

5.9.3 Mixed time advancement

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

convection-diffusion eq.

$(\phi = \psi e^{ikx_j})$

$$\frac{\partial \phi}{\partial t} = -c \frac{\partial \phi}{\partial x} \rightarrow \frac{d\psi}{dt} = -ick' \psi : \text{purely imaginary}$$

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \rightarrow \frac{d\psi}{dt} = -\alpha k'^2 \psi : \text{real & negative}$$

$$\frac{d\psi}{dt} = (-\alpha k'^2 - ick') \psi$$

complex number

- EE on convect. term + on diff. term

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

$\frac{\partial \phi^n}{\partial x} \propto \Delta x$ $\frac{\partial^2 \phi^n}{\partial x^2} \propto \Delta x^2$

$\Delta t \propto \Delta x^2$
not good!

- EE on conv. term + CN on diff. term

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

$\frac{\partial \phi^n}{\partial x} \propto \Delta x$ $O(\Delta t)$

CD2 → TDMA

$\Delta t \propto \Delta x$
not bad

- AB2 on conv. term + CN on diff. term

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\frac{c}{2} \left(3 \frac{\partial \phi^n}{\partial x} - \frac{\partial \phi^{n+1}}{\partial x} \right) + \frac{\alpha}{2} \left(\frac{\partial^2 \phi^{n+1}}{\partial x^2} + \frac{\partial^2 \phi^n}{\partial x^2} \right) + O(\Delta t^2)$$

CD2 \rightarrow TDMA

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

Stability analysis \rightarrow conditionally stable

store ϕ^n & ϕ^{n+1} ! not selfstarting. Δt fixed

- CN on all terms

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

CD2 \rightarrow TDMA absolutely stable.

* How about $c = \phi$?

$$\frac{\partial \phi}{\partial t} = -\phi \frac{\partial \phi}{\partial x} + \alpha \frac{\partial^2 \phi}{\partial x^2} : \text{nonlinear conv.-diff. eq.}$$

- CN on all terms

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

CD2

"fully implicit method". \rightarrow absolutely stable.

\rightarrow nonlinear algebraic eq's.

\rightarrow need iterations.

C

linearize this eq.

or solve nonlinear eq w/ iteration

- AB2 on conv. term + CN on diff. term.

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\frac{1}{2} \left(3\phi^n \frac{\partial \phi^n}{\partial x} - \phi^{n+1} \frac{\partial \phi^{n+1}}{\partial x} \right) + \frac{\alpha}{2} \left(\frac{\partial^2 \phi^{n+1}}{\partial x^2} + \frac{\partial^2 \phi^n}{\partial x^2} \right) + O(\Delta t^2)$$

$\Delta t \propto \Delta x$ explicit
 no iteration

$\frac{\Delta t \phi}{\Delta x} \leq 1$
 not self starting
 fixed Δt

store ϕ^n and ϕ^{n+1}

"semi-implicit method"

- AB2 on conv. & diff. terms.

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\frac{1}{2} \left(3\phi^n \frac{\partial \phi^n}{\partial x} - \phi^{n+1} \frac{\partial \phi^{n+1}}{\partial x} \right) + \frac{\alpha}{2} \left(3 \frac{\partial^2 \phi^{n+1}}{\partial x^2} - \frac{\partial^2 \phi^n}{\partial x^2} \right) + O(\Delta t^2)$$

fully explicit method

$\Delta t \propto \Delta x^2$

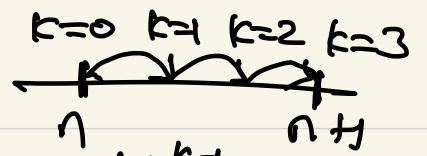
- RK3 on conv. term + CN on diff. term

$$\frac{\phi^k - \phi^{k-1}}{\Delta t} = \alpha_k \phi^{k-1} \frac{\partial \phi}{\partial x} + \beta_k \phi^{k-2} \frac{\partial \phi}{\partial x} + \alpha_k \frac{\partial^2 \phi}{\partial x^2} + \beta_k \frac{\partial^2 \phi}{\partial x^2} + O(\Delta t^2)$$

