Last time
Taylor's series on equally spaced nodes

Forward difference

$$\frac{d^n U_i}{dx^n} \cong \frac{\Delta^n U_i}{h^n} + 0(h)$$

Backward difference

$$\frac{d^n U_i}{dx^n} \cong \frac{\nabla^n U_i}{h^n} + 0(h)$$

Centered difference

$$\frac{d^n U_i}{dx^n} \cong \frac{\delta^n U_i}{(1 \text{ or } \underset{\uparrow}{2})h^n} + 0(h^2)$$

for odd n

Requires n + 1 points

and in general $\Delta^n U_i = \Delta(\Delta^{n-1} U_i)$

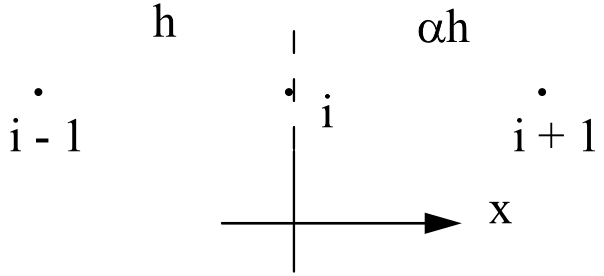
For greater accuracy one must add points

Uncentered: n + m points for $\approx \left.\frac{d^nU_i}{dx^n}\right|_i + 0(h^m)$

Centered: n+(m-1) points for $\approx \left.\frac{d^nU_i}{dx^n}\right|_i + 0(h^m)$
m must be even

For unequal spacing the centered approximation looses its meaning and accuracy is reduced to uncentered approximations

Alternative to Taylor Series : Polynomial Fit



Approximate U via
$\widehat{U} = ax^2 + bx + c$

3 unknowns (a, b, c) require 3 equations

$$\begin{aligned} U_{i-1} &= ah^2 + b(-h) + c \\ U_i &= c \\ U_{i+1} &= a(\alpha h)^2 + b(\alpha h) + c \end{aligned} \qquad \begin{bmatrix} h^2 & -h & 1 \\ 0 & 0 & 1 \\ (\alpha h)^2 & \alpha h & 1 \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{Bmatrix} U_{i-1} \\ U_i \\ U_{i+1} \end{Bmatrix}$$

Solve for a, b, c,

$$\begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \left\{ \begin{matrix} \{\alpha[U_{i-1}-U_i] + [U_{i+1}-U_i]\}/(\alpha^2+\alpha)h^2 \\ \{\alpha^2[U_{i-1}-U_i] + [U_{i+1}-U_i]\}/(\alpha^2+\alpha)h \\ U_i \end{matrix} \right\}$$

$$\frac{d\widehat{U}}{dx} = 2ax + b \qquad \frac{d^2\widehat{U}}{dx^2} = 2a$$

$$\frac{d^2\widehat{U}}{dx^2} = \frac{2[U_{i+1} - (1+\alpha)U_i + \alpha U_{i-1}]}{\alpha(\alpha+1)h^2}$$

i.e. The same as truncated Taylor Series

Loss of the leading error term is significant. By retaining the leading error in a Taylor Series one is continually reminded of the accuracy of the approximations and the origin of the formulation, (i.e. PDE) is more easily retained.

Alternate use of Error Term

$$\frac{dU_i}{dx} \sim \frac{\Delta U_i}{h} - \frac{h}{2}\frac{d^2U_i}{dx^2} + 0\ h^2$$

$$\longrightarrow \frac{\Delta^2 U_i}{h^2} + 0(h)$$

$$\frac{dU_i}{dx} \cong \frac{\Delta U_i}{h} - \frac{h}{2}\left[\frac{\Delta^2 U_i}{h^2} + 0(h)\right] + 0(h^2)$$

$$\cong \frac{\Delta U_i}{h} - \frac{\Delta^2 U_i}{2h} + 0\left(h^2\right)$$

$$\cong \frac{\left[\ U_{i+1} - U_i - \frac{1}{2}\left(U_{i+2} - 2U_{i+1} + U_i\right)\right]}{h} \ + \ 0\left(h\right)$$

