

CS601: Software Development for Scientific Computing

Autumn 2021

Week6:

- Structured Grids (Elliptic PDEs contd..)

Last Week..

- Intermediate C++
 - Class templates, STL, Operator overloading
- Structured Grids (Elliptic PDEs - introduction)

Elliptic Equation – Numerical Solution

1. Approximate the derivatives of $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$ using central differences
2. Choose step sizes δx and δy for x and y axis resp.
 1. Both x and y are independent variables here.
 2. Choose $\delta x = \delta y = h$
3. Write difference equation for approximating the PDE above

Elliptic Equation – Numerical Solution

1. Approximate the derivatives of $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$ using central differences

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{(u(x + \delta x, y) - 2u(x, y) + u(x - \delta x, y))}{(\delta x)^2}$$

$$\frac{\partial^2 u}{\partial y^2} \approx \frac{(u(x, y + \delta y) - 2u(x, y) + u(x, y - \delta y))}{(\delta y)^2}$$

Where, δx and δy are step sizes along x and y direction resp.

Elliptic Equation – Numerical Solution

- Substituting in $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$:

$$\frac{(u(x + \delta x, y) - 2u(x, y) + u(x - \delta x, y))}{(\delta x)^2}$$

+

$$\frac{(u(x, y + \delta y) - 2u(x, y) + u(x, y - \delta y))}{(\delta y)^2}$$

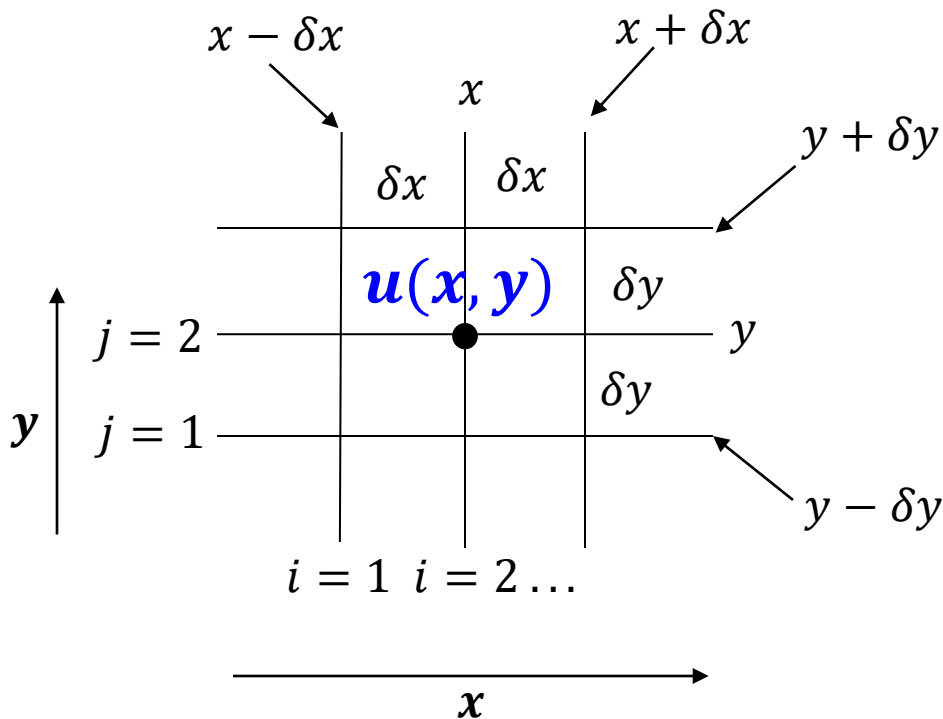
=

$$\frac{(u(x + \delta x, y) + u(x, y + \delta y) - 4u(x, y) + u(x - \delta x, y) + u(x, y - \delta y))}{(h)^2}$$

