CS601: Software Development for Scientific Computing

Autumn 2023

Week13: Solution Methods for Irregular Geometry (FEM)

Recap

Discretization

- All problems with ‘continuous’ quantities don’t require discretization
  - Most often they do.
- When discretization is done:
  - How refined is your discretization depends on certain parameters: step-size, cell shape and size. E.g.
    - Size of the largest cell (PDEs in FEM),
    - Step size in ODEs
  - Accuracy of the solution is of prime concern
    - Discretization always gives an approximate solution. Why?
    - Errors may creep in. Must provide an estimate of error.

Accuracy

- Discretization error
  - Is because of the way discretization is done
  - E.g. use more number of rays to minimize discretization error in ray tracing
- Solution error
  - The equation to be solved influences solution error
  - E.g. use more number of iterations in PDEs to minimize solution error
- Accuracy of the solution depends on both solution and discretization errors
- Accuracy also depends on cell shape

Error Estimate

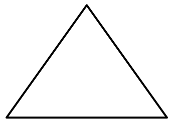
- You will have to deal with errors in the presence of discretization
  - Providing error estimate is necessary
- *Apriori* error estimate
  - Gives insight on whether a discretization strategy is suitable or not
  - Depends on discretization parameter
  - Properties of the (unknown) exact solution
  - Error is bound by: $\mathbf{Ch^p}$ where, C depends on exact solution, h is discretization parameter, and p is a fixed exponent. *Assumption: exact solution is differentiable, typically, p+1 times.*

Error Estimate

- *Aposteriori* error estimate
  - Is estimation of the error in computed (Approximate) solution and does not depend on information about exact solution
  - E.g. Sleipner-A oil rig disaster

Cell Shape

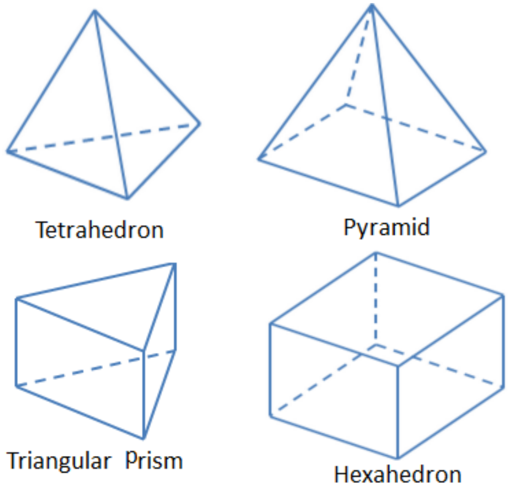
- 2D:



triangle

quadrilateral

- 3D: triangular or quadrilateral faced. E.g.

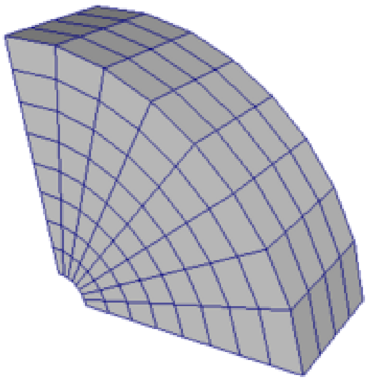


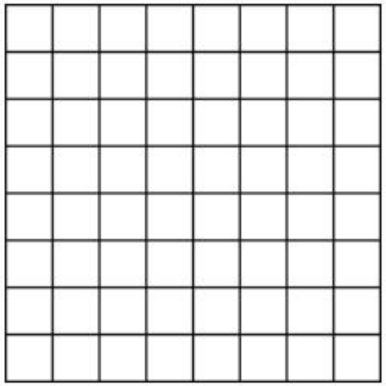
source: wikipedia

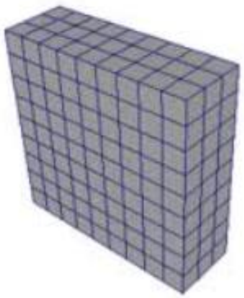
Tetrahedron: 4 vertices, 4 edges, 4△ faces
Pyramid: 5 vertices, 8 edges, 4 △ and 1 ▭ face
Triangular prism: 6 vertices, 9 edges, 2△ and 3▭ faces
Hexahedron: 8 vertices, 12 edges, 6 ▭ faces

Structured Grids

- Have regular connectivity between cells
  - i.e. every cell is connected to a predictable number of neighbor cells
- Quadrilateral (in 2D) and Hexahedra (in 3D) are most common type of cells
- Simplest grid is a rectangular region with uniformly divided rectangular cells (in 2D).







credits: nanohub.org

Structured Grids – Problem Statement

- Given:
  - A geometry
  - A mathematical model (partial differential equation (PDE))
  - Certain conditions / constraints / known values etc.
- Goal:
  1. Discretize into a grid of cells
  2. Approximate the PDE on the grid
  3. Solve the PDE on the grid

PDEs

- consider a function $u = u(x, t)$ satisfying the second-order PDE:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial t} + C\frac{\partial^2 u}{\partial t^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial t} + Fu = G\ ,$$

Where A-G are given functions. This is a PDE of type:

- Parabolic: if $B^2 - 4AC = 0$
- Elliptic: if $B^2 - 4AC < 0$
- Hyperbolic: if $B^2 - 4AC > 0$