$$\frac{dU_i}{dx} \cong \frac{-U_{i+2} + 4U_{i+1} - 3U_i}{2h} + 0\left(h^2\right)$$

i.e. The same as if derived directly from Taylor Series

Difference Formulas for Cross-Derivatives

a.) 2-D Taylor Series :

$$U(x+\Delta x, y+\Delta y) = U_{x,y} + \left(\Delta x\frac{\partial}{\partial x} + \Delta y\frac{\partial}{\partial y}\right)U_{x,y} + \frac{1}{2!}\left(\Delta x\frac{\partial}{\partial x} + \Delta y\frac{\partial}{\partial y}\right)^2 U_{x,y}$$

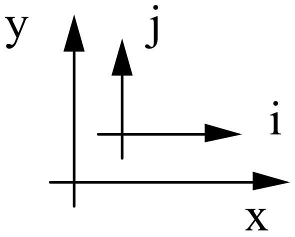
$$+\frac{1}{3!}\left(\Delta x\frac{\partial}{\partial x} + \Delta y\frac{\partial}{\partial y}\right)^3 U_{x,y} + \ldots + h.o.t.$$

Where $\left(\Delta x\frac{\partial}{\partial x} + \Delta y\frac{\partial}{\partial y}\right)^2 \equiv \Delta x^2\frac{\partial^2}{\partial x^2} + \Delta y^2\frac{\partial^2}{\partial y^2} + 2\Delta x\Delta y\frac{\partial^2}{\partial x\partial y}$ etc.

Procedure as in 1-D case: write Taylor series for all points in terms of U, $\frac{\partial U}{\partial x}, \frac{\partial U}{\partial y}$, … at point where $\frac{\partial^2 U}{\partial x \partial y}$ is wanted; mix together to get desired accuracy.

b.) Easier: Operate on 1-D formulas.

$$\frac{\partial^2 U}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial U}{\partial y}\right) \cong \frac{\partial}{\partial x}\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right) \cong \underbrace{\frac{\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)_{i+1} - \left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)_{i-1}}{2\Delta x}}_{\text{Intuitive ; What is leading error?}}$$



From 1-D: $\left(\frac{\partial U}{\partial y}\right) \cong \left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right) - \frac{(\Delta y)^2}{6}\frac{\partial^3 U}{\partial y^3} + \dots$

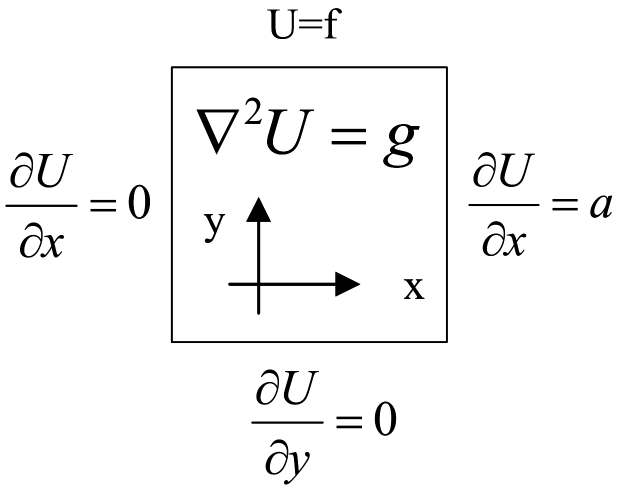
$$\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial y}\right) \cong \frac{\partial}{\partial x}\left(\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right) - \frac{(\Delta y)^2}{6}\frac{\partial^3 U}{\partial y^3} + \dots\right) \cong \left(\frac{\partial}{\partial x}\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right) - \frac{(\Delta y)^2}{6}\frac{\partial^4 U}{\partial x \partial y^3} + \dots\right)$$