$(\phi^0 = \phi^n) (\phi^3 = \phi^{n+1}) \quad (k=1, 2, 3)$

$$\left(\alpha_1 = \frac{4}{15}, \beta_1 = \frac{8}{15}, \boxed{\rho_1 = 0}; \quad \alpha_2 = \frac{1}{15}, \beta_2 = \frac{5}{12}, \beta_2 = -\frac{17}{60} \right.$$

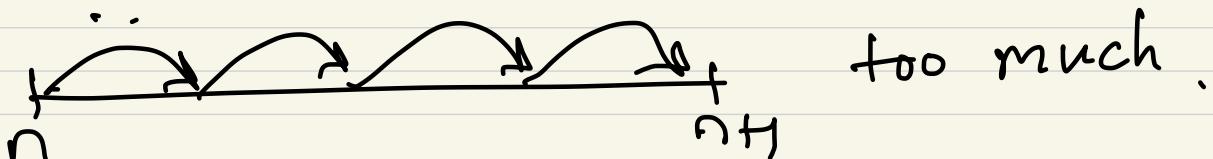
$$\left. \alpha_3 = \frac{1}{6}, \beta_3 = \frac{3}{4}, \beta_3 = -\frac{5}{12} \right)$$



self starting
 $\frac{\Delta t \phi}{\Delta x} \leq \sqrt{3} \quad \Delta t \propto \Delta x$

semi-implicit method
 change Δt during computation
 store ϕ^{k-1} & ϕ^{k-2}

- RK4 on conv. term + CN on diff. term



* Navier - Stokes eqs.

$$\left(\rho \frac{\partial u_i}{\partial t} + \sum_{j=1}^3 \rho u_j \frac{\partial u_i}{\partial x_j} \right) = - \frac{\partial P}{\partial x_i} + \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left(\mu \frac{\partial u_i}{\partial x_j} \right)$$

$\leftarrow \text{cn w/ ADI}$

$u_i = 1, 2, 3$

$\frac{\partial u_i}{\partial x_i} = 0$

coupled nonlinear second-order PDE.

$\nearrow 3D$

$\leftarrow \text{eqs. for } u_i \text{ & } P.$

AB2
RK3
CN

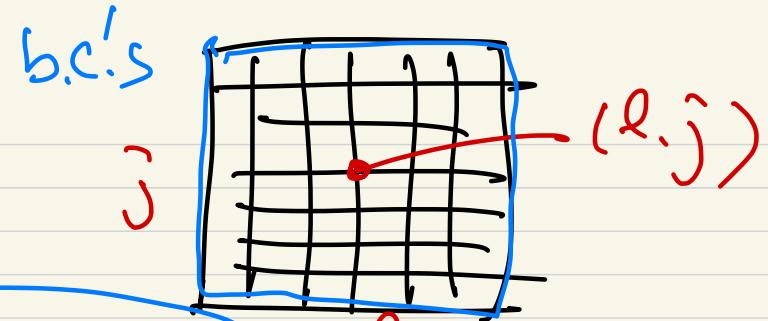
5.10 Elliptic PDEs

$$\left\{ \begin{array}{ll} \nabla^2 \phi = 0 & \text{Laplace eq.} \\ \nabla^2 \phi = f & \text{Poisson eq.} \\ \nabla^2 \phi + k^2 \phi = f & \text{Helmholtz eq.} \end{array} \right.$$

- $\nabla^2 \phi = f$
in $2D$, $\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f$

CD 2:

$$\frac{d_{l+1,j} - 2\phi_{l,j} + \phi_{l-1,j}}{\Delta x^2} + \frac{\phi_{l,j+1} - 2\phi_{l,j} + \phi_{l,j-1}}{\Delta y^2} = f_{l,j} \quad l=1,2,\dots,M-1, \quad j=1,2,\dots,N-1$$



$$(M-1)(N-1) \quad \begin{bmatrix} \phi_{11} \\ \phi_{21} \\ \phi_{31} \\ \vdots \\ \phi_{l-1,j} \\ \phi_{l,j} \\ \vdots \\ \phi_{M-1,N-1} \end{bmatrix} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