PDEs

- consider a function $u = u(x, t)$ satisfying the second-order PDE:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial t} + C\frac{\partial^2 u}{\partial t^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial t} + Fu = G \ ,$$

Where A-G are given functions. This is a PDE of type:

- Parabolic: if $B^2 - 4AC = 0$ Heat equation: $\partial_t u - \Delta u = f$
- Elliptic: if $B^2 - 4AC < 0$ Poisson problem: $-\Delta u = f$
- Hyperbolic: if $B^2 - 4AC > 0$

Wave equation: $\partial_t{}^2 u - \Delta u = f$

Approximating PDEs

Finite Difference Method

- Suppose $y = f(x)$
  - Forward difference approximation to the first-order derivative of f w.r.t. x is:

$$\frac{df}{dx} \approx \frac{\left(f(x+\delta x)-f(x)\right)}{\delta x}$$

  - Central difference approximation to the first-order derivative of f w.r.t. x is:

$$\frac{df}{dx} \approx \frac{\left(f(x+\delta x)-f(x-\delta x)\right)}{2\delta x}$$

  - Central difference approximation to the second-order derivative of f w.r.t. x is:

$$\frac{d^2f}{dx^2} \approx \frac{\left(f(x+\delta x)-2f(x)+f(x-\delta x)\right)}{(\delta x)^2}$$

Boundary Conditions and Classification

- Essential / Dirichlet
  - Value of the dependent variable is specified
  - E.g. temperature at the edges of the rod are constant 0°
- Neumann / Natural
  - Value of the dependent variable is specified as gradient of the dependent variable T e.g. dT/dx.
- Mixed / Robin
  - value of the dependent variable is specified as a function of the gradient. E.g. $-K(dTdx)x=L=hA(T-T\infty)$

Boundary and Initial Value Problems

- Boundary Value Problems
  - PDE contains independent variables that are only spatial in nature (do not contain time).
  - E.g. $\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$
- Initial Value Problems
  - PDE contains independent variables that are spatial and temporal in nature.
  - E.g. $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$

Definitions (Laplace Equation and Poisson Equation)

- Consider a region of interest R in, say, xy plane. The following is a *boundary-value problem*:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \qquad \text{,where}$$

f is a given function in R and

$u = g$,where

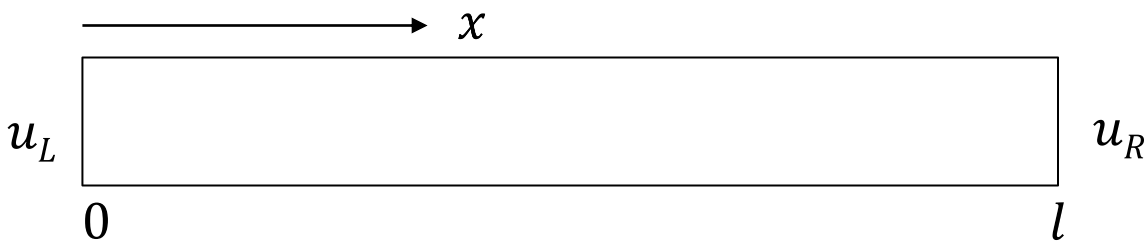
the function g tells the value of function u at boundary of R

- if $f = 0$ everywhere, then Eqn. (1) is Laplace's Equation
- if $f \neq 0$ somewhere in R, then Eqn. (1) is Poisson's Equation

Application: 1D Heat Equation

$$\partial_t u \ - \Delta u = f(x)$$

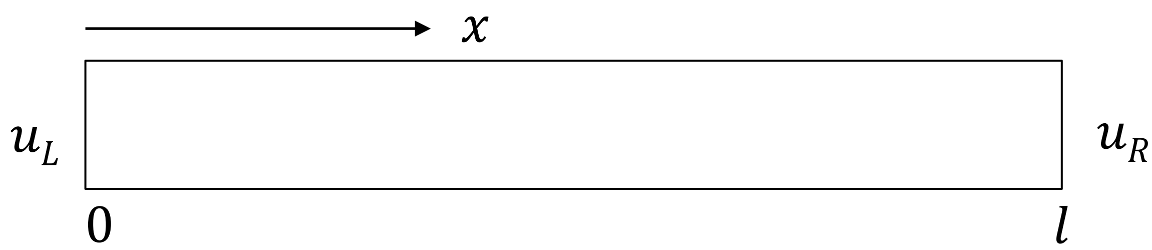
- Recall notation: $\Delta u \quad = \sum_{k=1}^{n} \partial_{kk} u$ $\qquad \frac{\partial u}{\partial t} = \ \partial_t u$
- Example: heat conduction through a rod



- $u = u(x, t)$ is the temperature of the metal bar at distance x from one end and at time t
- Goal: find u, temperature at different points along the length of the rod (i.e. from 0 to l)

1D Heat Equation - Equations

- Example: heat conduction through a rod



$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \qquad (0 < x < l, t > 0)$$

α is thermal diffusivity

$$u(0,t) = u_L \, , \quad t > 0$$
$$u(l,t) = u_R \, , \quad t > 0$$
$$u(x,0) = f(x)$$