$$= f(x, y)$$

Elliptic Equation – Numerical Solution

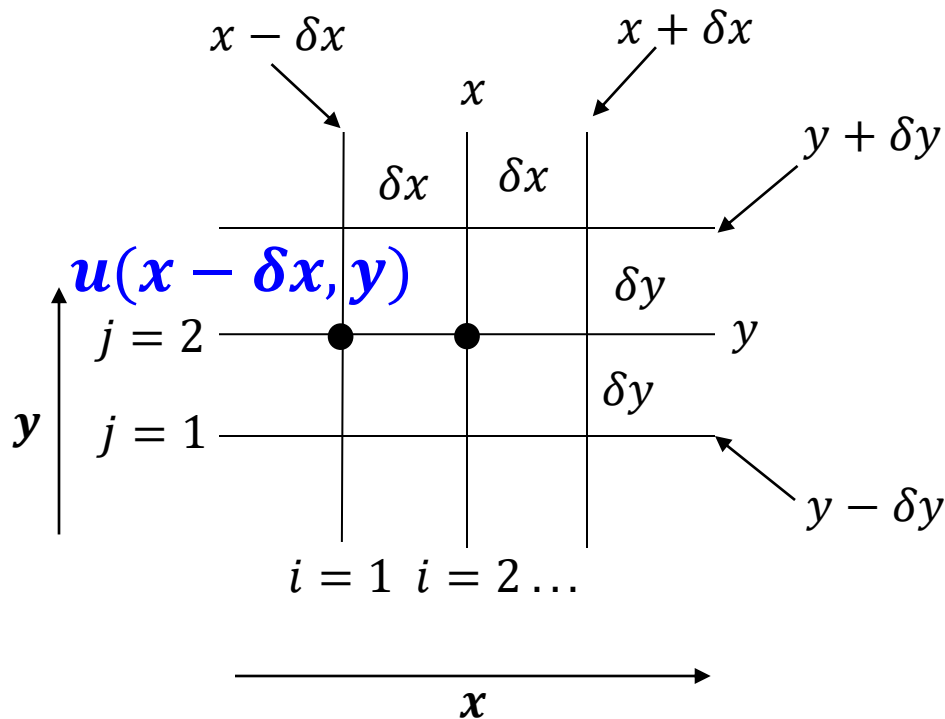
- Representing $u(x, y)$



Notation: $u_{i,j}$

Elliptic Equation – Numerical Solution

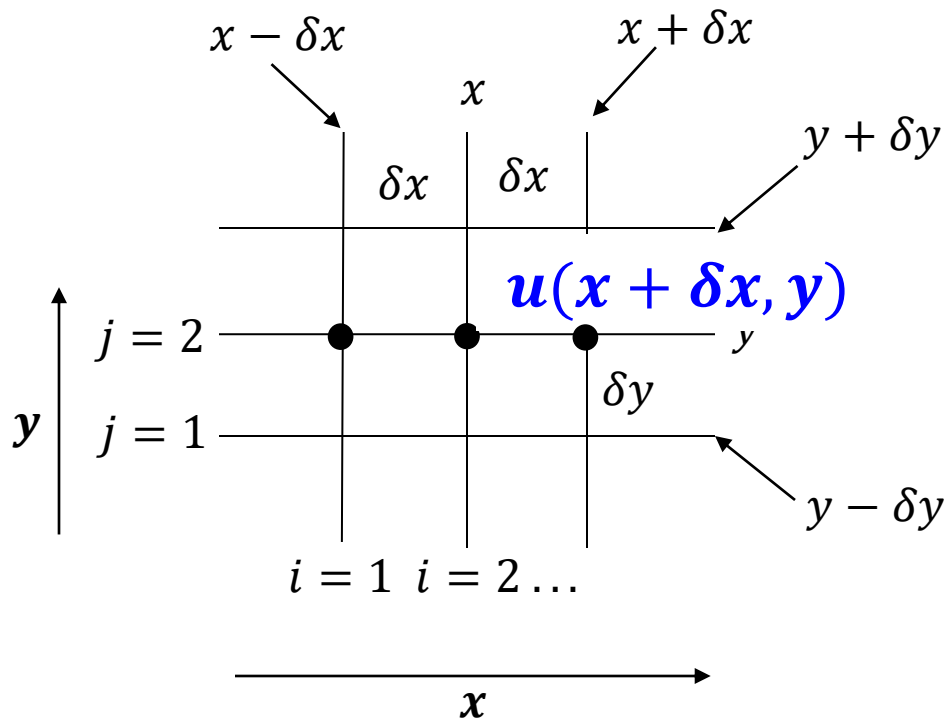
- Representing $u(x - \delta x, y)$



Notation: $u_{i-1,j}$

Elliptic Equation – Numerical Solution

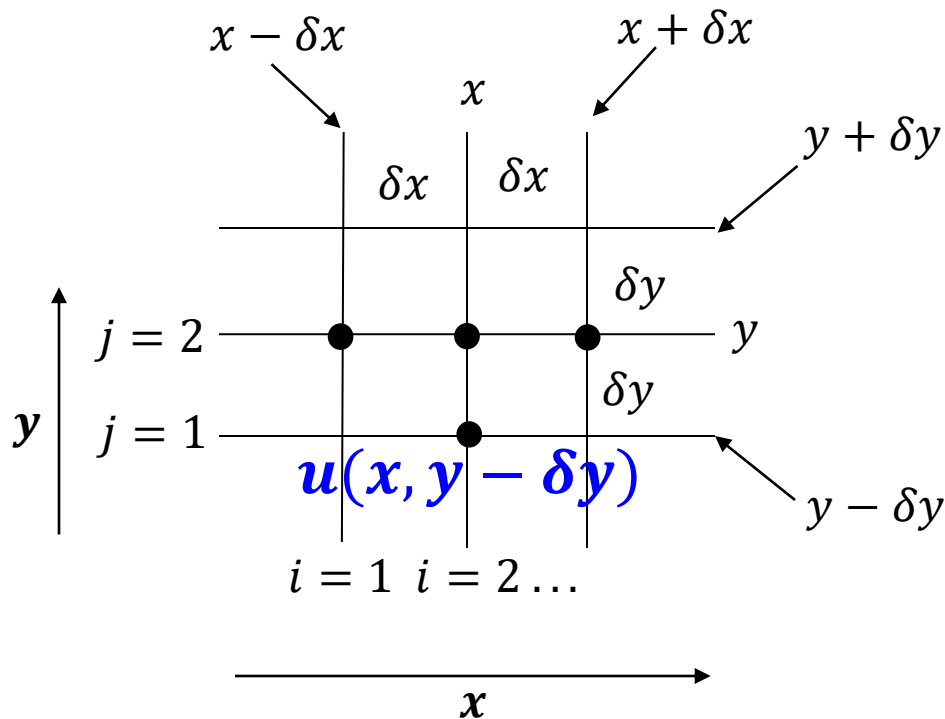
