delta t\right)}{\left(1 - \frac{1}{2} \lambda_y \Delta t\right)}$$

Finally:

$$\rho = \xi_2 \xi_1 = \left(\frac{1 - \frac{1}{2} a_x}{1 + \frac{1}{2} a_y}\right)\left(\frac{1 - \frac{1}{2} a_y}{1 + \frac{1}{2} a_x}\right) = \underbrace{\left(\frac{1 - \frac{1}{2} a_x}{1 + \frac{1}{2} a_x}\right)}_{\rho_x}\underbrace{\left(\frac{1 - \frac{1}{2} a_y}{1 + \frac{1}{2} a_y}\right)}_{\rho_y} = \rho_x \cdot \rho_y$$

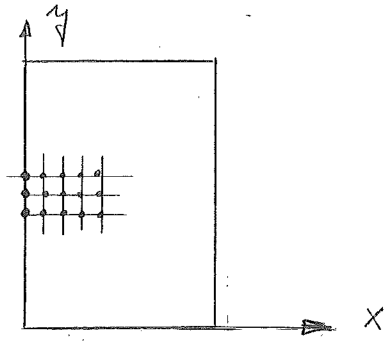
$\rho_x \equiv$ same as when applying CN scheme on $x \Rightarrow |\rho_x| \leq 1$

$\rho_y \equiv$ same as when applying CN scheme on $y \Rightarrow |\rho_y| \leq 1$

$\hookrightarrow |\rho| \leq 1 \Rightarrow$ scheme is unconditionally stable.

Treatment of boundary conditions

↳ We need to derive what is the proper condition to use for v^* so as to preserve the order of the scheme.



Example: case with v given on the boundaries

$$\left(I-\frac{1}{2}r_x\delta_x^2\right)v^* = \left(I+\frac{1}{2}r_y\delta_y^2\right)v^n \qquad (1)$$

$$\left(I-\frac{1}{2}r_y\delta_y^2\right)v^{n+1} = \left(I+\frac{1}{2}r_x\delta_x^2\right)v^* \qquad (2)$$

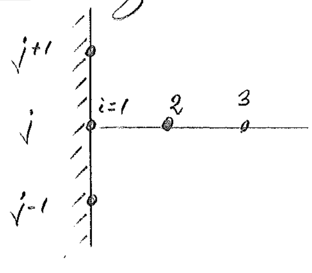
$$(1)\Longrightarrow \frac{1}{2}r_x\delta_x^2 v^* = v^* - \left(I+\frac{1}{2}r_y\delta_y^2\right)v^n \qquad (3)$$

Insert (3) into (2):

$$\left(I-\frac{1}{2}r_y\delta_y^2\right)v^{n+1} = v^* + \left(v^* - \left(I+\frac{1}{2}r_y\delta_y^2\right)v^n\right)$$
$$= 2v^* - \left(I+\frac{1}{2}r_y\delta_y^2\right)v^n$$

$$↳\ v^* = \frac{1}{2}\left[\left(I-\frac{1}{2}r_y\delta_y^2\right)v^{n+1} + \left(I+\frac{1}{2}r_y\delta_y^2\right)v^n\right]$$
$$= \frac{1}{2}\left(v^{n+1}+v^n\right) - \frac{1}{2}r_y\delta_y^2\left(v^{n+1}-v^n\right)$$ ≡ proper BC for v^* on the vertical boundaries

Example: left boundary



$v_{1,j}^n$ is given for all j and n as $v(x_1, y_j, t^n)$ is given

$$v_{1,j}^* = \frac{1}{2}\left[\left(v_{1,j}^{n+1} - \frac{1}{2}r_y\left(v_{1,j+1}^{n+1} - 2v_{1,j}^{n+1} + v_{1,j-1}^{n+1}\right)\right) + \left(v_{1,j}^n + \frac{1}{2}r_y\left(v_{1,j+1}^n - 2v_{1,j}^n + v_{1,j-1}^n\right)\right)\right]$$