Initial and boundary conditions

$$x(l - x)$$

1D Heat Equation - Analytical Solution

- Analytical Solution:

$$u(x,t) = \sum_{m=1}^{\infty} B_m e^{-m^2 \alpha \pi^2 t / l^2} \sin\left(\frac{m\pi x}{l}\right) ,$$

where, $B_m = 2/l \int_0^l f(s) \sin\left(\frac{m\pi s}{l}\right) ds$

But we are interested in a numerical solution

1D Heat Equation - Approximating Partial Derivatives

Plugging into $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$:

$$\frac{(u_j^{n+1} - u_j^n)}{\delta t} = \alpha \frac{(u_{j+1}^n - 2\, u_j^n + u_{j-1}^n)}{(\delta x)^2}$$

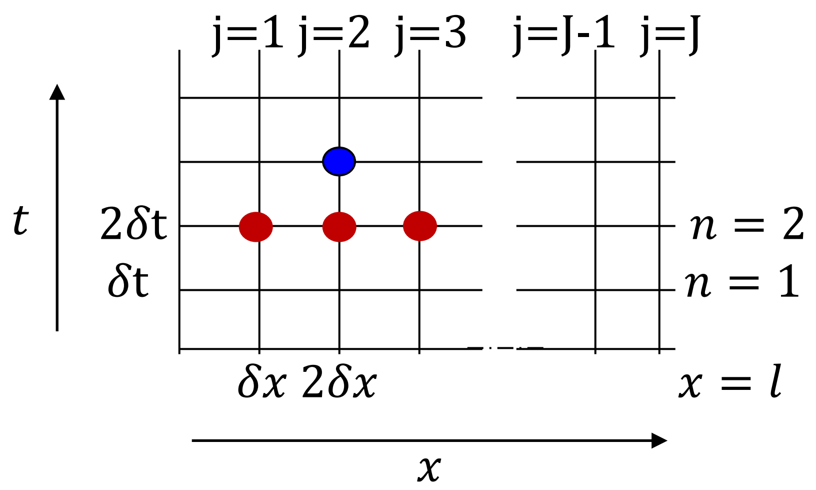
This is also called as difference equation because you are computing difference between successive values of a function involving discrete variables.

Recall: u_j^{n+1} denotes taking j steps along the length of the rod (x axis) and $n + 1$ time steps (t axis)

1D Heat Equation - Approximating Partial Derivatives

visualizing,

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

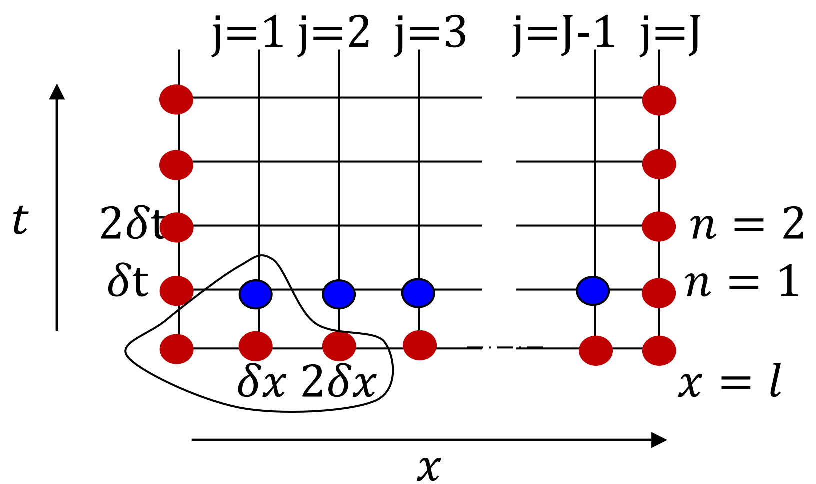


To compute the value of function at blue dot, you need 3 values indicated by the red dots – 3-point stencil

1D Heat Equation - Computation

visualizing,

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$



All the red dot values are known. We begin with computing the temp at blue dots (after time δt)

<u>Order of computation:</u> start from left and move to the right. Then move up (to the next time step, 2δt)

Explicit Difference Method: Stability

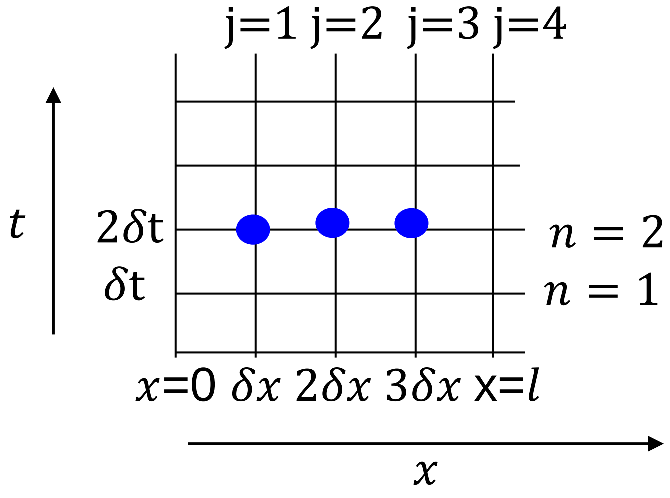
- Given: $l = 1,$
  $u(0, t) = u_L = 0,$
  $u(l, t) = u_R = 0,$
  $u(x, 0) = f(x) = x(l - x)$
  $\alpha = 1,$
- Choose: $\delta x = 0.25, \delta t = 0.075$
- Solve.