- Representing $u(x + \delta x, y)$



Notation: $u_{i+1,j}$

Elliptic Equation – Numerical Solution

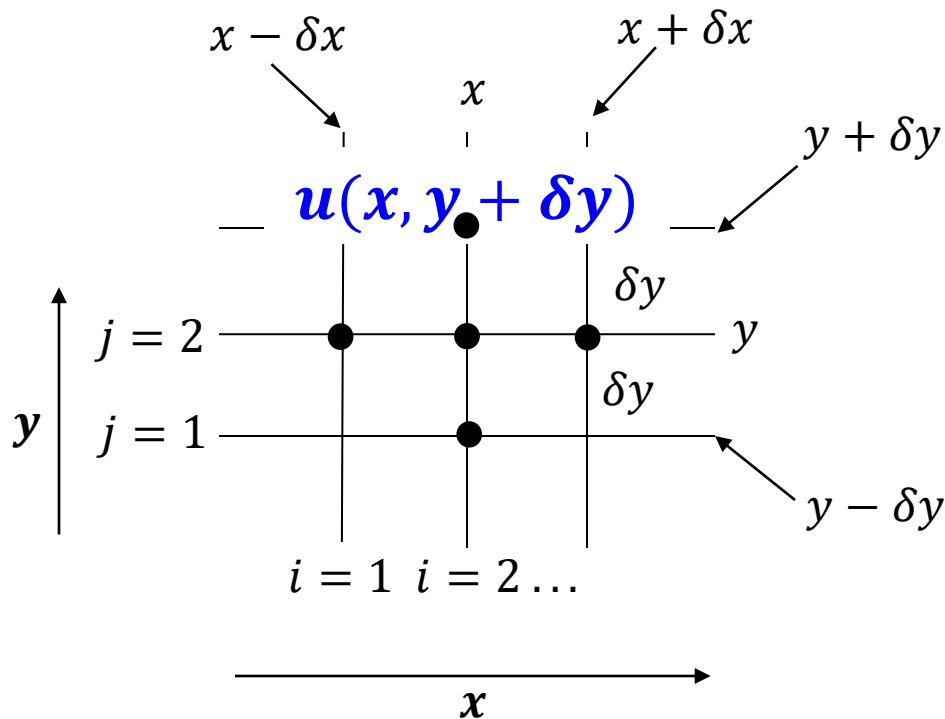
- Representing $u(x, y - \delta y)$



Notation: $u_{i,j-1}$

Elliptic Equation – Numerical Solution

- Representing $u(x, y + \delta y)$



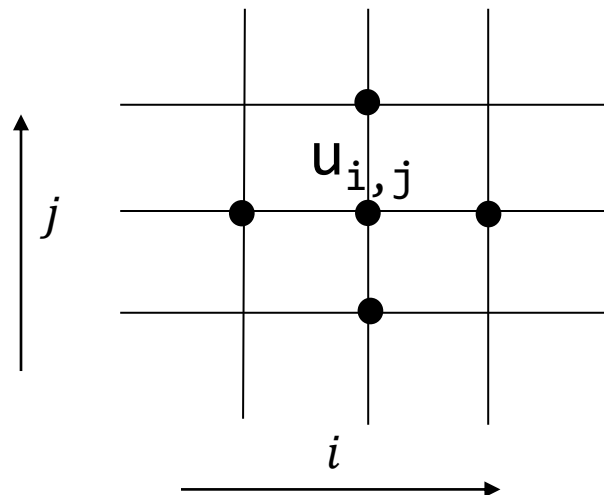
Notation: $u_{i,j+1}$

Elliptic Equation – Numerical Solution

- Rewriting:

$$\frac{(u(x + \delta x, y) + u(x, y + \delta y) - 4u(x, y) + u(x - \delta x, y) + u(x, y - \delta y))}{(h)^2} = f(x, y)$$

$$\frac{u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1}}{h^2} = f_{i,j}$$



5-point stencil

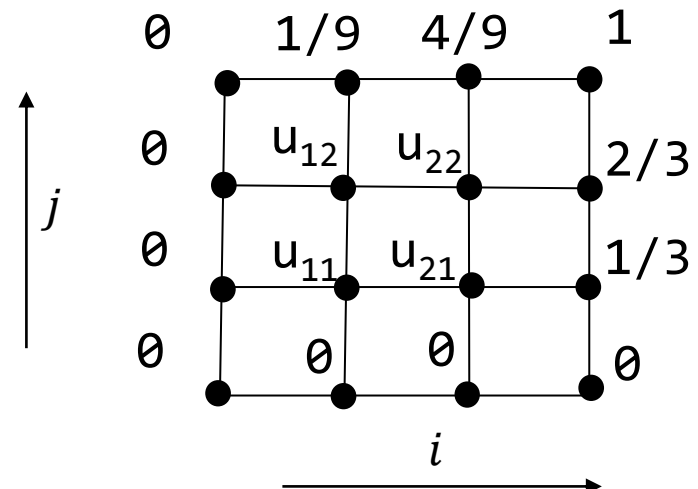
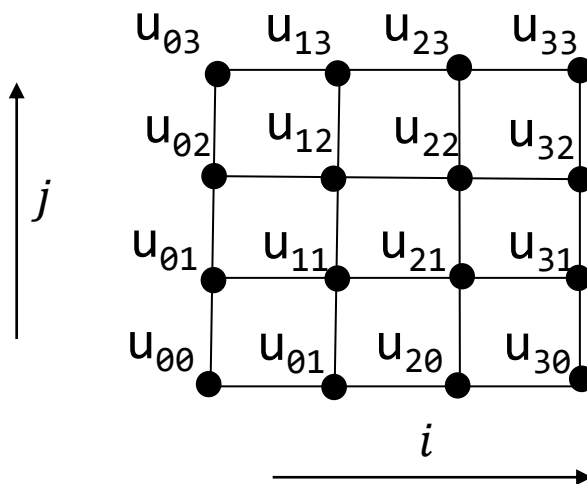
Elliptic Equation – Computing Stencil

- Consider the *boundary-value* problem:

$$u_{xx} + u_{yy} = 0 \text{ in the square } 0 < x < 1, 0 < y < 1$$

$$u = x^2y \text{ on the boundary, } h = 1/3$$

$$\frac{u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1}}{h^2} = 0$$



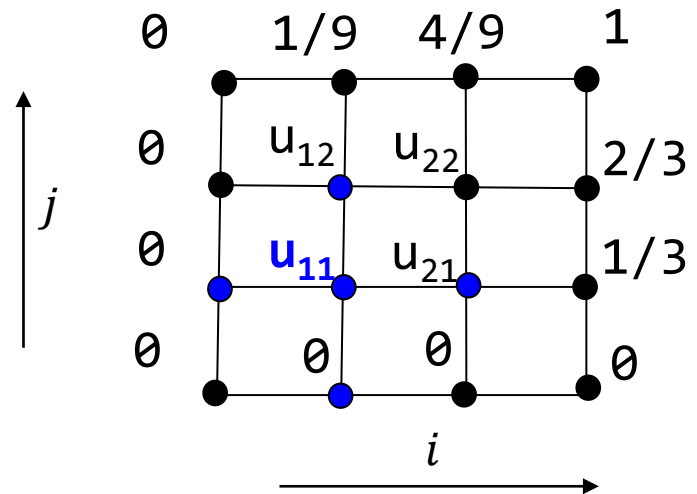
Elliptic Equation – Computing Stencil

- Computing u_{11}

$$(u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1} = \theta)$$

$$u_{21} + u_{12} - 4u_{11} + u_{01} + u_{10} = 0$$

$$u_{21} + u_{12} - 4u_{11} + \theta + \theta = 0$$



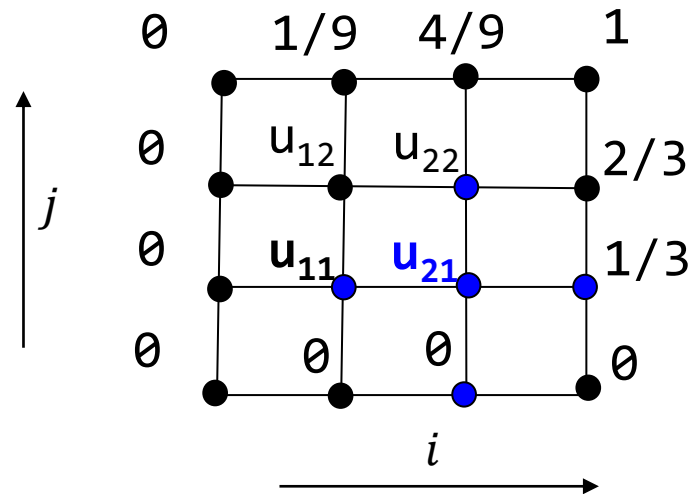
Elliptic Equation – Computing Stencil

- Computing u_{21}

$$(u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1} = 0)$$

$$u_{31} + u_{22} - 4u_{21} + u_{11} + u_{20} = 0$$

$$1/3 + u_{22} - 4u_{21} + u_{11} + 0 = 0$$



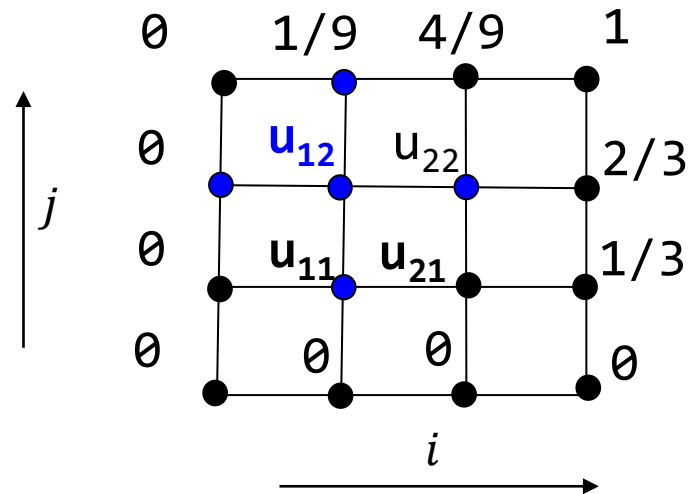
Elliptic Equation – Computing Stencil

- Computing u_{12}

$$(u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1} = 0)$$

$$u_{22} + u_{13} - 4u_{12} + u_{02} + u_{11} = 0$$

$$u_{22} + 1/9 - 4u_{12} + 0 + u_{11} = 0$$



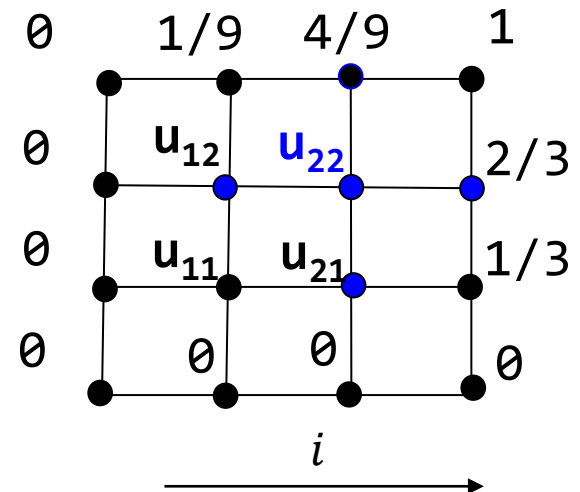
Elliptic Equation – Computing Stencil

- Computing u_{22}