(M-1)(N-1)

(M-1)(N-1)

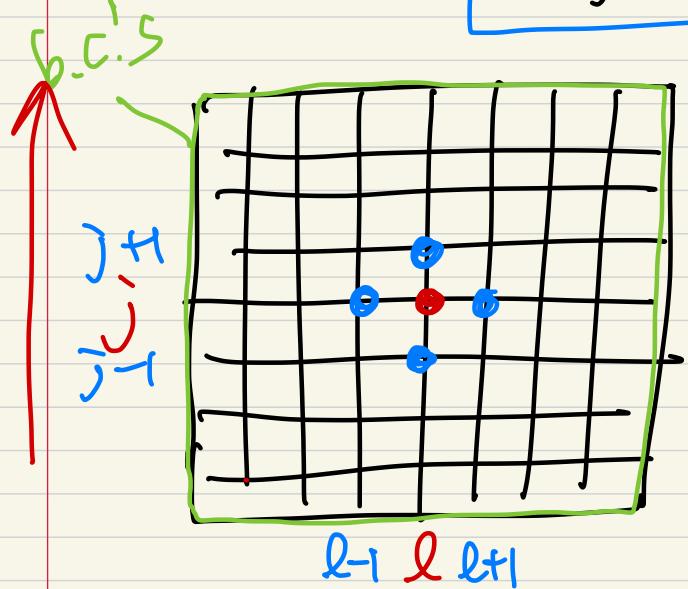
Block-tri-diagonal matrix \rightarrow difficult to solve directly
 $(M-1)(N-1) \times (M-1)(N-1)$

introduce iterative methods

$$\frac{\phi_{l+1,j}^k - 2\phi_{l,j}^k + \phi_{l-1,j}^k}{\Delta x^2} + \frac{\phi_{l,j+1}^k - 2\phi_{l,j}^k + \phi_{l,j-1}^k}{\Delta y^2} = f_{l,j}$$

K : iteration index

$$(\Delta x = \Delta y) \rightarrow \boxed{\phi_{l,j}^{k+1} = \frac{1}{4} (\phi_{l+1,j}^k + \phi_{l-1,j}^k + \phi_{l,j+1}^k + \phi_{l,j-1}^k) - \frac{\Delta x^2}{4} f_{l,j}}$$



Jacobi iteration

slow convergence.

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f \Rightarrow \boxed{\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} - f}$$

ellip. eq.

para. eq

As $t \rightarrow \infty$, steady sol. \rightarrow sol. of Poisson eq.

$$\boxed{\frac{\partial \phi}{\partial t} = 0}$$

We integrate para. eq. until reaching steady state
 $(\frac{\partial \phi}{\partial t} = 0)$

EE
CD2 ($\partial X = \partial Y$) $\rightarrow \frac{\phi_{l,j}^{n+1} - \phi_{l,j}^n}{\Delta t} = \frac{1}{\Delta x^2} (\phi_{l+1,j}^n - 2\phi_{l,j}^n + \phi_{l-1,j}^n + \phi_{l,j+1}^n - 2\phi_{l,j}^n + \phi_{l,j-1}^n)$

Stability limit: $\Delta t \leq \Delta x^2 / 4 \rightarrow \Delta t_{\max} = \frac{\Delta x^2}{C}$

$$\phi_{l,j}^{n+1} = \frac{1}{4} (\phi_{l+1,j}^n + \phi_{l-1,j}^n + \phi_{l,j+1}^n + \phi_{l,j-1}^n) - \frac{\Delta x^2}{C} f_{l,j}^n \quad X$$