Explicit Difference Method: Stability

- Compute time-step 2 values

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

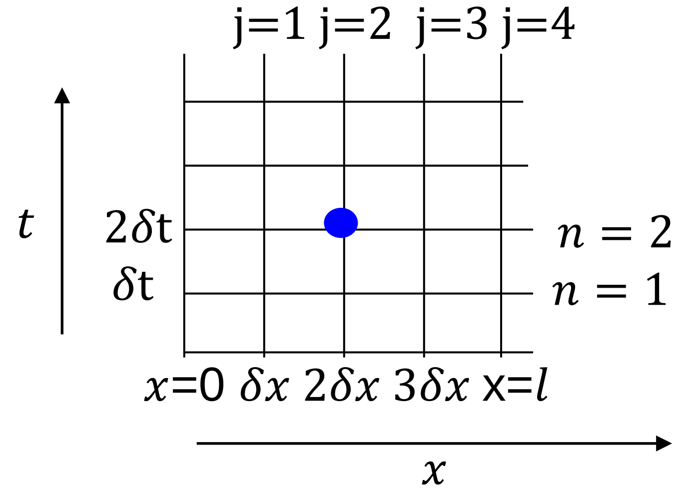
$$u_1^2 = u_1^1 + r(u_0^1 - 2u_1^1 + u_2^1) = 0.06851$$
$$u_2^2 = u_2^1 + r(u_1^1 - 2u_2^1 + u_3^1) = \mathbf{-0.05173}$$
$$u_3^2 = u_3^1 + r(u_2^1 - 2u_3^1 + u_4^1) = 0.06851$$



Explicit Difference Method: Stability

- Temperature at $2\delta x$ after $2\delta t$ time units went into negative! (when the boundaries were held constant at 0)
  - Example of *instability*

$u_2^2 = u_2^1 + r(u_1^1 - 2u_2^1 + u_3^1)$=**-0.05173**



The solution is stable (for heat diffusion problem) only if the approximations for $u(x,t)$ do not get bigger in magnitude with time

Explicit Difference Method: Stability

- The solution for heat diffusion problem is stable only if:

$$r \leq \frac{1}{2}$$

Therefore, choose your time step in such a way that:

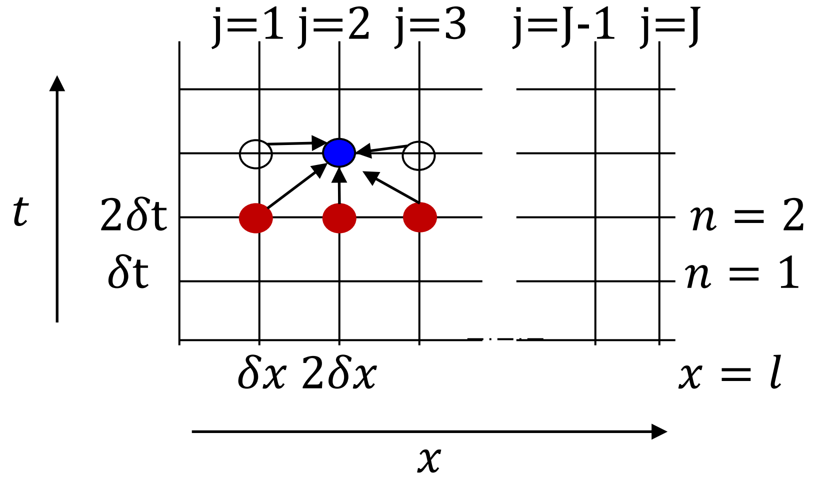
$$\delta t \leq \frac{\delta x^2}{2\alpha}$$

But this is a severe limitation!

Implicit Method: Stability

- Overcoming instability:

$$u_j^{n+1} = u_j^n \ + \ 1/2\, \mathrm{r}(\ u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}\ )$$



To compute the value of function at blue dot, you need 6 values indicated by the red dots (known) and 3 additional ones (unknown) above

Implicit Method: Stability

- Overcoming instability:

  $u_j^{n+1} = u_j^n \; + \; 1/2\, r(\, u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1} \,)$

- Extra work involved to determine the values of unknowns in a time step
  - Solve a system of simultaneous equations. Is it worth it?

Exercise

- Consider the *boundary-value* problem:

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

$u = x^2y$ on the boundary.

Is this Laplace equation or Poisson equation?

