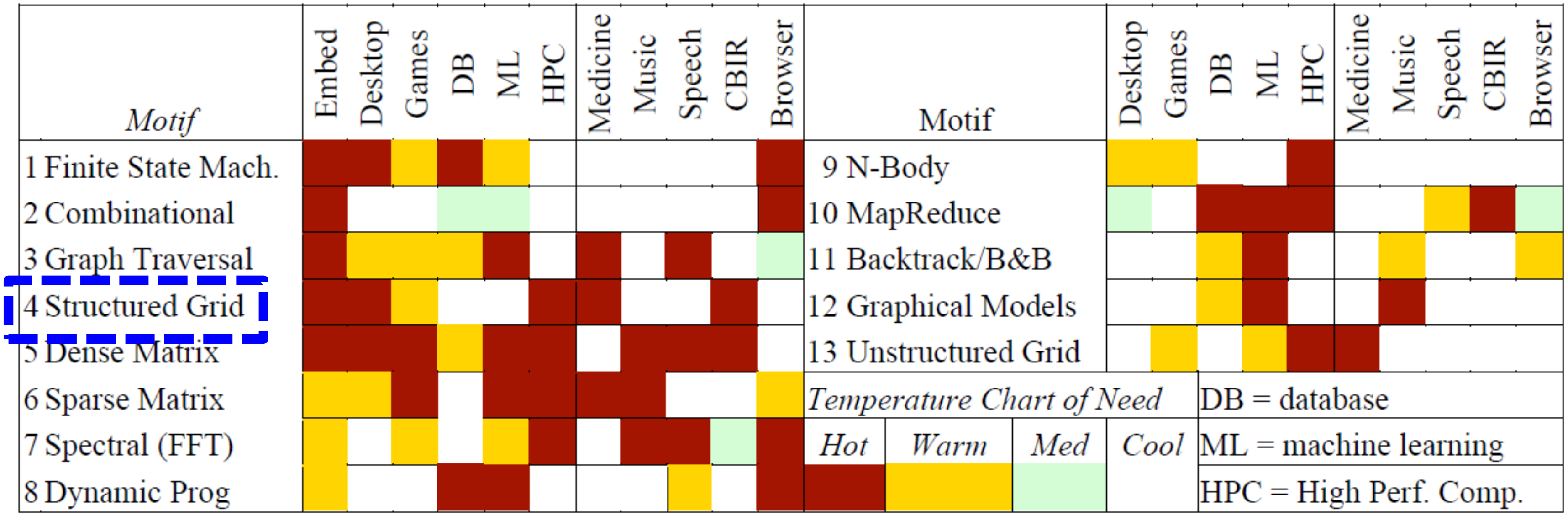
CS601: Software Development for Scientific Computing

Autumn 2023

Week12: Structured Grids

Matrix Algebra and Efficient Computation

- **Pic source: the Parallel Computing Laboratory at U.C. Berkeley: A Research Agenda Based on the Berkeley View (2008)**



Motif	Embed	Desktop	Games	DB	ML	HPC	Medicine	Music	Speech	CBIR	Browser
1 Finite State Mach.	🟥	🟥	🟨	🟥	🟨						🟥
2 Combinational	🟥			🟩	🟩						🟥
3 Graph Traversal	🟥	🟨	🟨	🟨	🟥		🟥		🟥		🟩
4 Structured Grid	🟥	🟥	🟨			🟥	🟥			🟥	
5 Dense Matrix	🟥	🟥	🟥	🟨	🟥	🟥		🟥	🟥	🟥	
6 Sparse Matrix	🟨	🟨	🟥		🟥	🟥	🟥	🟥			🟨
7 Spectral (FFT)	🟨		🟨		🟨	🟥		🟥	🟥	🟩	🟥
8 Dynamic Prog	🟨			🟥	🟥				🟨		🟥

Motif	Desktop	Games	DB	ML	HPC	Medicine	Music	Speech	CBIR	Browser
9 N-Body	🟨	🟨			🟥					
10 MapReduce	🟩		🟥	🟥	🟥			🟨	🟥	🟩
11 Backtrack/B&B			🟨	🟥			🟨			🟨
12 Graphical Models			🟨	🟥			🟥			
13 Unstructured Grid		🟨		🟨	🟥	🟥				

Temperature Chart of Need				DB = database
Hot	*Warm*	*Med*	*Cool*	ML = machine learning
🟥	🟨	🟩		HPC = High Perf. Comp.

Figure 4. Temperature Chart of the 13 Motifs. It shows their importance to each of the original six application areas and then how important each one is to the five compelling applications of Section 3.1. More details on the motifs can be found in (Asanovic, Bodik et al. 2006).

Next..

Discretization

- Cannot store/represent infinitely many continuous values
  - To model turbulent features of flow through a pipe, say, I am interested in `velocity` and `pressure` at all `points` in a region of interest
    1. Represent region of interest as a mesh of small discrete cells - ***discretization spacing***
    2. Solve equations for each cell

Example:

```
diameter of the pipe = 5cm
length=2.5cm
discretization spacing = 0.1mm
```

(volume of cylinder = $\pi r^2 h$)

Exercise: *how many variables do you need to declare?*

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

Exercise

- *does increasing mesh size always yield better accuracy?*

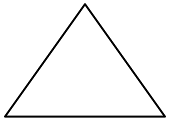
- *does decreasing cell size always yield better accuracy?*

- *How does changing mesh size affect computational cost?*

- *How does changing cell size affect computational cost?*

Cell Shape

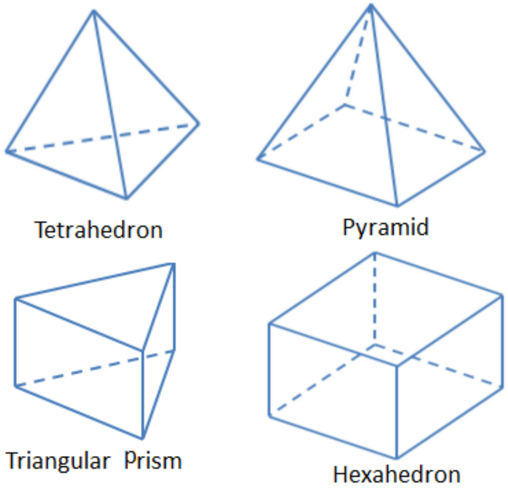
- 2D:



triangle

quadrilateral

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

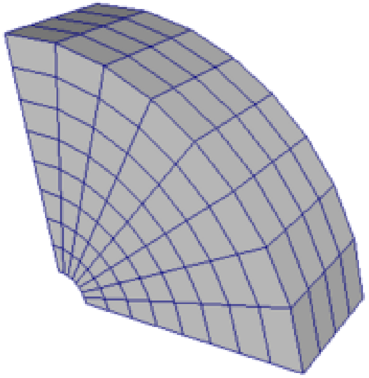


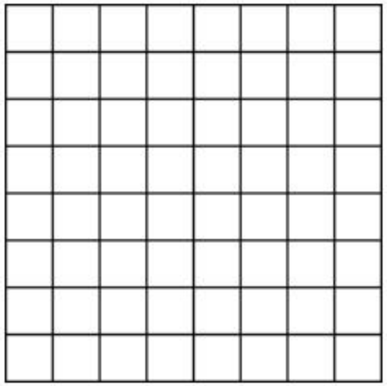
source: wikipedia

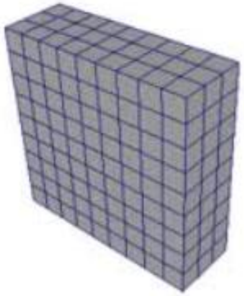
Tetrahedron: 4 vertices, 4 edges, 4△ faces
Pyramid: 5 vertices, 8 edges, 4 △ and 1 ▭ face
Triangular prism: 6 vertices, 9 edges, 2△ and 3▭ faces
Hexahedron: 8 vertices, 12 edges, 6 ▭ faces

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)
  - Certain conditions / constraints / known values etc.
- Goal:
  - Discretize into a grid of cells
  - Approximate the PDE on the grid
  - Solve the PDE on the grid

Structured Grids - Representation

- Because of regular connectivity between cells
  - Cells can be identified with indices (x,y) or (x,y,z) and neighboring cell info can be obtained.
  - How about identifying a cell here?