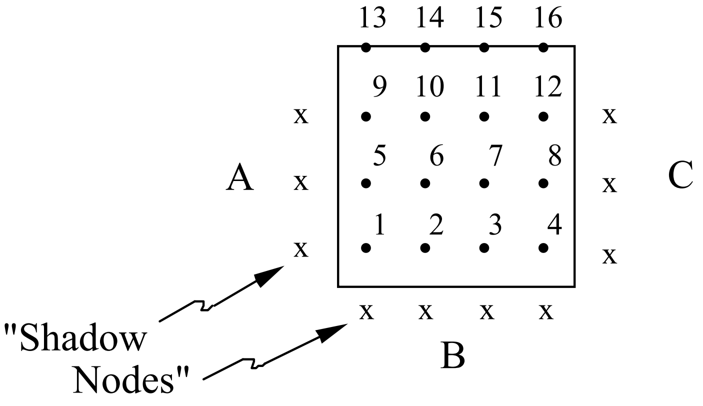
$$\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial y}\right) \cong \left(\frac{\left(\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)_{i+1} - \left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)_{i-1}\right)}{2\Delta x} - \frac{(\Delta x)^2}{6}\frac{\partial^3\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)}{\partial x^3} - \frac{(\Delta y)^2}{6}\frac{\partial^4 U}{\partial x \partial y^3} + \dots\right)$$

$$\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial y}\right) \cong \left(\frac{\left(\left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)_{i+1} - \left(\frac{U_{j+1} - U_{j-1}}{2\Delta y}\right)_{i-1}\right)}{2\Delta x} - \frac{(\Delta x)^2}{6}\frac{\partial^4 U}{\partial x^3 \partial y} - \frac{(\Delta y)^2}{6}\frac{\partial^4 U}{\partial x \partial y^3} + \dots\right)$$

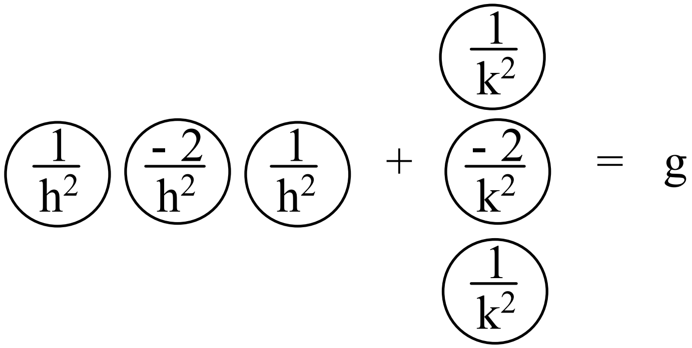
So the leading error terms are symmetrical.

Consider an Elliptic PDE (Poisson's Eqn.)



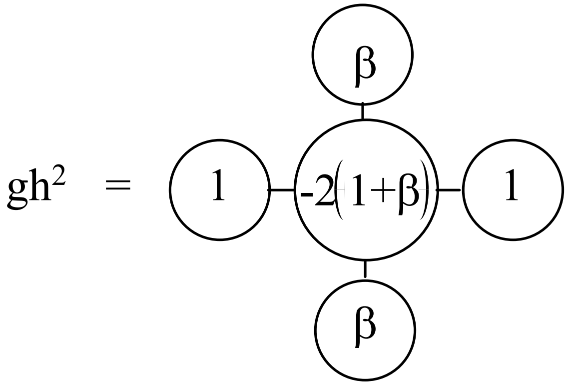


$$\text{PDE}: \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = g \cong \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} + \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{k^2}$$



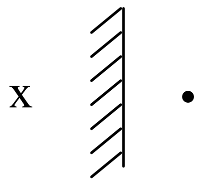
Define $\beta = \frac{h^2}{k^2}$

“Computational Molecule”