Elliptic Equation – Numerical Solution for a 2D Problem

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 and 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

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

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

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

Elliptic Equation – Numerical Solution

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

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

$$+$$

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

$$=$$

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

$$= f(x, y)$$

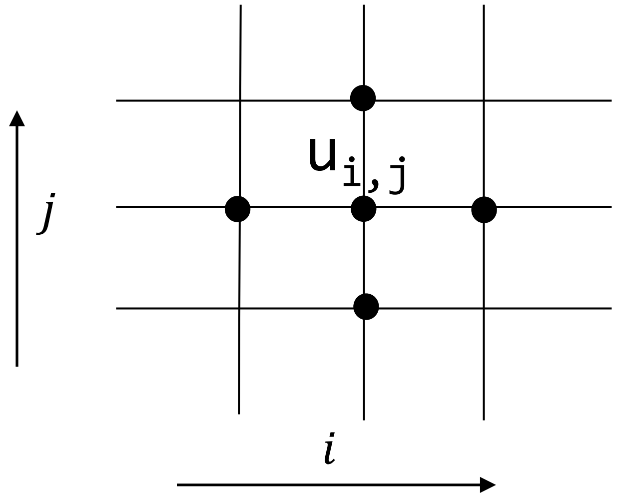
Elliptic Equation – Numerical Solution

- Rewriting:

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

$$= f(x,y)$$

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



5-point stencil

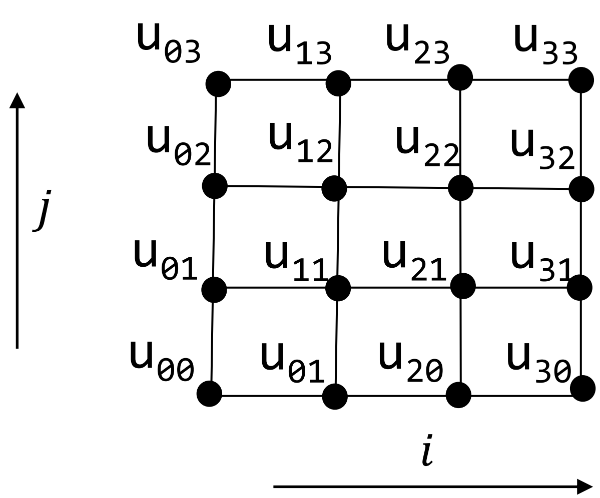
Elliptic Equation – Computing Stencil

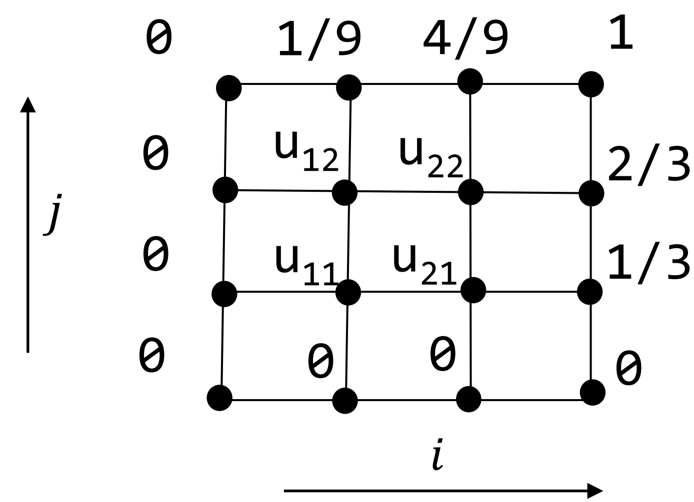
- Consider the *boundary-value* problem:

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

$u = x^2y$ on the boundary, $h = 1/3$

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





Elliptic Equation – Computing Stencil

- System of Equations

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

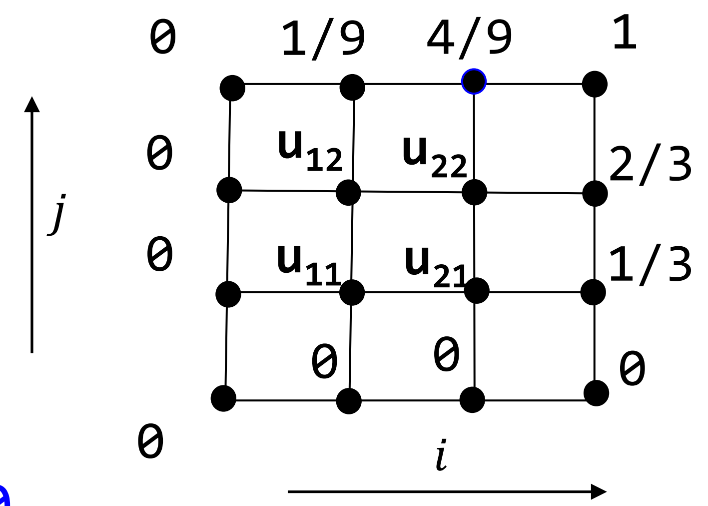
Right Top Center Left Bottom

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

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

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

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



Elliptic Equation – Computing Stencil

- Computing System of Equations:

$$u_{21} + u_{12} - 4u_{11} + 0 + 0 = 0$$
$$1/3 + u_{22} - 4u_{21} + u_{11} + 0 = 0$$
$$u_{22} + 1/9 - 4u_{12} + 0 + u_{11} = 0$$
$$2/3 + 4/9 - 4u_{22} + u_{12} + u_{21} = 0$$

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

A x = B

Ax=B

Matrix A has only coefficients

	1	
1	**-4**	**1**
	1	

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

- Matrix A has this format (shown here for h=5)
- Lot of Zeros!
- Five non-zero bands
  - Top-left to bottom-right diagonals
- Main diagonal is all -4 (from center of the stencil)

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

Left

- 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

Right

- 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

Bottom

- 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

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 . . . 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.