    Given:

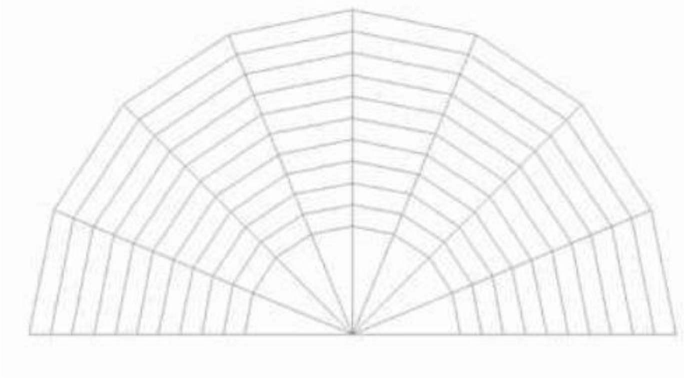
    $\xi =$ ("Xi") radius

    η = ("Eta") angle

    Compute:

$$x = \left(\frac{1}{2} + \xi\right)\cos(\pi\eta)$$

$$y = \left(\frac{1}{2} + \xi\right)\sin(\pi\eta)$$



Structured Grids - Representation

- Assume that we have a grid.
- Task:
  - Approximate Partial Differential Equations (PDEs)
  - Solve/Implement PDEs (turning PDEs into large set of algebraic equations)

Mathematical Model of the Grid

- Partial Differential Equations (PDEs):
  - Navier-Stokes equations to model water, blood flow, weather forecast, aerodynamics etc.
  - Elasticity (Lame-Navier equations)
  - Nutrient transport in blood flow
  - Heat conduction: *how heat conducts/diffuses through a material given the temperature at boundaries?*
  - Mechanics: *how does a mass reach from point p1 to point p2 in shortest time under gravitational forces?*

Notation and Terminology

- $\frac{\partial u}{\partial x} = \ \partial_x u$
- $\frac{\partial^2 u}{\partial x \partial y} = \ \partial_{xy} u$
- $\frac{\partial u}{\partial t} = \ \partial_t u$, t usually denotes time.
- Laplace operator $(\mathbf{L})$: of a two-times continuously differentiable scalar-valued function $u: \mathbb{R}^n \to \mathbb{R}$

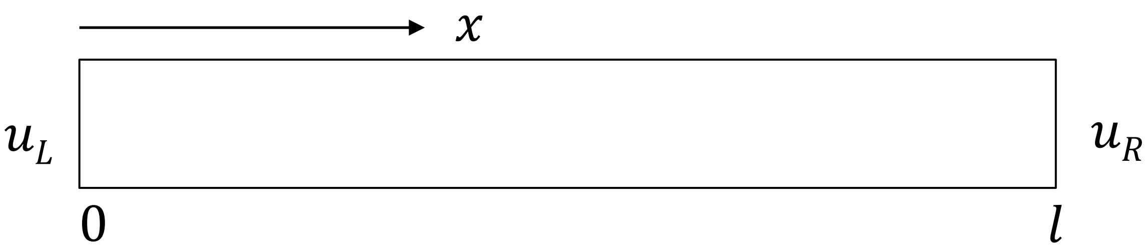
$$\Delta u \quad = \sum_{k=1}^{n} \partial_{kk} u$$

Important PDEs

- Three important types (*not a complete categorization by any means*):
  - Poisson problem: $-\Delta u = f$ (elliptic)
  - Heat equation: $\partial_t u \; - \Delta u = f$ (parabolic. Here, $\partial_t u = \frac{\partial u}{\partial t}$ = partial derivative w.r.t. time)
  - Wave equation: $\partial_t{}^2 u \; - \Delta u = f$ (Hyperbolic. Here, $\partial_t{}^2 u = \frac{\partial^2 u}{\partial t \partial t}$ = second-order partial derivative w.r.t. time)

Application: Heat Equation

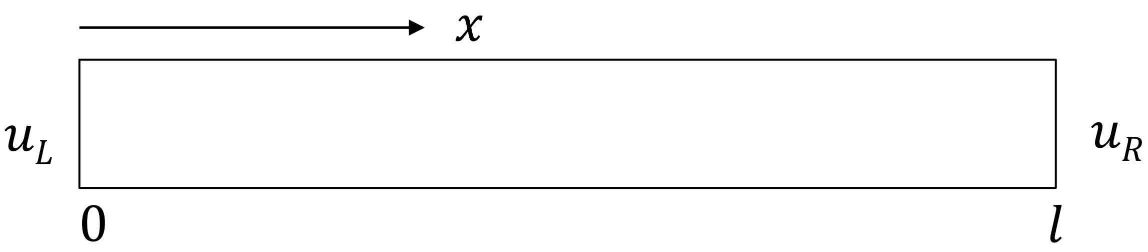
- Example: heat conduction through a rod



- $u = u(x,t)$ is the temperature of the metal bar at distance x from one end and at time t
- Goal: find u

Initial and Boundary Conditions

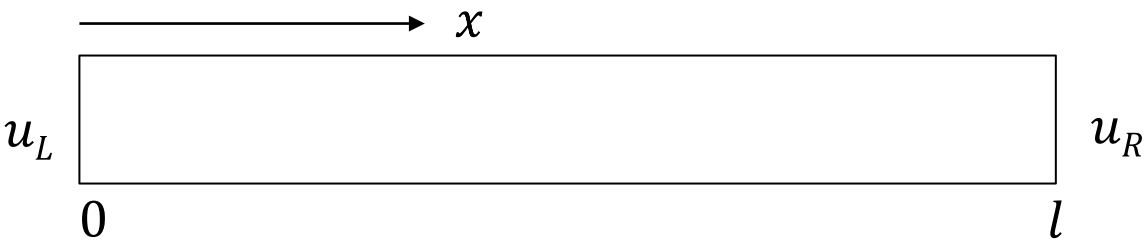
- Example: heat conduction through a rod



- Metal bar has length l and the ends are held at constant temperatures u_L at the left and u_R at the right
- Temperature distribution at the initial time is known $f(x)$, with $f(0) = u_L$ and $f(l) = u_R$

Equations

- Example: heat conduction through a rod



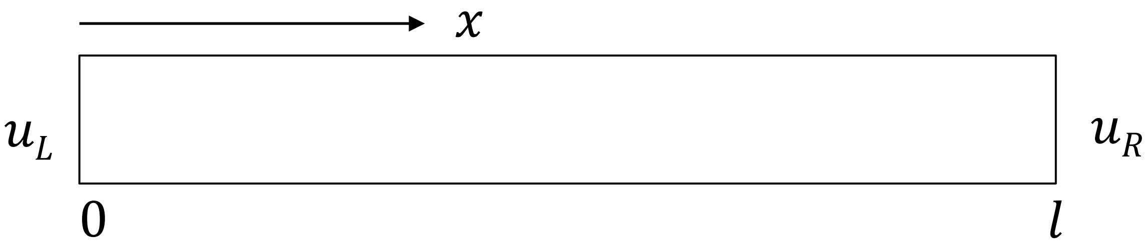
$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \qquad (0 < x < l, t > 0)$$

α is thermal diffusivity

(a constant if the material is homogeneous and isotropic.
copper = 1.14 cm^2 s^{-1}, aluminium = 0.86 cm^2 s^{-1})