$$(u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1} = 0)$$

$$u_{32} + u_{23} - 4u_{22} + u_{12} + u_{21} = 0$$

$$2/3 + 4/9 - 4u_{22} + u_{12} + u_{21} = 0$$

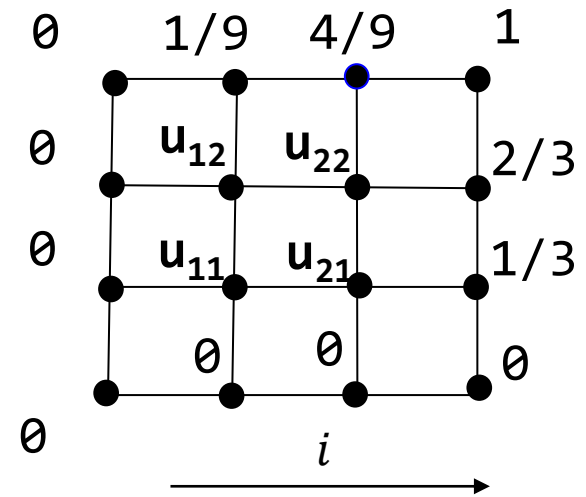


Elliptic Equation – Computing Stencil

- System of Equations

$$(u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1} = 0)$$

Right	Top	Center	Left	Bottom	
↓	↓	↓	↓	↓	
$u_{21} + u_{12} - 4u_{11} + 0 + 0 = 0$					
$1/3 + u_{22} - 4u_{21} + u_{11} + 0 = 0$					
$u_{22} + 1/9 - 4u_{12} + 0 + u_{11} = 0$					
$2/3 + 4/9 - 4u_{22} + u_{12} + u_{21} = 0$					



Elliptic Equation – Computing Stencil

- Computing System of Equations:

$$u_{21} + u_{12} - 4u_{11} + 0 + 0 = 0$$

$$1/3 + u_{22} - 4u_{21} + u_{11} + 0 = 0$$

$$u_{22} + 1/9 - 4u_{12} + 0 + u_{11} = 0$$

$$2/3 + 4/9 - 4u_{22} + u_{12} + u_{21} = 0$$

$$\begin{pmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix} = \begin{pmatrix} 0 \\ -1/3 \\ -1/9 \\ -10/9 \end{pmatrix} \quad \mathbf{Ax=B}$$

A
x
=
B

Matrix A has only coefficients

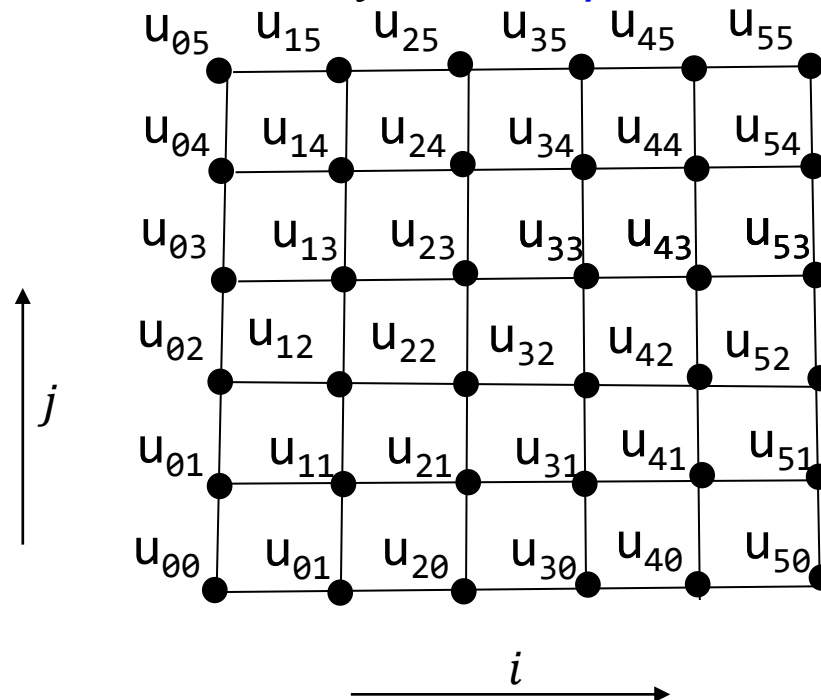
$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -4 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