Same as Jacobi iteration \rightarrow very slow convergence

$$\nabla^2 \phi = f$$

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi - f$$

not
very
popular

EE + CD2

$$\frac{\phi^{n+1} - \phi^n}{\delta t} = \nabla^2 \phi^n - f$$

↳ Jacobi iteration

CN + CD2

$$\frac{\phi^{n+1} - \phi^n}{\delta t} = \frac{1}{2} \nabla^2 (\phi^{n+1} + \phi^n) - f + \Theta(\delta t^2)$$

ADI + approx. fact.

no limit in δt



CN: $\delta t \uparrow \rightarrow (6 \rightarrow -1)$

IE + CD2

better than CN

$$\frac{\phi^{n+1} - \phi^n}{\delta t} = \nabla^2 \phi^{n+1} - f + \Theta(\delta t)$$

ADI + approx. fact.

$$\phi^n = \sigma^n \phi^0 M$$

5.10.1 Iterative solution methods

$Ax = b \rightarrow x = A^{-1}b$ direct sol. $\leftarrow \Theta(M^3N^3)$ operations expensive

$$\rightarrow A = A_1 - A_2$$

$$\rightarrow A_1 x = A_2 x + b \quad - \textcircled{*}$$

$$A_1 x^{k+1} = A_2 x^k + b \quad - \textcircled{**}$$

$$\rightarrow \boxed{x^{k+1} = A_1^{-1} A_2 x^k + A_1^{-1} b}$$

k : iteration index

A_1 should be easy to invert.

$$\text{Error : } \varepsilon^k = x - x^k$$

$$\textcircled{*} - \textcircled{**} : A_1(x - x^{k+1}) = A_2(x - x^k)$$

$$\rightarrow A_1 \varepsilon^{k+1} = A_2 \varepsilon^k$$

$$\rightarrow \varepsilon^{k+1} = A_1^{-1} A_2 \varepsilon^k \rightarrow \varepsilon^k = (A_1^{-1} A_2)^k \varepsilon^0 \quad (\lambda_{\max} < 1)$$

↑

For convergence, $\varepsilon^k \rightarrow 0$

\rightarrow Eigenvalues of $A_1^{-1} A_2$ should have modulus less than 1.

5.10.2 Point Jacobi method

$$\nabla^2 \phi = f \xrightarrow{\text{CD2}} A\phi = b$$

$$A = A_1 - A_2$$

A_1 : diagonal matrix D

the simplest choice for A_1

$$A_1 = D = \begin{bmatrix} -4 & & & \\ & -4 & & \\ & & \ddots & \\ 0 & & & \ddots \end{bmatrix}$$

$$A_1^{-1} = D^{-1} = \begin{bmatrix} -\frac{1}{4} & & & \\ & -\frac{1}{4} & & \\ & & \ddots & \\ 0 & & & \ddots \end{bmatrix}$$

$$A_2 = \left[\begin{array}{cc|cc|c} 0 & -1 & 1 & -1 & \\ -1 & 0 & -1 & 1 & \\ \hline -1 & -1 & 0 & -1 & \\ & & -1 & 0 & -1 \\ & & & & \ddots \end{array} \right]$$

$$A_1^{-1} A_2 = D^{-1} A_2 = -\frac{1}{4} A_2$$

$$A = \left[\begin{array}{cc|cc|c} -4 & 1 & 0 & 1 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 \\ \hline \ddots & \ddots & \ddots & 0 & 0 & 1 \\ 1 & 1 & 1 & -4 & 1 & 1 \\ & & & \ddots & \ddots & 1 \\ 0 & & & 1 & 1 & 1 \\ \hline & & & & \ddots & \ddots \end{array} \right]$$

$$\phi^{(k+1)} = -\frac{1}{4} A_2 \phi^{(k)} - \frac{1}{4} b$$

$$\rightarrow \boxed{\phi_{l,j}^{(k+1)} = \frac{1}{4} (\phi_{l+1,j}^k + \phi_{l-1,j}^k + \phi_{l,j+1}^k + \phi_{l,j-1}^k) - \frac{1}{4} b_{l,j}}$$