Note: when BC is not function of t, we have: $v_{1,j}^* = v_{1,j}$

when BC is not function of y, we have: $v_{1,j}^* = \frac{1}{2}\left(v_1^{n+1} + v_1^n\right)$

ADI Douglas - Rachford

$$(I - r_x \delta_x^2)\, u^* = (I + r_y \delta_y^2)\, u^n \qquad (1)$$

$$(I - r_y \delta_y^2)\, u^{n+1} = u^* - r_y \delta_y^2\, u^n \qquad (2)$$

Composite form:

$$(I - r_x \delta_x^2)(I - r_y \delta_y^2)\, u^{n+1} = \underbrace{(I - r_x \delta_x^2)\, u^*}_{(1)} - (I - r_x \delta_x^2)\, r_y \delta_y^2\, u^n$$

$$= (I + r_y \delta_y^2)\, u^n - r_y \delta_y^2\, u^n + r_x r_y \delta_x^2 \delta_y^2\, u^n$$

$$= (I + r_x r_y \delta_x^2 \delta_y^2)\, u^n$$

$$\left(I - (r_x \delta_x^2 + r_y \delta_y^2) + r_x r_y \delta_x^2 \delta_y^2\right) u^{n+1} = (I + r_x r_y \delta_x^2 \delta_y^2)\, u^n$$

This is basically the Euler scheme, with a higher order error term: $r_x r_y \delta_x^2 \delta_y^2 (u^{n+1} - u^n) \simeq r_x r_y \Delta t\, \delta_x^2 \delta_y^2 \left(\frac{\partial u}{\partial t}\Big|^{n+1/2}\right)$

↳ scheme is $O(\Delta t)$ still.

Stability:

$$\xi_1 = \frac{(1 - a_y)}{(1 + a_x)}$$

$$\rho = \frac{1}{(1 + a_y)}(\xi_1 + a_y) = \frac{1}{(1 + a_y)}\left(\left(\frac{1 - a_y}{1 + a_x}\right) + a_y\right) = \frac{1 + a_y a_x}{(1 + a_y)(1 + a_x)}$$

$|\rho| \le 1 \Rightarrow$ uncond. stable

Boundary conditions

$$(2) \Rightarrow u^* = (I - r_y \delta_y^2)\, u^{n+1} + r_y \delta_y^2\, u^n$$

$$= u^{n+1} - r_y \delta_y^2 (u^{n+1} - u^n)$$

ADI Mitchell-Fairweather

$$\boxed{\begin{aligned} &\left(I - \tfrac{1}{2}\left(r_x - \tfrac{1}{6}\right)\delta_x^2\right) U^* = \left(I + \tfrac{1}{2}\left(r_y + \tfrac{1}{6}\right)\delta_y^2\right) U^n \quad (1)\\ &\left(I - \tfrac{1}{2}\left(r_y - \tfrac{1}{6}\right)\delta_y^2\right) U^{n+1} = \left(I + \tfrac{1}{2}\left(r_x + \tfrac{1}{6}\right)\delta_x^2\right) U^* \quad (2)\end{aligned}}$$

Composite Form

$$\left(I - \tfrac{1}{2}\left(r_x - \tfrac{1}{6}\right)\delta_x^2\right)\left(I - \tfrac{1}{2}\left(r_y - \tfrac{1}{6}\right)\delta_y^2\right) U^{n+1} = \left(1 + \tfrac{1}{2}\left(r_x + \tfrac{1}{6}\right)\delta_x^2\right)\left(1 + \tfrac{1}{2}\left(r_y + \tfrac{1}{6}\right)\delta_y^2\right) U^n$$

↳ $O\left((\Delta t)^2, (\Delta x)^4, (\Delta y)^4\right)$

Stability: uncond. stable | Boundary conditions (exercise)

Methods "Locally One-Dimensional" (LOD)

Yanenko (1971)