Equations

- Example: heat conduction through a rod



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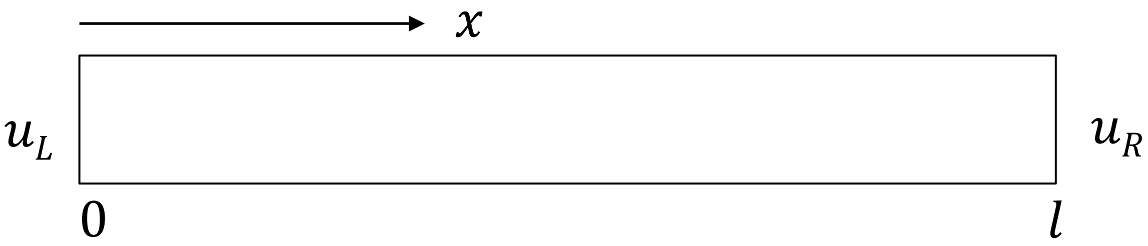
- *Exercise: what kind of a PDE is this? (Poisson/Heat/Wave?)*

Equations

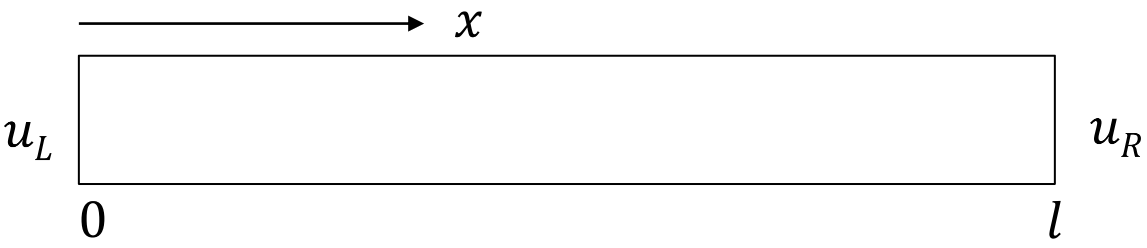
- Example: heat conduction through a rod



$\partial_t u = \alpha \Delta u$ as per the notation mentioned earlier

Equations

- Example: heat conduction through a rod



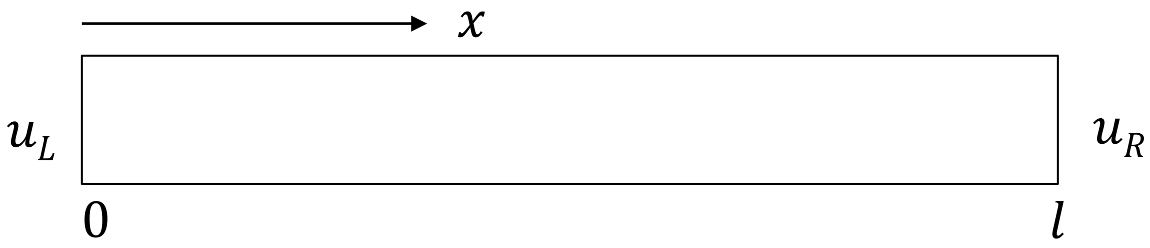
$$\partial_t u = \alpha \Delta u$$

Can also be written as:

$$\partial_t u - \alpha \Delta u = 0$$

Equations

- Example: heat conduction through a rod



$\partial_t u - \alpha \Delta u = 0$,

Based on initial and boundary conditions:

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

Equations

- Summarizing:
  1. $\partial_t u - \alpha \Delta u = 0$, 0<x<l, t>0
  2. $u(0,t) = u_L, t > 0$
  3. $u(l,t) = u_R\ , t > 0$
  4. $u(x,0) = \ f(x), 0 < x < l$

- Solution:

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

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

Equations

- Summarizing:
  1. $\partial_t u - \alpha \Delta u = 0$, 0<x<l, t>0
  2. $u(0,t) = u_L, t > 0$
  3. $u(l,t) = u_R\,, t > 0$
  4.

But we are interested in a numerical solution

- Solution:

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

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

Approximating Partial Derivatives

- 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:

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

Approximating Partial Derivatives

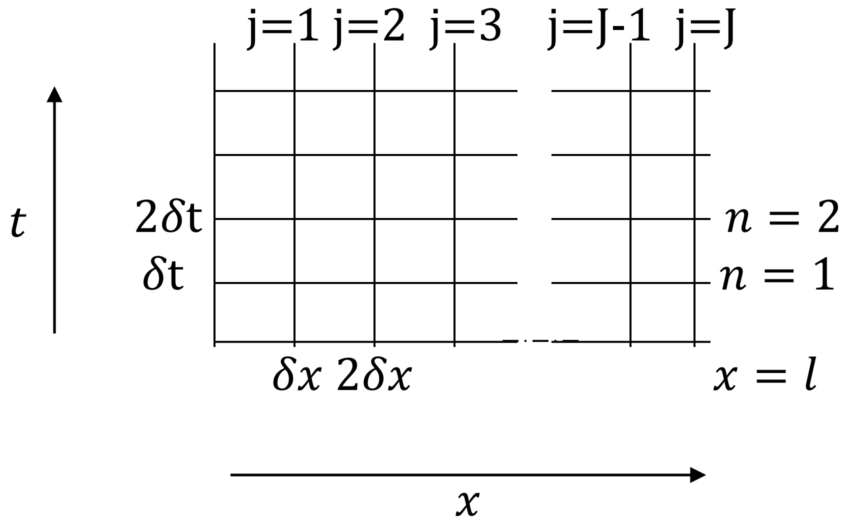
- In example heat application $f = u = u(x, t)$ and $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$
  - First, approximating $\frac{\partial u}{\partial t}$:

    $\frac{\partial u}{\partial t} \approx \frac{\left(u(x,t+\delta t)-u(x,t)\right)}{\delta t}$, where δt is a small increment in time
  - Next, approximating $\frac{\partial^2 u}{\partial x^2}$:

    $\frac{\partial^2 u}{\partial x^2} \approx \frac{\left(u(x+\delta x,t)-2u(x,t)+u(x-\delta x,t)\right)}{(\delta x)^2}$, where δx is a small increment in space (along the length of the rod)

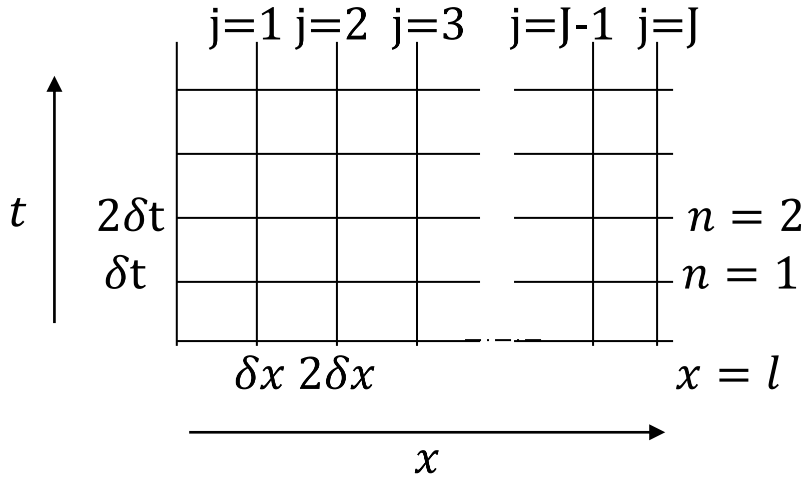
Approximating Partial Derivatives

- Divide length l into J equal divisions: $\delta x = l/J$ (space step)
- Choose an appropriate δt (time step)



Approximating Partial Derivatives

- Find sequence of numbers which approximate u at a sequence of (x, t) points (i.e. at the intersection of horizontal and vertical lines below)



- Approximate the exact solution $u(j \times \delta x, n \times \delta t)$ using the approximation for partial derivatives mentioned earlier

Approximating Partial Derivatives

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

$$= \frac{(u_j^{n+1} - u_j^n)}{\delta t}$$

where u_j^{n+1} denotes taking j steps along x direction and $n + 1$ steps along t direction

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

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

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.