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

L D U

Background – Jacobi Iteration

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

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

$\Rightarrow DX^{(k+1)} = -(L+U)X^{k}+B$ **(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. $$\begin{pmatrix} -4 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & -4 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix}^{\mathbf{1}} = -\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{pmatrix}^{\mathbf{0}} + \begin{pmatrix} 0 \\ -1/3 \\ -1/9 \\ -10/9 \end{pmatrix},$$

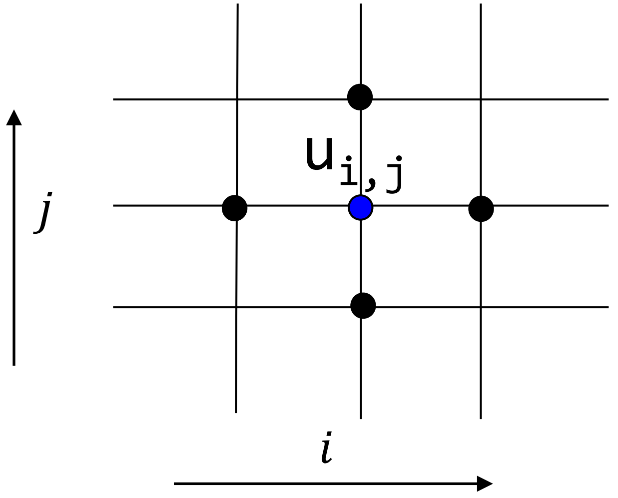
u_{ij} 's value in $(\mathbf{1})^{st}$ iteration is computed based on u_{ij} values computed in $(\mathbf{0})^{th}$ iteration

Background – Jacobi Iteration

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

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

- Center's value is updated. Why?



5-point stencil

Computing Stencil

- $\boldsymbol{u_{right} + u_{top} - 4u_{center} + u_{left} + u_{bottom} = 0}$

  $\Rightarrow \boldsymbol{u_{center} = 1/4(u_{right} + u_{top} + u_{left} + u_{bottom})}$

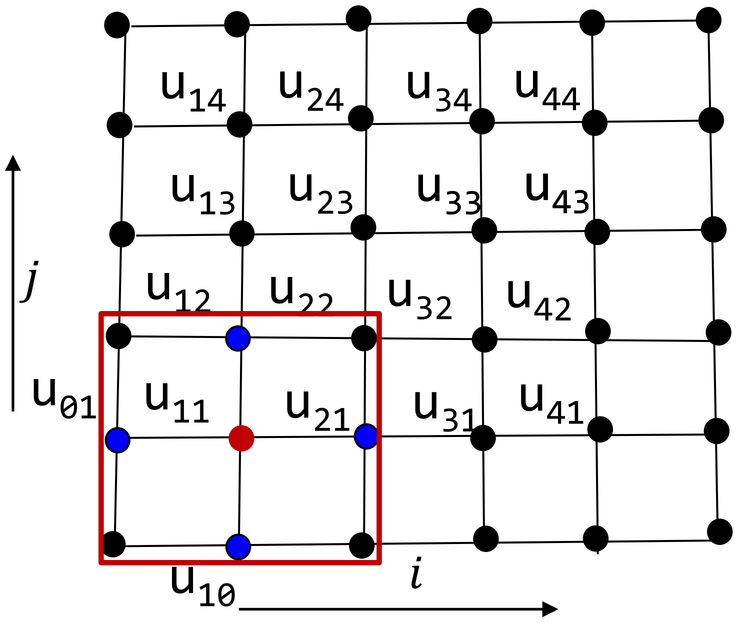
- Applying Jacobi Iteration:

$$\boldsymbol{u_{center}^{(k+1)} = 1/4(u_{right}^{(k)} + u_{top}^{(k)} + u_{left}^{(k)} + u_{bottom}^{(k)})}$$

Computing Stencil

- Example: applying Jacobi Iteration:

$$u_{center}^{(k+1)} = 1/4(u_{right}^{(k)} + u_{top}^{(k)} + u_{left}^{(k)} + u_{bottom}^{(k)})$$



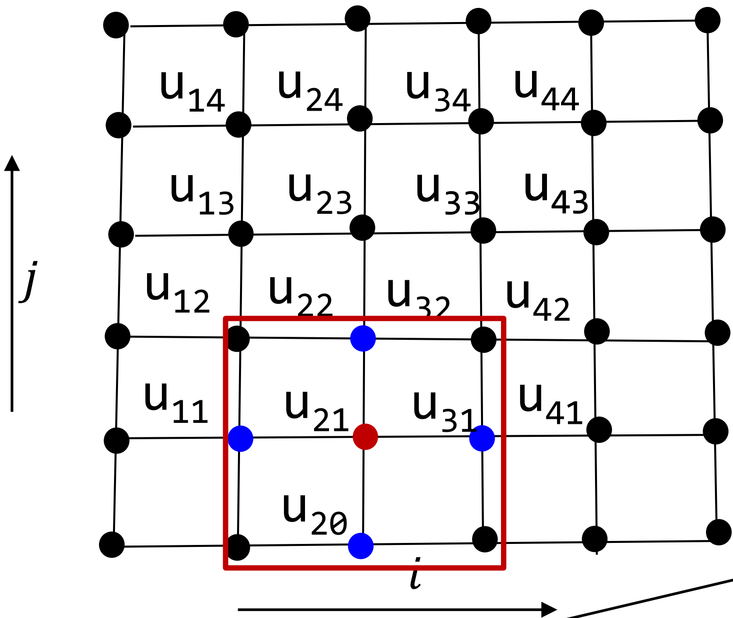
<u>Iteration 1</u>

1) Compute u_{11} using initial guess for u_{12} and u_{21}. u_{01} and u_{10} are known from boundary conditions