Elliptic Equation – Computing Stencil

- Consider the *boundary-value* problem:

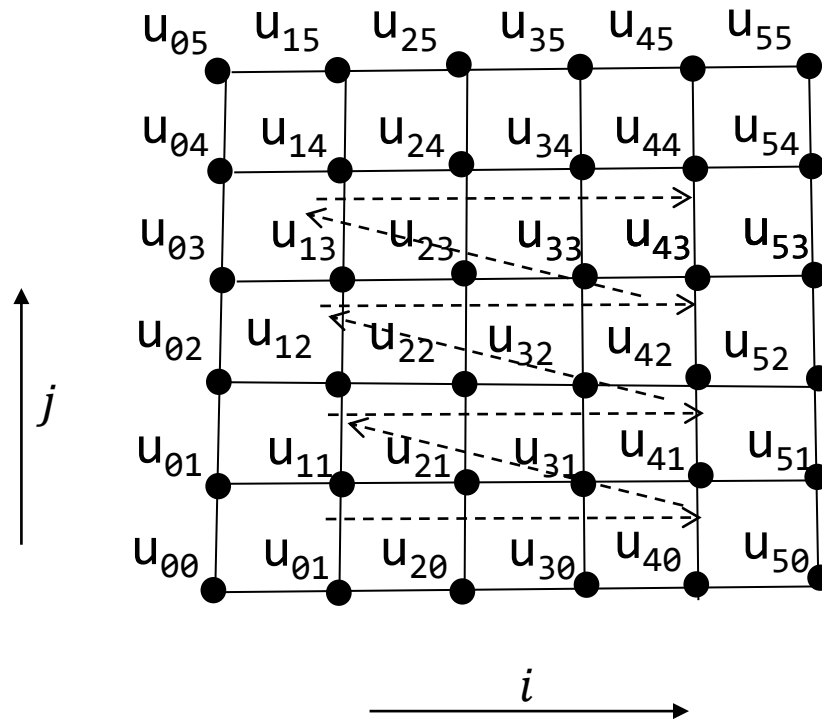
$$u_{xx} + u_{yy} = 0 \text{ in the square } 0 < x < 1, 0 < y < 1$$

$$u = x^2y \text{ on the boundary, } h = 1/5$$



Elliptic Equation – Computing Stencil

- Computing stencil (boundary values are all given): 16 unknowns (u_{11} to u_{44}), So, 16 equations.



Elliptic Equation – Computing Stencil

-4	1	0	0	1								
1	-4	1	0	0	1							
0	1	-4	1	0	0	1						
0	0	1	-4	1	0	0	1					
1	0	0	1	-4	1	0	0	1				
	1	0	0	1	-4	1	0	0	1			
		1	0	0	1	-4	1	0	0	1		
			1	0	0	1	-4	1	0	0	1	
				1	0	0	1	-4	1	0	0	1

- Lot of Zeros!
- Five non-zero bands
 - Top-left to bottom-right diagonals
- Main diagonal is all -4 (from center of the stencil)
- What about others?

Elliptic Equation – Computing Stencil

-4	1	0	0	1								
1	-4	1	0	0	1							
0	1	-4	1	0	0	1						
0	0	1	-4	1	0	0	1					
1	0	0	1	-4	1	0	0	1				
	1	0	0	1	-4	1	0	0	1			
		1	0	0	1	-4	1	0	0	1		
			1	0	0	1	-4	1	0	0	1	
				1	0	0	1	-4	1	0	0	1

- Lot of Zeros!
- Five non-zero bands
 - Top-left to bottom-right diagonals
- Main diagonal is all -4 (from center of the stencil)
- What about others?

Left

Elliptic Equation – Computing Stencil

-4	1	0	0	1								
1	-4	1	0	0	1							
0	1	-4	1	0	0	1						
0	0	1	-4	1	0	0	1					
1	0	0	1	-4	1	0	0	1				
	1	0	0	1	-4	1	0	0	1			
		1	0	0	1	-4	1	0	0	1		
			1	0	0	1	-4	1	0	0	1	
				1	0	0	1	-4	1	0	0	1

- Lot of Zeros!
- Five non-zero bands
 - Top-left to bottom-right diagonals
- Main diagonal is all -4 (from center of the stencil)
- What about others?