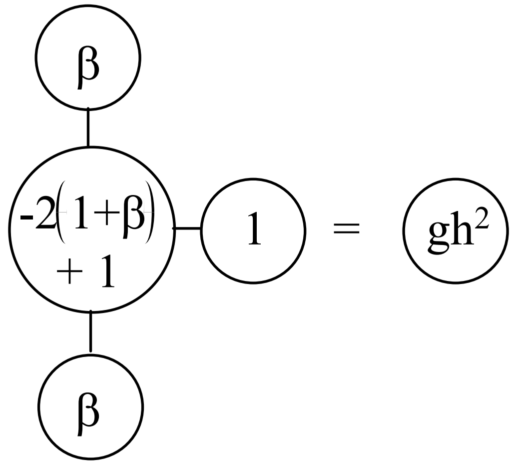
<u>Valid at all interior nodes</u>

Boundary A : $\frac{\partial U}{\partial x} = 0$



$$\frac{U_{\bullet} - U_x}{h} = 0 \Rightarrow$$

i.e. $U_x = U_{\bullet}$

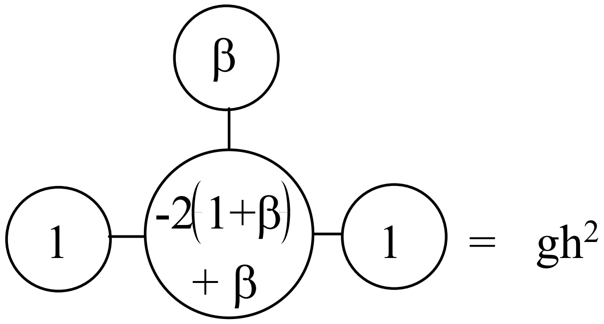


β

$-2(1+\beta) + 1$ — 1 $=$ gh^2

β

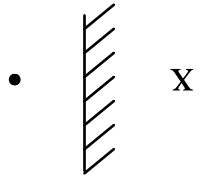
Boundary B :



β

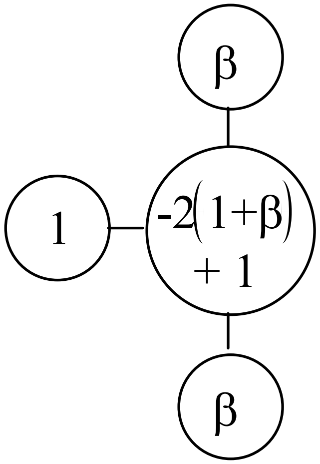
1 — $-2(1+\beta) + \beta$ — 1 $=$ gh^2

Boundary C :



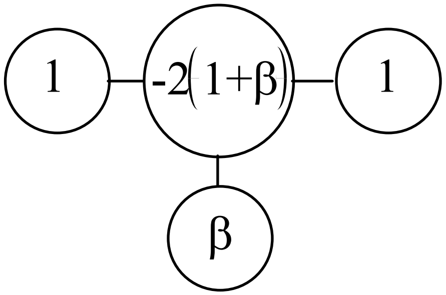
$$\frac{U_x - U_\bullet}{h} = a$$

$$U_x = U_\bullet + ah$$



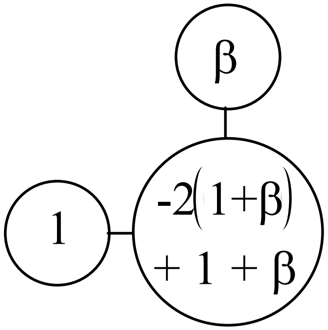
$$= -ah + gh^2$$

Top Row (nodes 9-12)