LOD Euler

$$\begin{cases} \dfrac{U^* - U^n}{\Delta t} = \epsilon \dfrac{\delta_x^2}{(\Delta x)^2} U^* & (1)\\[2ex] \dfrac{U^{n+1} - U^*}{\Delta t} = \epsilon \dfrac{\delta_y^2}{(\Delta y)^2} U^{n+1} & (2)\end{cases}$$

$$\boxed{\begin{aligned} &(I - r_x \delta_x^2) U^* = U^n \\ &(I - r_y \delta_y^2) U^{n+1} = U^* \end{aligned}}$$

(1) $\xi_1 = \dfrac{1}{(1+a_x)}$ uncond. stable

(2) $\xi_2 = \dfrac{1}{(1+a_y)}$ uncond. stable

Composite form

$$(I - r_x \delta_x^2)(I - r_y \delta_y^2) U^{n+1} = U^n$$

↳ This is basically the Euler scheme, with higher order error term: $r_x r_y \delta_x^2 \delta_y^2 U^{n+1}$. This is not as good as $r_x r_y \delta_x^2 \delta_y^2 (U^{n+1} - U^n)$!

$\rho = \dfrac{1}{(1+a_y)} \cdot \dfrac{1}{(1+a_x)}$ uncond. stable | BC: (2) $\Rightarrow U^* = (I - r_y \delta_y^2) U^{n+1}$
$= U^{n+1} - r_y \delta_y^2 U^{n+1}$

LOD Crank Nicolson

$$\boxed{\begin{aligned} \left(I-\tfrac{1}{2} r_x \delta_x^2\right) U^* &= \left(I+\tfrac{1}{2} r_x \delta_x^2\right) U^n \\ \left(I-\tfrac{1}{2} r_y \delta_y^2\right) U^{n+1} &= \left(I+\tfrac{1}{2} r_y \delta_y^2\right) U^* \end{aligned}}$$

(1) $\xi_1 = \left(\dfrac{1-\frac{1}{2} a_x}{1+\frac{1}{2} a_x}\right)$ uncond. stable

(2) $\xi_2 = \left(\dfrac{1-\frac{1}{2} a_y}{1+\frac{1}{2} a_y}\right)$ uncond. stable

Composite Form:

$$\left(I-\tfrac{1}{2} r_x \delta_x^2\right)\left(I-\tfrac{1}{2} r_y \delta_y^2\right) U^{n+1} = \left(I-\tfrac{1}{2} r_x \delta_x^2\right)\left(I+\tfrac{1}{2} r_y \delta_y^2\right) U^*$$

as δ_x^2 and δ_y^2 commute

$$= \left(I+\tfrac{1}{2} r_y \delta_y^2\right)\left(I-\tfrac{1}{2} r_x \delta_x^2\right) U^*$$

$$= \left(I+\tfrac{1}{2} r_y \delta_y^2\right)\left(I+\tfrac{1}{2} r_x \delta_x^2\right) U^n$$

Scheme is $O((\Delta t)^2)$. as Crank-Nicolson.

$$\rho = \left(\frac{1-\frac{1}{2} a_y}{1+\frac{1}{2} a_y}\right)\left(\frac{1-\frac{1}{2} a_x}{1+\frac{1}{2} a_x}\right)$$ uncond. stable.

BC:

$$(1) \Rightarrow \tfrac{1}{2} r_x \delta_x^2 U^* = U^* - \left(I+\tfrac{1}{2} r_x \delta_x^2\right) U^n$$

↳ we cannot insert that into (2) !

↳ Impossible to find a proper condition on U^* so as to preserve the order of the scheme at the boundary?