Approximating Partial Derivatives

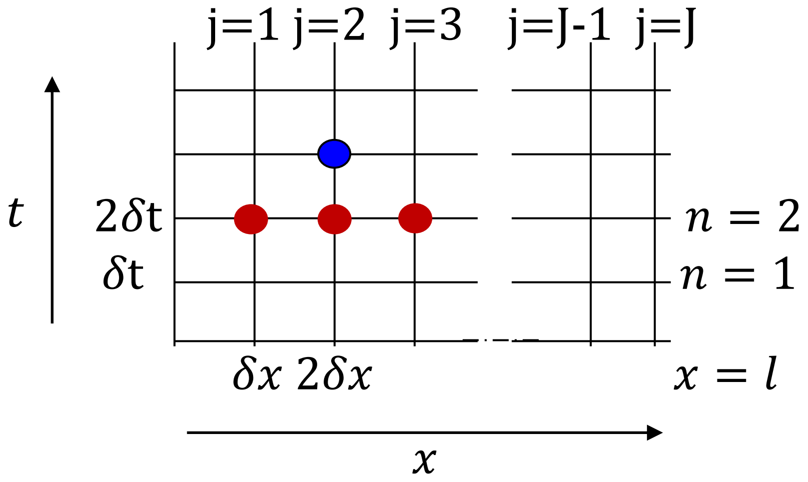
Simplifying:

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

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

Approximating Partial Derivatives

- Initial and boundary conditions tell us that:
  $u(0,t) = u_L$,
  $u(l,t) = u_R$,
  $u(x,0) = f(x)$

- $u_0^0, u_1^0\, u_2^0, \ldots.\, u_J^0$ are known (at time t=0, the temperature at all points along the distance is known as indicated by $f(x)$ = f_j).
- u_0^1 is $u_{L,}\, u_J^1$ is u_R
- Now compute points on the grid from left-to-right:

Approximating Partial Derivatives

- Now compute points on the grid from left-to-right:

$$u_1^1 = u_1^0 + r(u_0^0 - 2u_1^0 + u_2^0)$$
$$u_2^1 = u_2^0 + r(u_1^0 - 2u_2^0 + u_3^0)$$

.

.

$$u_{J-1}^1 = u_{J-1}^0 + r\left(u_{J-2}^0 - 2u_{J-1}^0 + u_J^0\right)$$

- This constitutes the computation done in the first time step.
- Now do the second time step computation…and so on..

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

- Initialize u_j^0 values from initial and boundary conditions i.e. *get time-step 0 values*

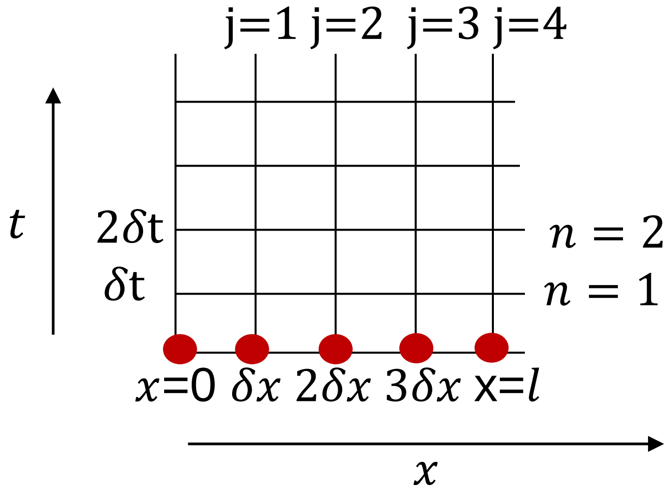
u_0^0 = 0

$u_1^0 = f(\delta x) = \delta x(l - \delta x)$ = .1875

$u_2^0 = f(2\delta x) = 2\delta x(l - 2\delta x)$ = .25

$u_3^0 = f(3\delta x) = 3\delta x(l - 3\delta x)$ = .1875

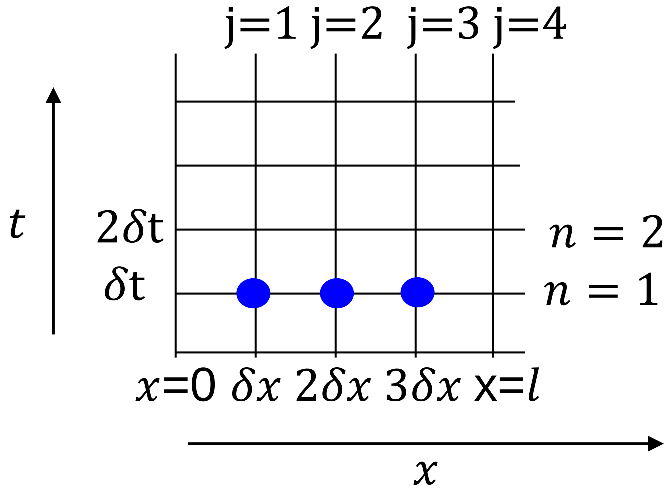
u_4^0 = 0



Explicit Difference Method: Stability

- Compute time-step 1 values

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

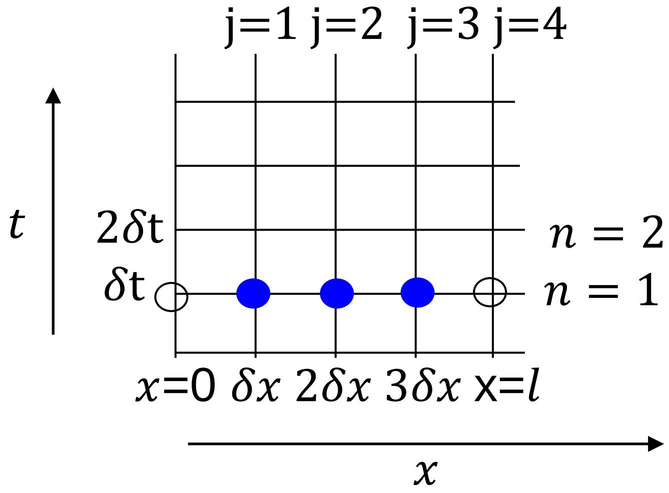


Explicit Difference Method: Stability

- Compute time-step 1 values

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

What about values of $u(x,t)$ at ○ ?



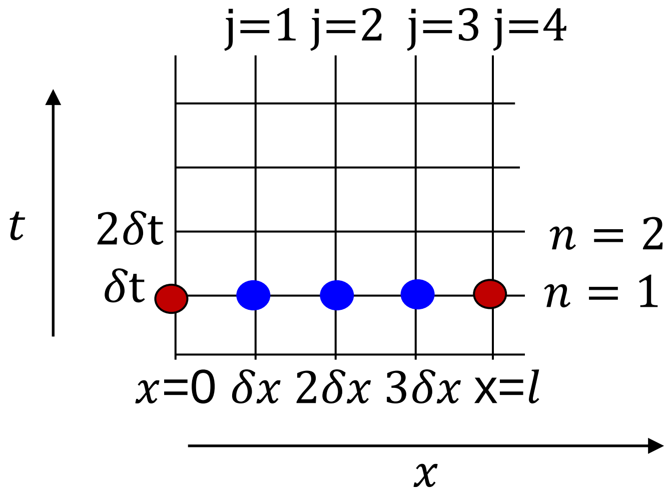
Explicit Difference Method: Stability

- Compute time-step 1 values

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

What about values of $u(x,t)$ at ○ ?