point Jacobi method

$$\lambda \text{ for } D^T A_2 : \lambda_{l,j} = \frac{1}{2} \left[\cos \frac{l\pi}{M} + \cos \frac{j\pi}{N} \right] \quad l=1, 2, \dots, M-1 \\ j=1, 2, \dots, N-1$$

$$\lambda_{\max} = \frac{1}{2} \left[\cos \frac{\pi}{M} + \cos \frac{\pi}{N} \right] = 1 - \frac{1}{4} \left(\frac{\pi^2}{M^2} + \frac{\pi^2}{N^2} \right) + \dots$$

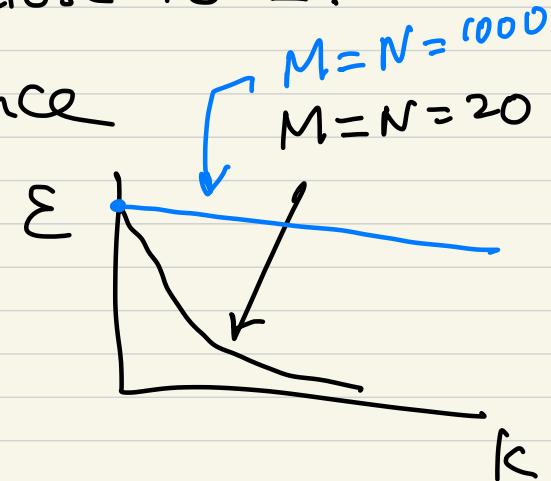
$$(\cos x = 1 - \frac{1}{2!} x^2 + \frac{1}{4!} x^4 + \dots)$$

for large $M \& N$, max eigenvalue is close to 1.

$$\varepsilon^k \sim \lambda_{\max} \varepsilon^0 \rightarrow \text{slow convergence}$$

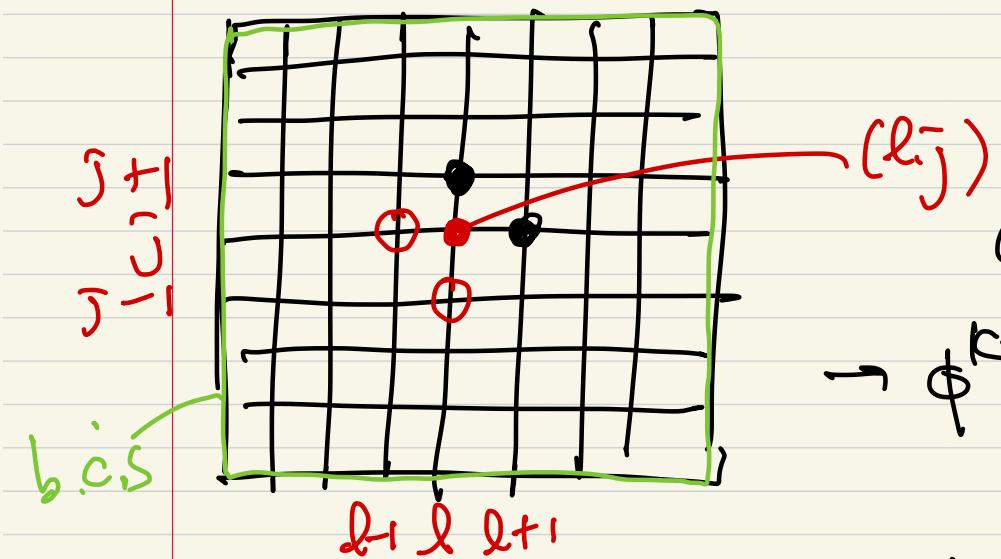
w/ large $M \& N \Rightarrow \lambda_{\max} \rightarrow 1$!

\therefore look for 'marginal' solution.