Stability

Defs: $a_x = 4\eta_x \sin^2\left(\frac{k\Delta x}{2}\right) = -\lambda_x \Delta t$

$a_y = 4\eta_y \sin^2\left(\frac{l\Delta y}{2}\right) = -\lambda_y \Delta t$

- **Euler implicit**: $O(\Delta t)$

$$\left(I - (\eta_x \delta_x^2 + \eta_y \delta_y^2)\right) v^{n+1} = v^n \qquad \rho = \frac{1}{1+(a_x+a_y)} \qquad \text{uncond.}$$

- **Crank-Nicolson**: $O((\Delta t)^2)$

$$\left(I - \tfrac{1}{2}(\eta_x \delta_x^2 + \eta_y \delta_y^2)\right) v^{n+1} = \left(I + \tfrac{1}{2}(\eta_x \delta_x^2 + \eta_y \delta_y^2)\right) v^n \qquad \rho = \frac{\left(1-\frac{1}{2}(a_x+a_y)\right)}{\left(1+\frac{1}{2}(a_x+a_y)\right)} \qquad \text{uncond.}$$

- **ADI (Peaceman-Rachford)**: $O((\Delta t)^2)$

$$\begin{cases} \left(I - \frac{1}{2}\eta_x \delta_x^2\right) v^* = \left(I + \frac{1}{2}\eta_y \delta_y^2\right) v^n & \xi_1 = \dfrac{(1-\frac{1}{2}a_y)}{(1+\frac{1}{2}a_x)} \\ \left(I - \frac{1}{2}\eta_y \delta_y^2\right) v^{n+1} = \left(I + \frac{1}{2}\eta_x \delta_x^2\right) v^* & \xi_2 = \dfrac{(1-\frac{1}{2}a_x)}{(1+\frac{1}{2}a_y)} \end{cases}$$

Composite:

$$\left(I - \tfrac{1}{2}\eta_x \delta_x^2\right)\left(I - \tfrac{1}{2}\eta_y \delta_y^2\right) v^{n+1} = \left(I + \tfrac{1}{2}\eta_x \delta_x^2\right)\left(I + \tfrac{1}{2}\eta_y \delta_y^2\right) v^n$$

$$\rho = \xi_2 \cdot \xi_1 = \frac{(1-\frac{1}{2}a_x)}{(1+\frac{1}{2}a_y)} \cdot \frac{(1-\frac{1}{2}a_y)}{(1+\frac{1}{2}a_x)} = \frac{(1-\frac{1}{2}a_x)}{(1+\frac{1}{2}a_x)} \cdot \frac{(1-\frac{1}{2}a_y)}{(1+\frac{1}{2}a_y)} \qquad \text{uncond.}$$

- **ADI (Douglas-Rachford)**: $O(\Delta t)$

$$\begin{cases} \left(I - \eta_x \delta_x^2\right) v^* = \left(I + \eta_y \delta_y^2\right) v^n & \xi_1 = \dfrac{(1-a_y)}{(1+a_x)} \\ \left(I - \eta_y \delta_y^2\right) v^{n+1} = v^* - \eta_y \delta_y^2 v^n \end{cases}$$

Composite:

$$\left(I - \eta_x \delta_x^2\right)\left(I - \eta_y \delta_y^3\right) v^{n+1} = \left(I + \eta_x \eta_y \delta_x^2 \delta_y^2\right) v^n$$

$$\rho = \frac{1}{(1+a_y)}\left(\xi_1 + a_y\right) = \frac{(1+a_y a_x)}{(1+a_y)(1+a_x)} \qquad \text{uncond.}$$

Stability

ADI (Mitchell - Fairweather) : $\mathcal{O}\left((\Delta t)^2, (\Delta x)^4, (\Delta y)^4\right)$

$$\begin{cases} \left(I - \frac{1}{2}\left(r_x - \frac{1}{6}\right)\delta_x^2\right) U^* = \left(I + \frac{1}{2}\left(r_y + \frac{1}{6}\right)\delta_y^2\right) U^n \\ \left(I - \frac{1}{2}\left(r_y - \frac{1}{6}\right)\delta_y^2\right) U^{n+1} = \left(I + \frac{1}{2}\left(r_x + \frac{1}{6}\right)\delta_x^2\right) U^* \end{cases}$$

Composite :

$$\left(I - \frac{1}{2}\left(r_x - \frac{1}{6}\right)\delta_x^2\right)\left(I - \frac{1}{2}\left(r_y - \frac{1}{6}\right)\delta_y^2\right) U^{n+1} = \left(I + \frac{1}{2}\left(r_x + \frac{1}{6}\right)\delta_x^2\right)\left(I + \frac{1}{2}\left(r_y + \frac{1}{6}\right)\delta_y^2\right) U^n$$

uncond.