Right

Elliptic Equation – Computing Stencil

-4	1	0	0	1								
1	-4	1	0	0	1							
0	1	-4	1	0	0	1						
0	0	1	-4	1	0	0	1					
1	0	0	1	-4	1	0	0	1				
	1	0	0	1	-4	1	0	0	1			
		1	0	0	1	-4	1	0	0	1		
			1	0	0	1	-4	1	0	0	1	
				1	0	0	1	-4	1	0	0	1

- Lot of Zeros!
- Five non-zero bands
 - Top-left to bottom-right diagonals
- Main diagonal is all -4 (from center of the stencil)
- What about others?

Bottom

Elliptic Equation – Computing Stencil

-4	1	0	0	1							
1	-4	1	0	0	1						
0	1	-4	1	0	0	1					
0	0	1	-4	1	0	0	1				
1	0	0	1	-4	1	0	0	1			
	1	0	0	1	-4	1	0	0	1		
		1	0	0	1	-4	1	0	0	1	
			1	0	0	1	-4	1	0	0	1
				1	0	0	1	-4	1	0	0
					1	0	0	1	-4	1	0
						1	0	0	1	-4	1
							1	0	0	1	-4
								1	0	0	1
									1	0	0
										1	0
											1

Top

- Lot of Zeros!
- Five non-zero bands
 - Top-left to bottom-right diagonals
- Main diagonal is all -4 (from center of the stencil)
- What about others?

Computing Stencil – Iterative Methods

- Jacobi and Gauss-Seidel
 - Start with an initial guess for the unknowns u^0_{ij}
 - Improve the guess u^1_{ij}
 - Iterate: derive the new guess, u^{n+1}_{ij} , from old guess u^n_{ij}
- Solution (Jacobi):
 - Approximate the *value of the center* with old values of (left, right, top, bottom)

Background – Jacobi Iteration

- **Goal:** find solution to system of equations represented by $AX=B$
- **Approach:** find sequence of approximations $X^0, X^1, X^2, \dots, X^n$, which gradually approach X .
 - X^0 is called initial guess, X^i 's called *iterates*
- **Method:**
 - Split A into $A=L+D+U$ e.g.

$$\begin{pmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} + \begin{pmatrix} -4 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & -4 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

\uparrow
L

\uparrow
D

\uparrow
U

Background – Jacobi Iteration

- **Compute:** $AX=B$ is $(L+D+U)X=B$

$$\Rightarrow DX = -(L+U)X+B$$

$$\Rightarrow DX^{(k+1)} = -(L+U)X^k+B \quad \textbf{(iterate step)}$$

$$\Rightarrow X^{(k+1)} = D^{-1} (-(L+U)X^k) + D^{-1}B$$

(As long as D has no zeros in the diagonal $X^{(k+1)}$ is obtained)

- E.g.
$$\begin{pmatrix} -4 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & -4 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix}^{\mathbf{1}} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix}^{\mathbf{0}} + \begin{pmatrix} 0 \\ -1/3 \\ -1/9 \\ -10/9 \end{pmatrix},$$

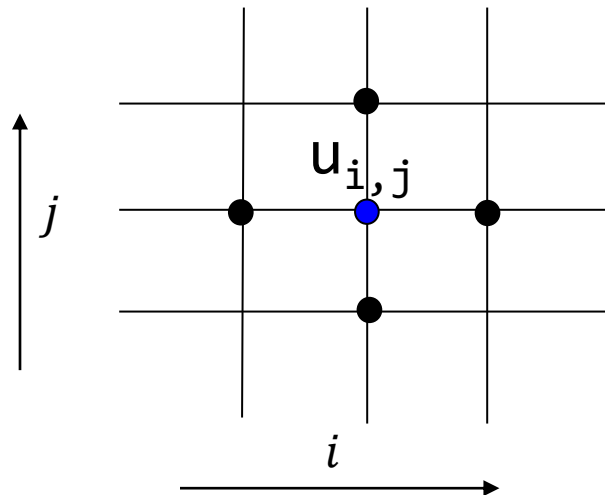
u_{ij} 's value in ($\mathbf{1}$)st iteration is computed based on u_{ij} values computed in ($\mathbf{0}$)th iteration

Background – Jacobi Iteration

- E.g.
$$\begin{pmatrix} -4 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & -4 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix}^{k+1} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix}^k + \begin{pmatrix} 0 \\ -1/3 \\ -1/9 \\ -10/9 \end{pmatrix},$$

u_{ij} 's value in $(k+1)^{st}$ iteration is computed based on u_{ij} values computed in $(k)^{th}$ iteration

- Center's value is updated. Why?



5-point stencil