$$= -\beta f + gh^2$$

Corners : ex. node 4

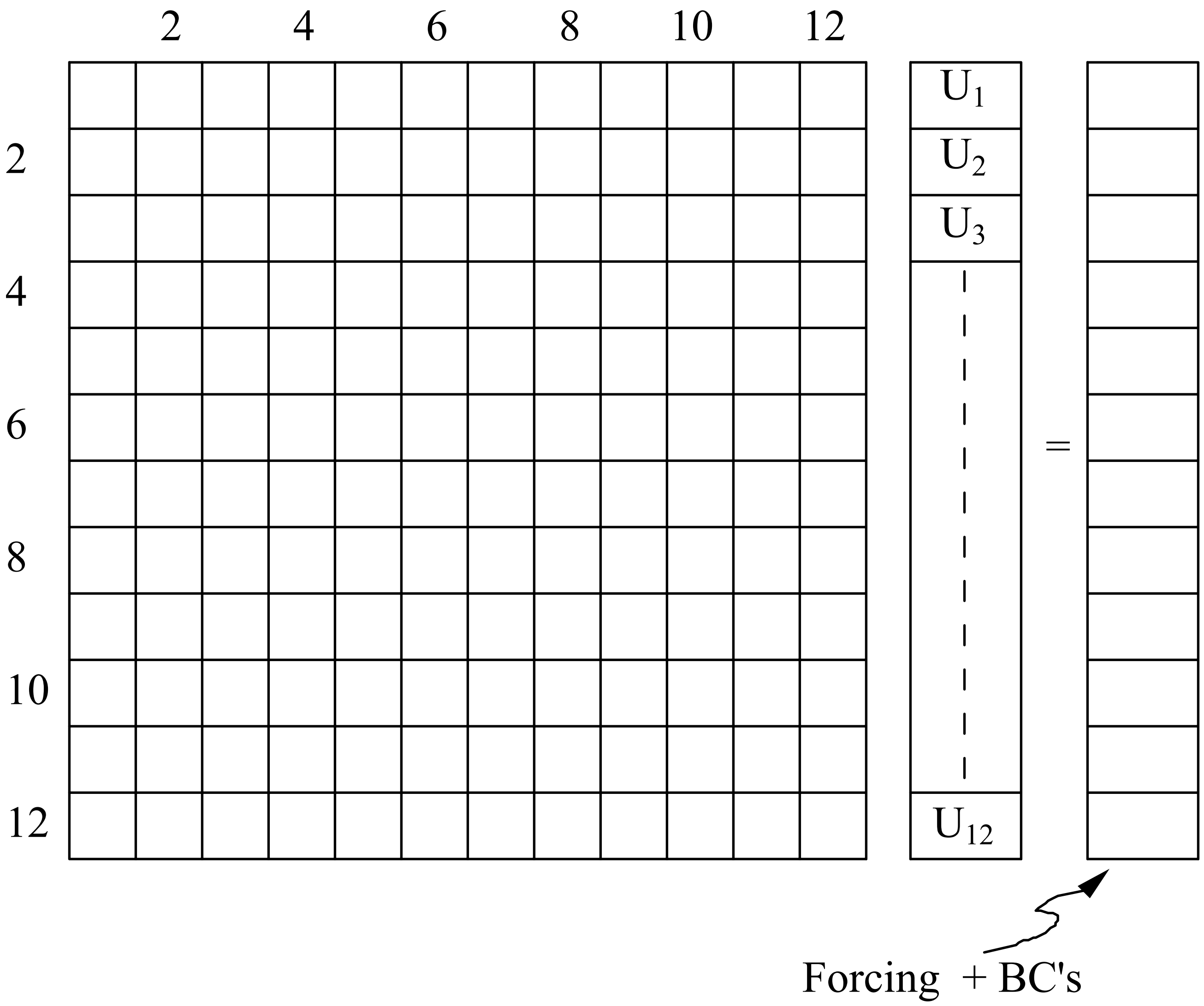


$= -ah + gh^2$

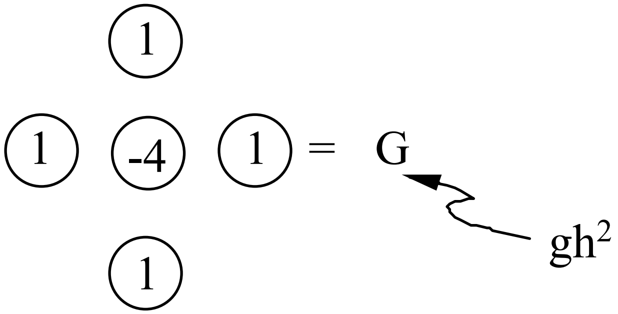
Basic Rule :

Type I Boundary : Do not use the PDE
Type II, III : Use PDE plus BC, together

The node spacing adjacent to the Type II boundaries are spaced at a $\Delta x/2$ format. This is NOT required. It IS accurate, however, the unknown values (u) on the boundary are not calculated. This may be a disadvantage. Similarly, if the geometry does not lend itself to this spacing conveniently - do not use it. The alternate strategy is to place nodes directly on the boundary. If nodes are on the boundary then the shadow node contributions do not usually move to the diagonal.