LOD Euler : $\mathcal{O}(\Delta t)$

$$\begin{cases} (I - r_x \delta_x^2) U^* = U^n \\ (I - r_y \delta_y^2) U^{n+1} = U^* \end{cases}$$

$$\xi_1 = \frac{1}{(1 + a_x)} \qquad \xi_2 = \frac{1}{(1 + a_y)}$$

Composite :

$$(I - r_x \delta_x^2)(I - r_y \delta_y^2) U^{n+1} = U^n$$

$$\rho = \xi_2 \cdot \xi_1 = \frac{1}{(1 + a_y)} \cdot \frac{1}{(1 + a_x)}$$

uncond

LOD Crank-Nicolson : $\mathcal{O}((\Delta t)^2)$

$$\begin{cases} \left(I - \frac{1}{2} r_x \delta_x^2\right) U^* = \left(I + \frac{1}{2} r_x \delta_x^2\right) U^n \\ \left(I - \frac{1}{2} r_y \delta_y^2\right) U^{n+1} = \left(I + \frac{1}{2} r_y \delta_y^2\right) U^* \end{cases}$$

$$\xi_1 = \frac{\left(1 - \frac{1}{2} a_x\right)}{\left(1 + \frac{1}{2} a_x\right)} \qquad \xi_2 = \frac{\left(1 - \frac{1}{2} a_y\right)}{\left(1 + \frac{1}{2} a_y\right)}$$

Composite : (Seulement si δ_x^2 et δ_y^2 commutent)

$$\left(1 - \frac{1}{2} r_x \delta_x^2\right)\left(1 - \frac{1}{2} r_y \delta_y^2\right) U^{n+1} = \left(1 + \frac{1}{2} r_y \delta_y^2\right)\left(1 + \frac{1}{2} r_x \delta_x^2\right) U^n$$

$$\rho = \xi_2 \cdot \xi_1 = \frac{\left(1 - \frac{1}{2} a_y\right)}{\left(1 + \frac{1}{2} a_y\right)} \cdot \frac{\left(1 - \frac{1}{2} a_x\right)}{\left(1 + \frac{1}{2} a_x\right)}$$

uncond

Stability

- Trivial extension of ADI Peaceman-Rashford to 3-D : $O(\Delta t)$!

$$\begin{cases} \left(I-\frac{1}{3}\eta_x\delta_x^2\right)U^{*} = \left(I+\frac{1}{3}\left(\eta_y\delta_y^2+\eta_z\delta_z^2\right)\right)U^{n} \\ \left(I-\frac{1}{3}\eta_y\delta_y^2\right)U^{**} = \left(I+\frac{1}{3}\left(\eta_z\delta_z^2+\eta_x\delta_x^2\right)\right)U^{*} \\ \left(I-\frac{1}{3}\eta_z\delta_z^2\right)U^{n+1} = \left(I+\frac{1}{3}\left(\eta_x\delta_x^2+\eta_y\delta_y^2\right)\right)U^{**} \end{cases}$$

Bad!

$$\rho = \xi_3\cdot\xi_2\cdot\xi_1 = \frac{\left(1-\frac{1}{3}(a_x+a_y)\right)}{\left(1+\frac{1}{3}a_z\right)}\cdot\frac{\left(1-\frac{1}{3}(a_z+a_x)\right)}{\left(1+\frac{1}{3}a_y\right)}\cdot\frac{\left(1-\frac{1}{3}(a_y+a_z)\right)}{\left(1+\frac{1}{3}a_x\right)}$$

No!