5.10.3 Gauss - Seidel method (GS)

$$CD2: \phi_{l,j}^{k+1} = \frac{1}{4} (\phi_{l+1,j}^k + \phi_{l-1,j}^k + \phi_{l,j+1}^k + \phi_{l,j-1}^k) - \frac{1}{4} b_{l,j}$$



$$A = A_1 - A_2 = (D - L) - U$$

$$(D - L) \phi^{k+1} = U \phi^k + b$$

$$\rightarrow \phi^{k+1} = (D - L)^{-1} U \phi^k + (D - L)^{-1} b$$

$$\text{Eigenvalue of } A_1^{-1} A_2 \text{ : } \lambda_{l,j} = \frac{1}{4} \left(\cos \frac{l\pi}{M} + \cos \frac{j\pi}{N} \right)^2$$

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

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

$$\lambda_{GS} = \lambda_J^2$$

$$\varepsilon_{GS}^k = \lambda_{GS}^k \varepsilon^0 = (\lambda_J^2)^k \varepsilon^0 = \lambda_J^{2k} \varepsilon^0 = \varepsilon_J^{2k}$$

$\therefore GS$ is twice faster than Jacobi.

CRAY
vector
machine

5.10.4 Successive over Relaxation (SOR) scheme $\nabla^2 \phi = f$

$$\text{Let } d = \phi^{k+1} - \phi^k$$

$$\phi^{k+1} = \phi^k + d \cdot \omega$$

ω : relaxation factor $(\omega > 1)$

$(\omega < 1 : \text{under-relaxation}$
for nonlinear eq.)

GS

$$(D-L)\phi^{k+1} = U\phi^k + b$$

$$D\phi^{k+1} = L\phi^{k+1} + U\phi^k + b \rightarrow \phi^{k+1} = D^{-1}L\phi^{k+1} + D^{-1}U\phi^k + D^{-1}b$$

$$\text{SOR: } \phi^{k+1} = \phi^k + [D^{-1}L\phi^{k+1} + D^{-1}U\phi^k + D^{-1}b - \phi^k] \cdot \omega$$

$$\rightarrow (I - \omega D^{-1}L)\phi^{k+1} = [(1-\omega)I + \omega D^{-1}U]\phi^k + \omega D^{-1}b$$

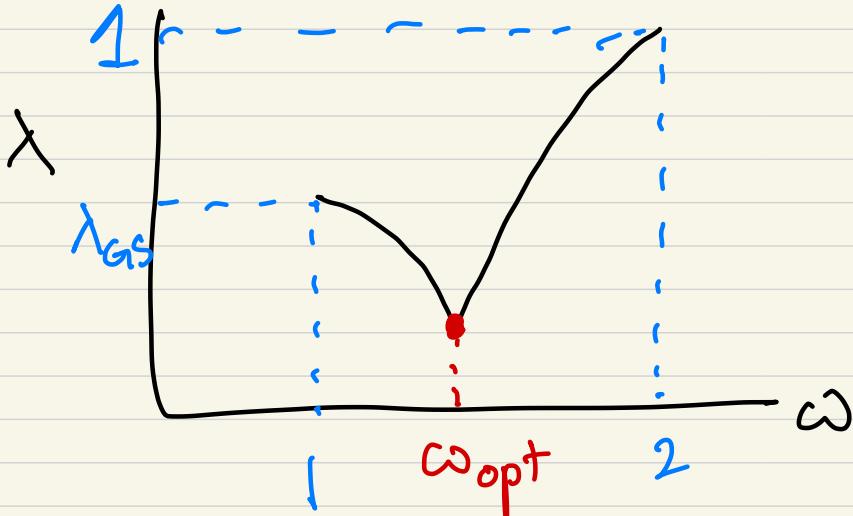
$$\rightarrow \boxed{\phi^{k+1} = (I - \omega D^{-1}L)^{-1}[(1-\omega)I + \omega D^{-1}U]\phi^k + (I - \omega D^{-1}L)^{-1}\omega D^{-1}b}$$