Get it from boundary conditions



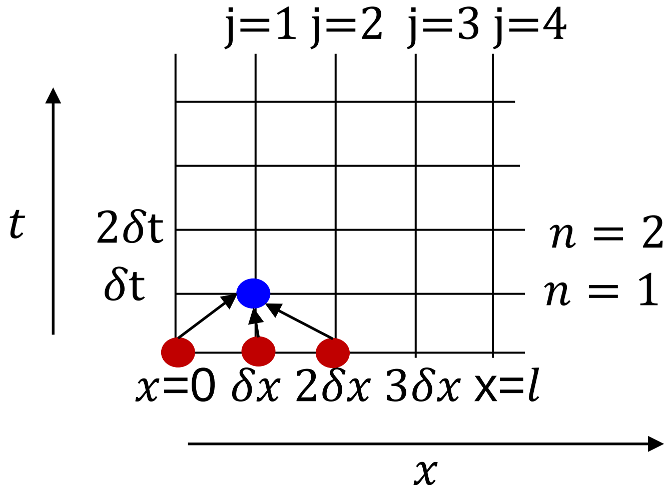
Explicit Difference Method: Stability

- Compute time-step 1 values

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

$r = \alpha\delta t/(\delta x)^2$ = 1.2

u_1^1 = $u_1^0 + r(u_0^0 - 2u_1^0 + u_2^0)$ = 0.03678



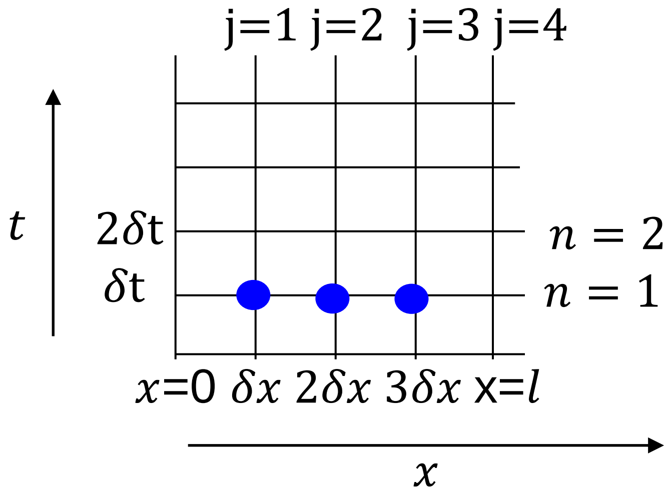
Explicit Difference Method: Stability

- Compute time-step 1 values

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

$$r = \alpha\delta t/(\delta x)^2 = 1.2$$

$$u_1^1 = u_1^0 + r(u_0^0 - 2u_1^0 + u_2^0) = 0.03678$$
$$u_2^1 = u_2^0 + r(u_1^0 - 2u_2^0 + u_3^0) = 0.1$$
$$u_3^1 = u_3^0 + r(u_2^0 - 2u_3^0 + u_4^0) = 0.03678$$

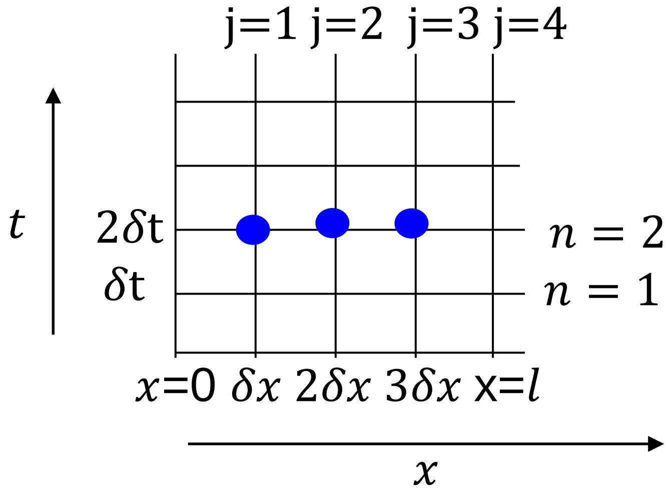


Explicit Difference Method: Stability

- Compute time-step 2 values

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

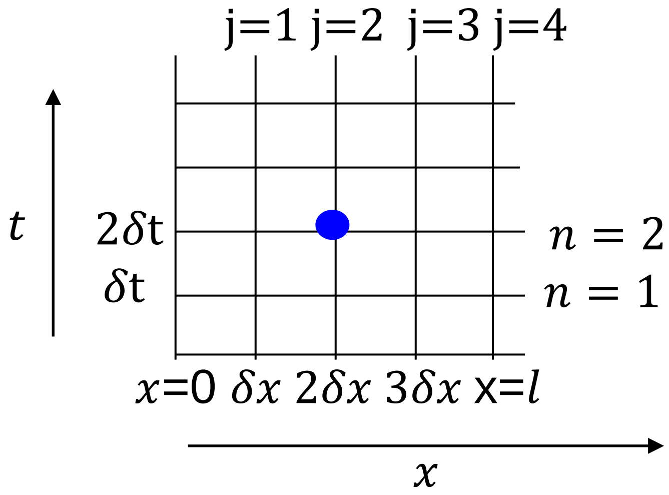
$u_1^2 = u_1^1 + r(u_0^1 - 2u_1^1 + u_2^1)$=0.06851
$u_2^2 = u_2^1 + r(u_1^1 - 2u_2^1 + u_3^1)$=**-0.05173**
$u_3^2 = u_3^1 + r(u_2^1 - 2u_3^1 + u_4^1)$=0.06851



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*

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



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:

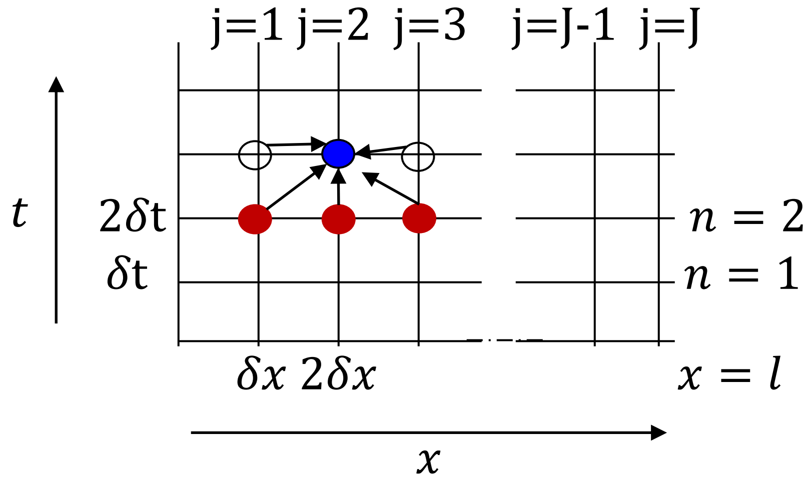
$$\delta t \leq \frac{\delta x^2}{2\alpha}$$

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?

Suggested Reading

- *J.W. Thomas. Numerical Partial Differential Equations: Finite Difference Methods*
- *Parabolic PDEs: https://learn.lboro.ac.uk/archive/olmp/olmp_resources/pages/workbooks_1_50_jan2008/Workbook32/32_4_prblc_pde.pdf*

PDEs - Recap

- 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 $B^2 – 4AC > 0$

Important PDEs - Recap

Laplace operator $(\mathbf{L})$: of a two-times continuously differentiable scalar-valued function $u: \mathbb{R}^n \to \mathbb{R}$

$$\Delta u \quad = \sum_{k=1}^{n} \partial_{kk} u$$

- **Poisson problem**: $-\Delta u = f$ (elliptic, independent of time.)
- **Heat equation**: $\partial_t u - \Delta u = f$ (parabolic. Here, $\partial_t u = \frac{\partial u}{\partial t}$ = partial derivative w.r.t. time)
- **Wave equation**: $\partial_t{}^2 u - \Delta u = f$ (Hyperbolic. Here, $\partial_t{}^2 u = \frac{\partial^2 u}{\partial t \partial t}$ = second-order partial derivative w.r.t. time)

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

- 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

Exercise

- Consider the *boundary-value* problem:

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

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

Is this Laplace equation or Poisson equation?