- ADI Douglas-Rachford : $O(\Delta t)$

$$\begin{cases} \left(I-\eta_x\delta_x^2\right)U^{*} = \left(I+\left(\eta_y\delta_y^2+\eta_z\delta_z^2\right)\right)U^{n} \\ \left(I-\eta_y\delta_y^2\right)U^{**} = U^{*}-\eta_y\delta_y^2U^{n} \\ \left(I-\eta_z\delta_z^2\right)U^{n+1} = U^{**}-\eta_z\delta_z^2U^{n} \end{cases} \qquad \xi_1 = \frac{1-(a_y+a_z)}{(1+a_x)}$$

Composite:

$$\left(I-\eta_x\delta_x^2\right)\left(I-\eta_y\delta_y^2\right)\left(I-\eta_z\delta_z^2\right)U^{n+1} =$$

$$\left(I+\left(\eta_x\eta_y\delta_x^2\delta_y^2+\eta_y\eta_z\delta_y^2\delta_z^2+\eta_z\eta_x\delta_z^2\delta_x^2\right)-\eta_x\eta_y\eta_z\delta_x^2\delta_y^2\delta_z^2\right)U^{n}$$

$$\rho = \frac{1}{(1+a_z)}\left(\frac{1}{(1+a_y)}\left(\xi_1+a_y\right)+a_z\right) = \frac{1+(a_xa_y+a_ya_z+a_za_x)+a_xa_ya_z}{(1+a_z)(1+a_y)(1+a_x)}$$

uncond

- ADI Douglas-Brian: $O((\Delta t)^2)$

$$\left(I-\frac{1}{2}\eta_x\delta_x^2\right)U^{*} = \left(I+\frac{1}{2}\eta_x\delta_x^2+\left(\eta_y\delta_y^2+\eta_z\delta_z^2\right)\right)U^{n}$$

$$\left(I-\frac{1}{2}\eta_y\delta_y^2\right)U^{**} = \left(I+\frac{1}{2}\left(\eta_x\delta_x^2+\eta_y\delta_y^2\right)+\eta_z\delta_z^2\right)U^{n}+\frac{1}{2}\eta_x\delta_x^2U^{*}$$

$$\left(I-\frac{1}{2}\eta_z\delta_z^2\right)U^{n+1} = \left(I+\frac{1}{2}\left(\eta_x\delta_x^2+\eta_y\delta_y^2+\eta_z\delta_z^2\right)\right)U^{n}+\frac{1}{2}\eta_x\delta_x^2U^{*}+\frac{1}{2}\eta_y\delta_y^2U^{**}$$

Composite:

$$\left(I-\frac{1}{2}\eta_x\delta_x^2\right)\left(I-\frac{1}{2}\eta_y\delta_y^2\right)\left(I-\frac{1}{2}\eta_z\delta_z^2\right)U^{n+1} =$$

$$\left(I+\frac{1}{2}\left(\eta_x\delta_x^2+\eta_y\delta_y^2+\eta_z\delta_z^2\right)+\frac{1}{4}\left(\eta_x\eta_y\delta_x^2\delta_y^2+\eta_y\eta_z\delta_y^2\delta_z^2+\eta_z\eta_x\delta_z^2\delta_x^2\right)-\frac{1}{8}\eta_x\eta_y\eta_z\delta_x^2\delta_y^2\delta_z^2\right)U^{n}$$

$$\rho = \frac{1-\frac{1}{2}(a_x+a_y+a_z)+\frac{1}{4}(a_xa_y+a_ya_z+a_za_x)+\frac{1}{8}a_xa_ya_z}{\left(1+\frac{1}{2}a_x\right)\left(1+\frac{1}{2}a_y\right)\left(1+\frac{1}{2}a_z\right)} = \frac{\left(\left(1-\frac{1}{2}a_x\right)\left(1-\frac{1}{2}a_y\right)\left(1-\frac{1}{2}a_z\right)+\frac{1}{4}a_xa_ya_z\right)}{\left(1+\frac{1}{2}a_x\right)\left(1+\frac{1}{2}a_y\right)\left(1+\frac{1}{2}a_z\right)}$$

uncond.

This scheme is the proper extension of the ADI Peaceman-Rashford to 3D.