2
4
6
8
10
12
2
4
6
8
10
12
U_1
U_2
U_3
U_{12}
=
Forcing + BC's

For $\beta = 1$: $(h = k)$

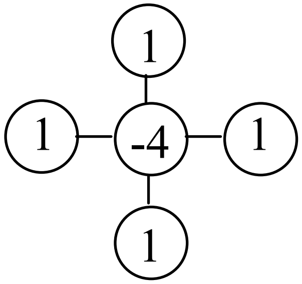


Solution Strategies

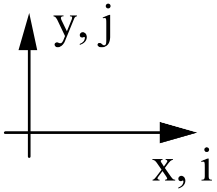
Direct:
- Exact algebraic solution in finite # of steps
- Non-repetitive
- Complicated coding
- Exploit sparse / banded structure
- Node numbering : dictates the banded structure
- LU Decomposition popular
  - Preserves bandwidth
  - "Back Substitution" step easy relative to decomposition ∴ numerous solutions to the same matrix can be gotten cheaply.

Iterative:

- Exact algebraic solution only after ∞ # of steps
- Monotonously repetitive
- Coding simple; proceed directly from <u>molecule</u>
- Exploit sparseness; banded structure irrelevant
- Retain double subscripts U_{ij}
- Node numbering important:
  - Dictates <u>order</u> in which iterations proceed
  - $\therefore$ Can determine convergence properties
- “Point” versus $\underbrace{\text{"Block" or "Line"}}_{\text{Matrix Inversion (usually 3-Diag)}}$ methods:



$$= gh^2 = G$$



$$U_{i+1,\,j} + U_{i-1,\,j} + U_{i,\,j+1} + U_{i,\,j-1} - 4U_{i,\,j} = G$$

Jacobi : "Solve" for $U_{i,\,j}$

$$U_{i,j}^{n+1} = \frac{1}{4}\left[U_{i+1,\,j} + U_{i-1,\,j} + U_{i,\,j+1} + U_{i,\,j-1} - G\right]^n$$

- Easy
- Need 2 arrays $U^n,\ U^{n+1}$
- Iteration independent of node #'s / order of calculation

Gauss - Seidel : Use latest info within Jacobi

$$U_{i,j}^{n+1} = \frac{1}{4}\left[U^n_{i+1,\,j} + \underline{U^{n+1}_{i-1,\,j}} + U^n_{i,\,j+1} + \underline{U^{n+1}_{i,\,j-1}} - G\right]$$

- Easy
- Only one array
- Ordering makes difference!

<u>S.O.R.</u> : Accelerate / Dampen the Gauss - Seidel :

$$\widetilde{U}_{i,j}^{n+1} \equiv \text{ Gauss - Seidel "estimate" for } U_{i,j}^{n+1}$$

$$U_{i,j}^{n+1} = \underbrace{\omega\widetilde{U}_{i,j}^{n+1} + (1 - \omega)U_{i,j}^{n}} = U_{i,j}^{n} + \omega\left(\widetilde{U}_{i,j}^{n+1} - U_{i,j}^{n}\right)$$

$$U_{i,j}^{n+1} = \omega\left[\frac{1}{4}[U_{i+1,j}^{n} + U_{i-1,j}^{n+1} + U_{i,j+1}^{n} + U_{i,j-1}^{n+1} - G]\right] + (1-\omega)U_{i,j}^{n}$$

where $\boxed{0 < \omega < 2}$