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 and x and y are independent variables here.
   2. Choose δx= δy = 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

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

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

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

Elliptic Equation – Numerical Solution

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

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

$$+$$

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

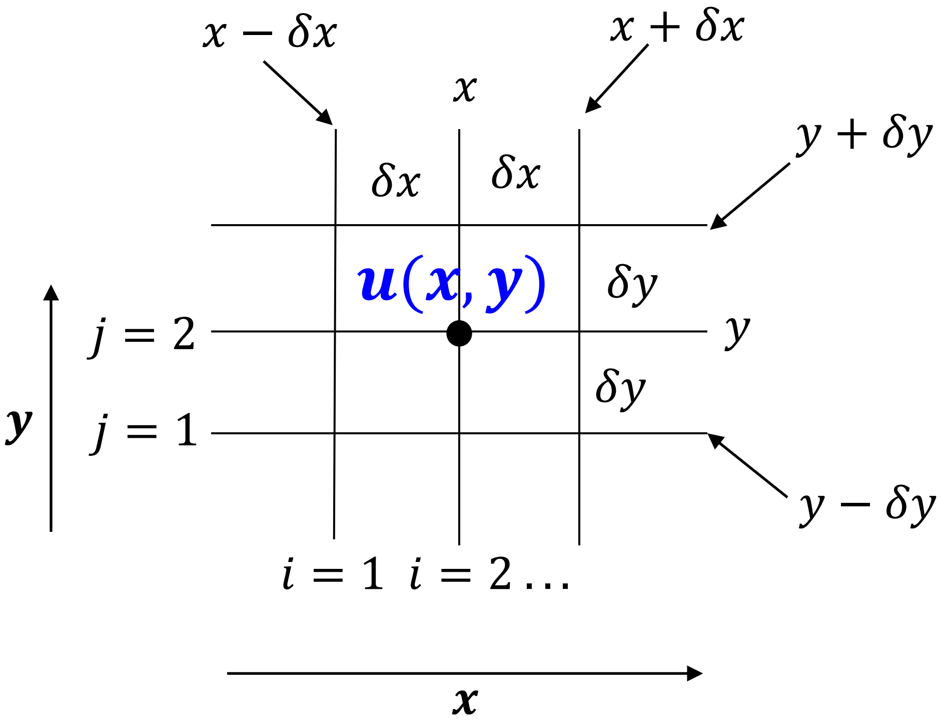
$$=$$

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

$$= f(x, y)$$

Elliptic Equation – Numerical Solution

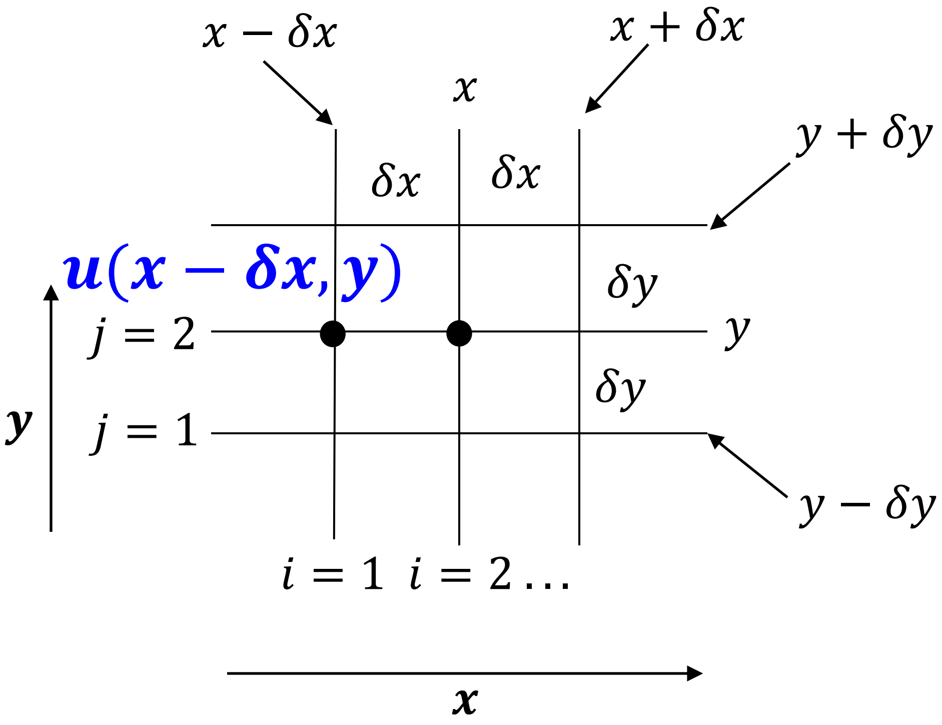
- Representing $u(x, y)$



Notation: $\mathbf{u}_{\mathbf{i,j}}$

Elliptic Equation – Numerical Solution

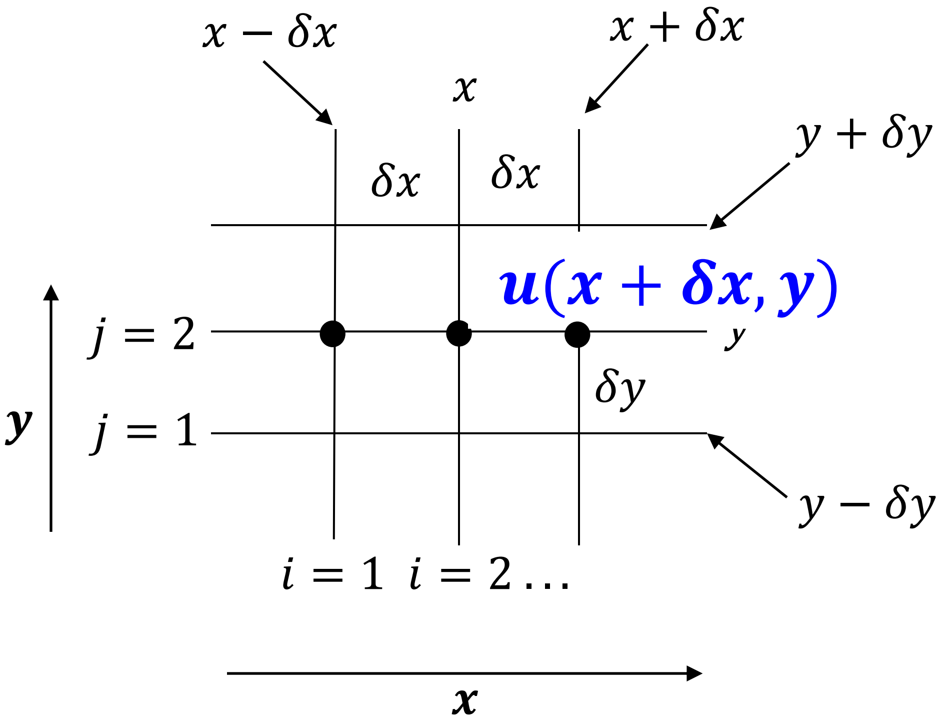