$$\text{GSOR} = A_1^T A_2$$

$$\text{for Poisson operator, } \lambda_{\text{SOR}} = \frac{1}{4}(\mu\omega + \sqrt{\mu^2\omega^2 - 4(\omega-1)})^2$$

$$\text{where } \mu = \lambda_J, (\lambda_J = \frac{1}{2}(\cos \frac{J\pi}{M} + \cos \frac{J\pi}{N}))$$

optimum ω ? minimize $\lambda \Rightarrow \frac{d\lambda}{d\omega} = 0 \rightarrow$ no solution



$$\frac{d\lambda}{d\omega} \rightarrow \infty \Rightarrow \omega_{\text{opt}} = \frac{2}{1 + \sqrt{1 - \mu_{\max}^2}}$$

As $M \& N \uparrow$, $\mu_{\max} \rightarrow 1$
 $\Rightarrow \omega_{\text{opt}} \rightarrow 2$.

$$\omega = 1 : \lambda_{\text{SOR}} = \mu^2 = \lambda_J^2 = \lambda_{\text{GS}}$$

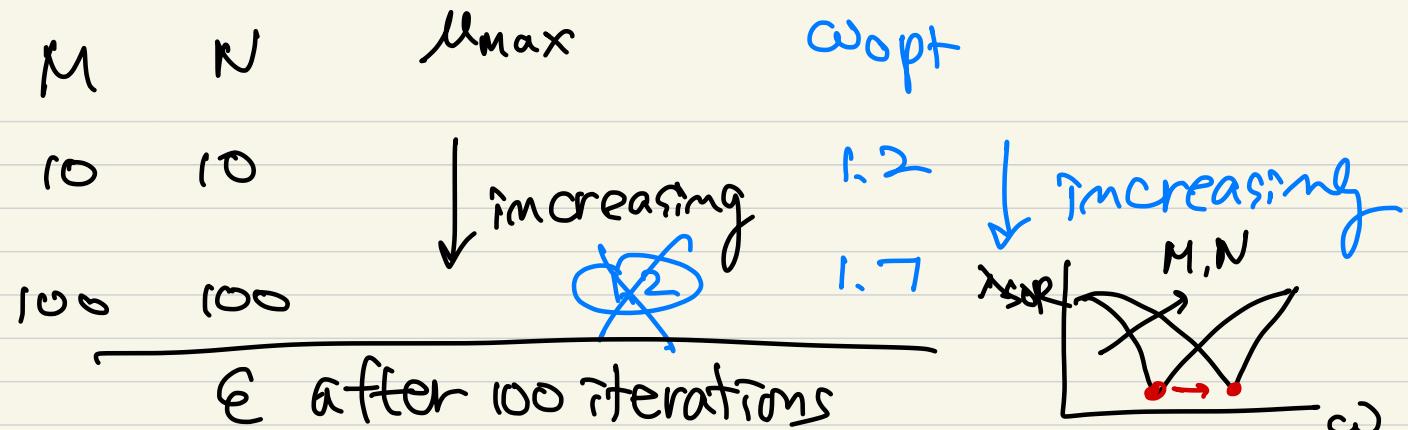
$$\omega = 2 : \lambda_{\text{SOR}} = \frac{1}{4} (2\mu + \sqrt{4\mu^2 - 4})^2 = \frac{1}{4} (2\mu + \sqrt{4(1-\mu^2)})^2$$

$$\rightarrow |\lambda_{\text{SOR}}|^2 = \dots = 1.$$

$$\Rightarrow \boxed{1 < \omega < 2 \text{ for SOR}} \rightarrow \omega_{\text{opt}} = 1.7 \approx 1.9$$

For problems w/ irregular geometries and non-uniform mesh,
 ω_{opt} cannot be obtained analytically, and thus ω_{opt} must
be found by numerical experiment.

$$\nabla^2 \phi = f$$



$M=N=100$

Jacobi

GS

SOR ω / $\omega = 1.75$

0.887

0.786

5×10^{-7}

ϵ

$\omega = 1.1$

1.6

1.7