Computing Stencil

- Example: applying Jacobi Iteration:

$$u_{center}^{(k+1)} = 1/4(u_{right}^{(k)} + u_{top}^{(k)} + u_{left}^{(k)} + u_{bottom}^{(k)})$$



<u>Iteration 1</u>

1) Compute u_{11} using initial guess for u_{12} and u_{21}. u_{01} and u_{10} are known from boundary conditions

2) Compute u_{21} using initial guess for u_{11}, u_{31}, and u_{22}. u_{20} are known from boundary conditions

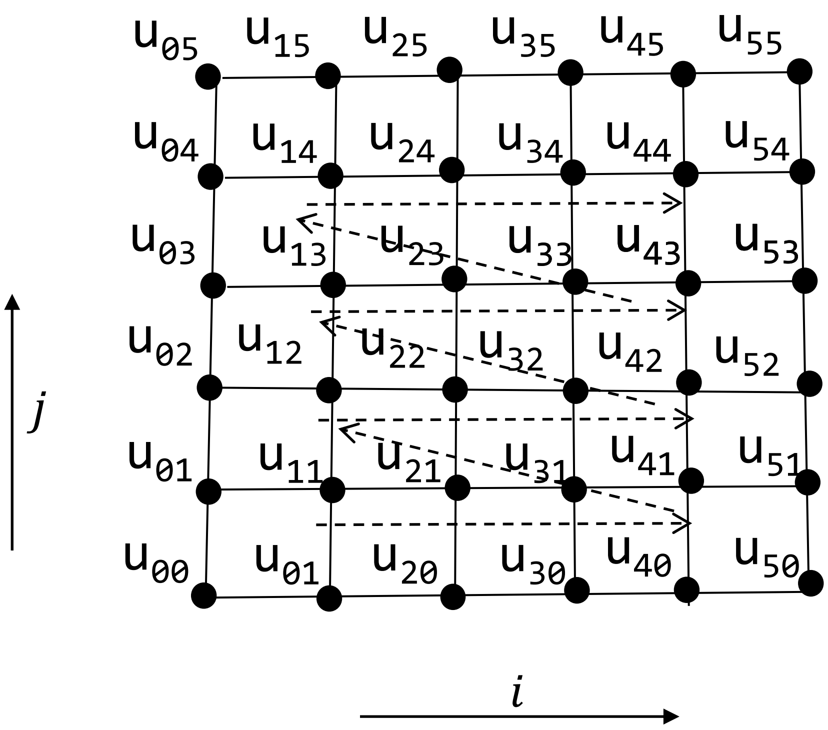
In 2), note that the initial guess for u_{11} is used even though u_{11} was updated just before in 1)

Today: Computing Stencil

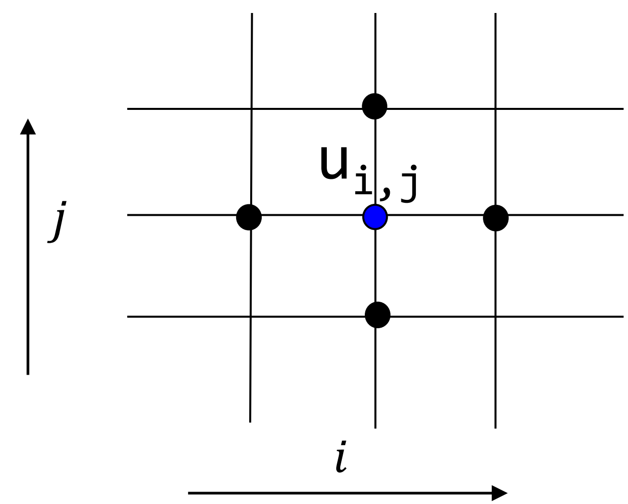
- Jacobi and Gauss-Seidel (Solution approach)
  - Start with an initial guess for the unknowns u^0_{ij}
  - Improve the guess u^1_{ij}
  - Iterate: derive the new guess, u^{n+1}_{ij} , from old guess u^n_{ij}
- Solution (Jacobi):
  - Approximate the *value of the center* with *old values* of (left, right,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

Elliptic Equation – Computing Stencil

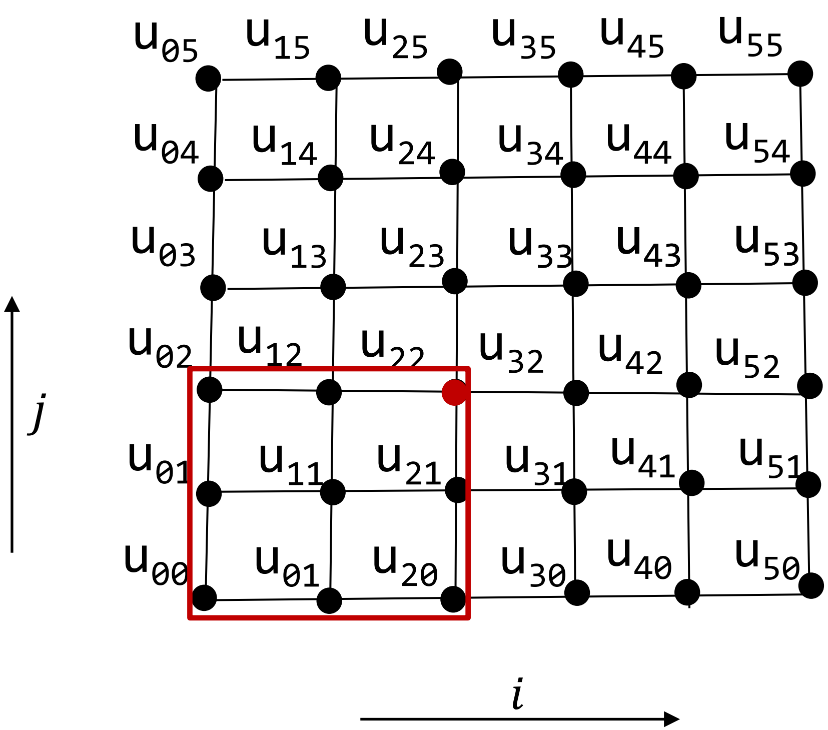
- In every iteration, suppose we follow the computing order as shown (dashed):



In any iteration, what are all the points of a 5-point stencil already updated while computing u_{ij} ?

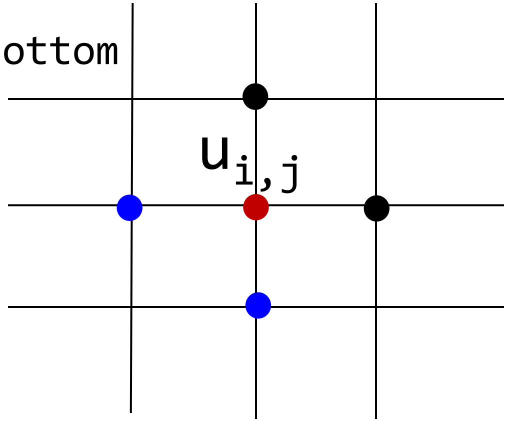


Elliptic Equation – Computing Stencil



What are the points that are already computed at $u_{i,j}$*?*

u_{left}, u_{bottom}



Background – Gauss-Seidel Iteration

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

  $\Rightarrow$ (L+D)X = -UX+B

  $\Rightarrow$ $(L+D)X^{(k+1)} = -UX^{k}+B$ **(iterate step)**

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

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

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

Computing Stencil – Gauss-Seidel

- Gauss-Seidel: Applying for 2D Laplace Equation

$$u_{center}^{(k+1)} = 1/4(u_{right}^{(k)} + u_{top}^{(k)} + u_{left}^{(k+1)} + u_{bottom}^{(k+1)})$$

- Gauss-Seidel: Observations
  - For a given problem and initial guess, Gauss-seidel *converges faster* than Jacobi
  - An iteration in Jacobi can be parallelized but not gauss-seidel

IMPORTANT – Numbering the grid points

- Computing System of Equations: **Ax=B**

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

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

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

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

u11 u21 u12 u22

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

A x = B

IMPORTANT – Numbering the grid points

- Computing System of Equations: **Ax=B**

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

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

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

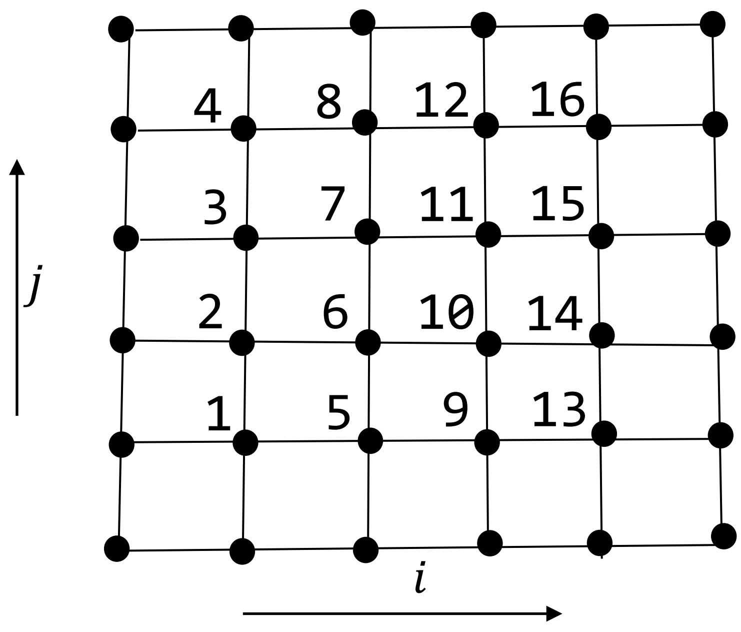
$$2/3 + 4/9 - 4u_{22} + u_{12} + u_{21} = 0$$

u11 u12 u21 u22

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

A x = B

IMPORTANT – Numbering the grid points



1	2	3	4	5	6	7	8	9	....
-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	0	0	1	-4	1	0
				1	0	0	1	-4	1

- Refer to class notes for FEM