- Representing $u(x - \delta x, y)$



Notation: $\mathbf{u}_{\mathbf{i-1,j}}$

Elliptic Equation – Numerical Solution

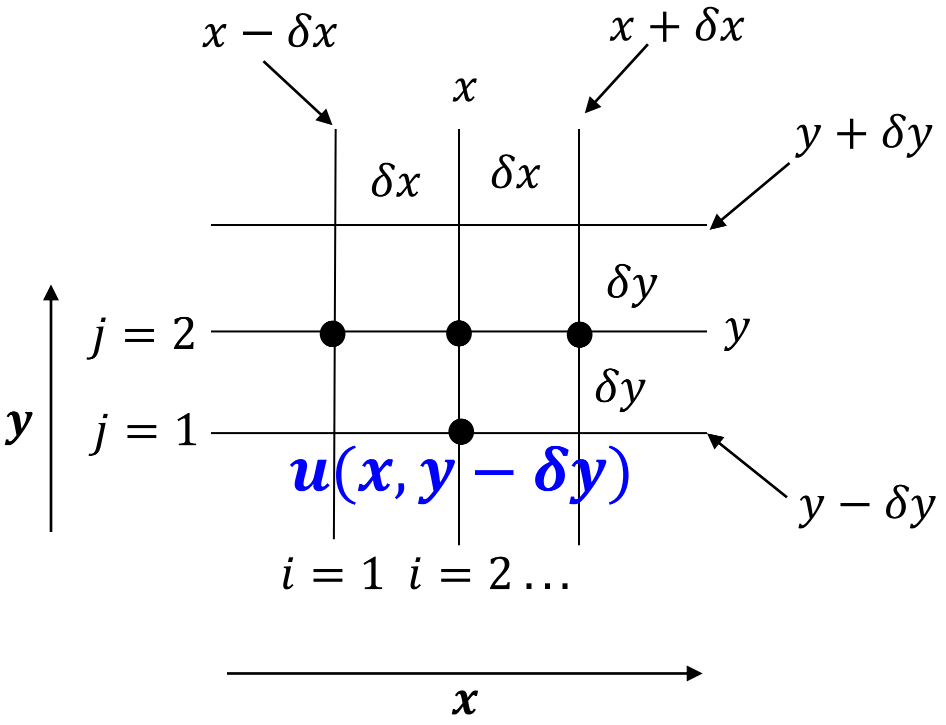
- Representing $u(x + \delta x, y)$



Notation: $\mathbf{u}_{\mathbf{i+1,j}}$

Elliptic Equation – Numerical Solution

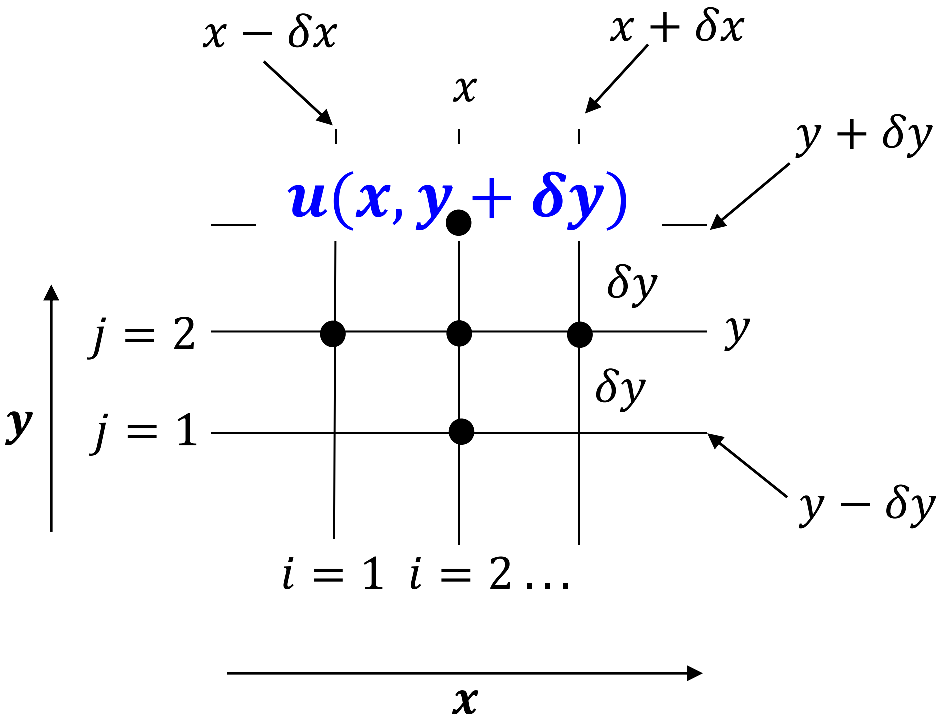
- Representing $u(x, y - \delta y)$



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

Elliptic Equation – Numerical Solution

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



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

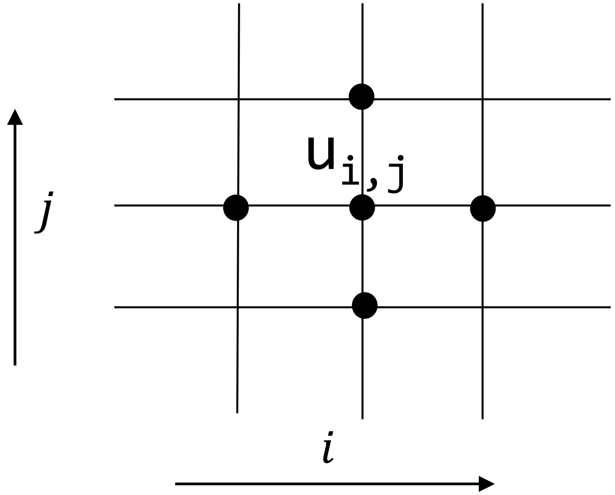
Elliptic Equation – Numerical Solution

- Rewriting:

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

$$= f(x,y)$$

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



5-point stencil

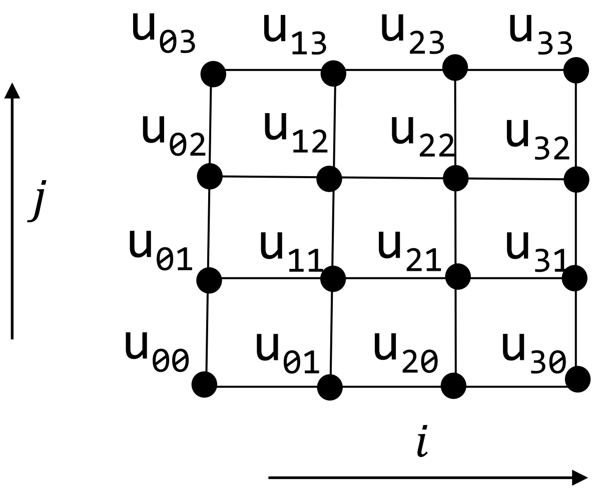
Elliptic Equation – Computing Stencil

- Consider the *boundary-value* problem:

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

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

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

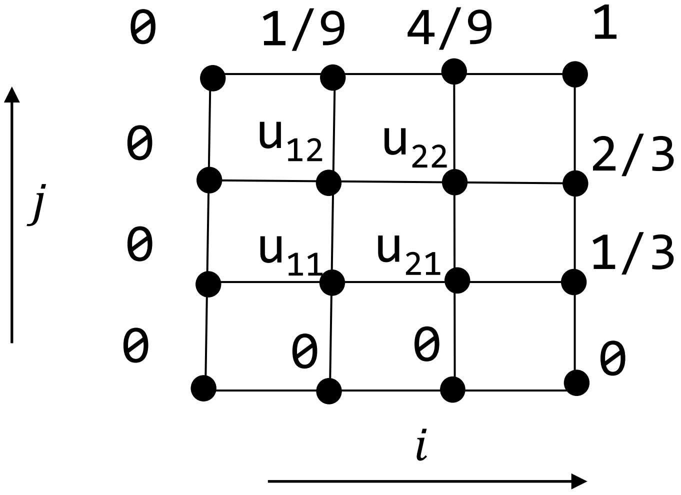


u_{03} u_{13} u_{23} u_{33}

u_{02} u_{12} u_{22} u_{32}

u_{01} u_{11} u_{21} u_{31}

u_{00} u_{01} u_{20} u_{30}



0 1/9 4/9 1

0 u_{12} u_{22} 2/3

0 u_{11} u_{21} 1/3

0 0 0 0

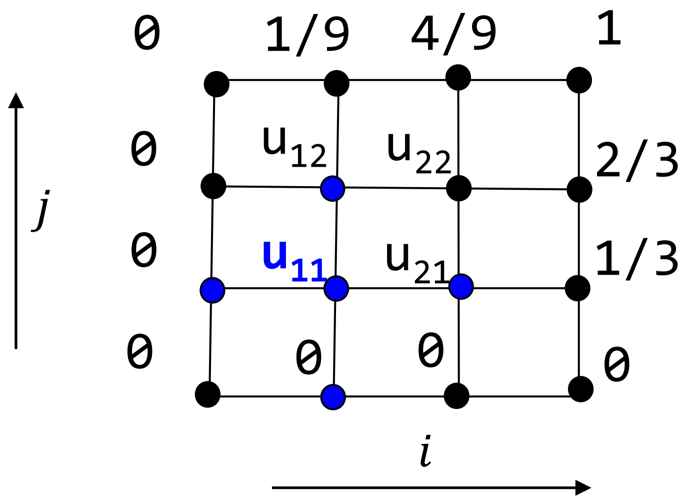
Elliptic Equation – Computing Stencil

- Computing u_{11}

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

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

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



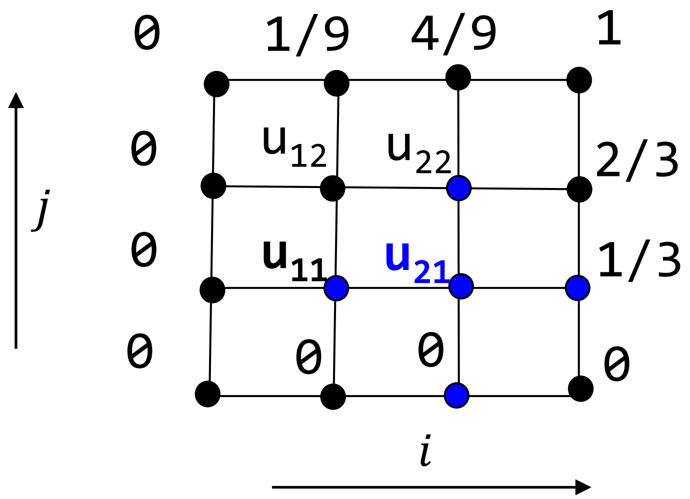
Elliptic Equation – Computing Stencil

- Computing u_{21}

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

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

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



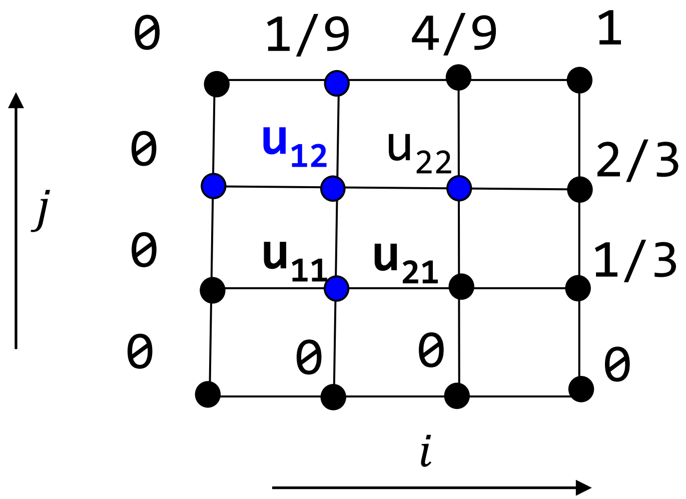
Elliptic Equation – Computing Stencil

- Computing u_{12}

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

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

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



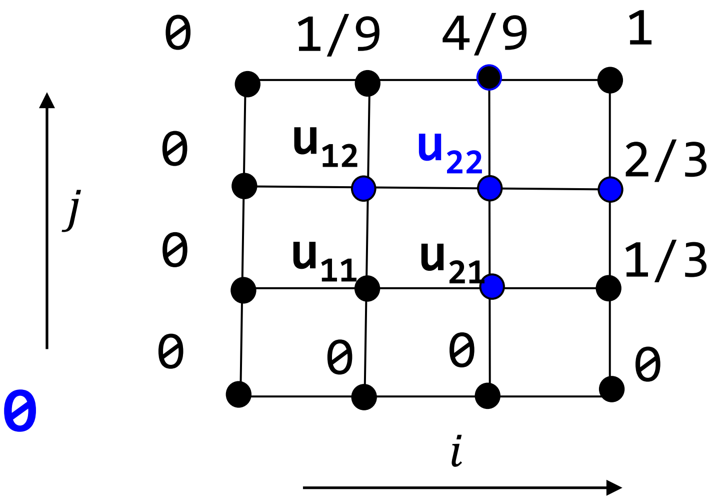
Elliptic Equation – Computing Stencil

- Computing u_{22}

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

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

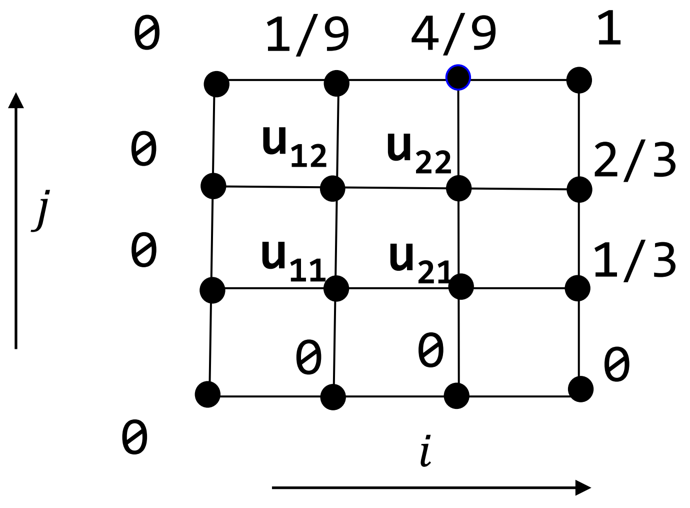
$$2/3 + 4/9 - 4u_{22} + u_{12} + u_{21} = 0$$



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:

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

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

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

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

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

Ax=B

A x = B

Matrix A has only coefficients

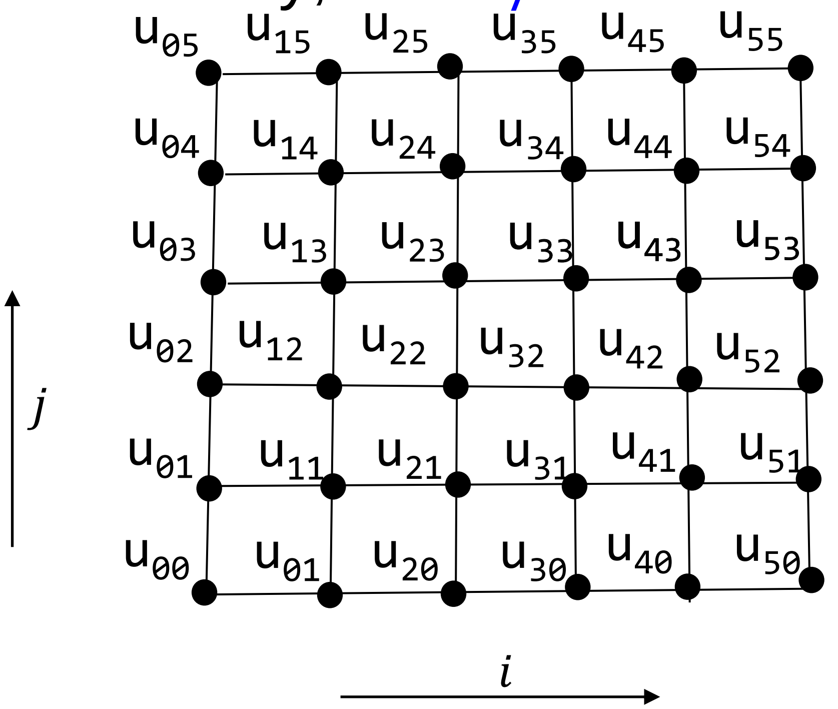
$$\begin{array}{ccc} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{array}$$

Elliptic Equation – Computing Stencil

- Consider the *boundary-value* problem (here u_{xx} denotes $\partial^2 u/\partial x^2$):

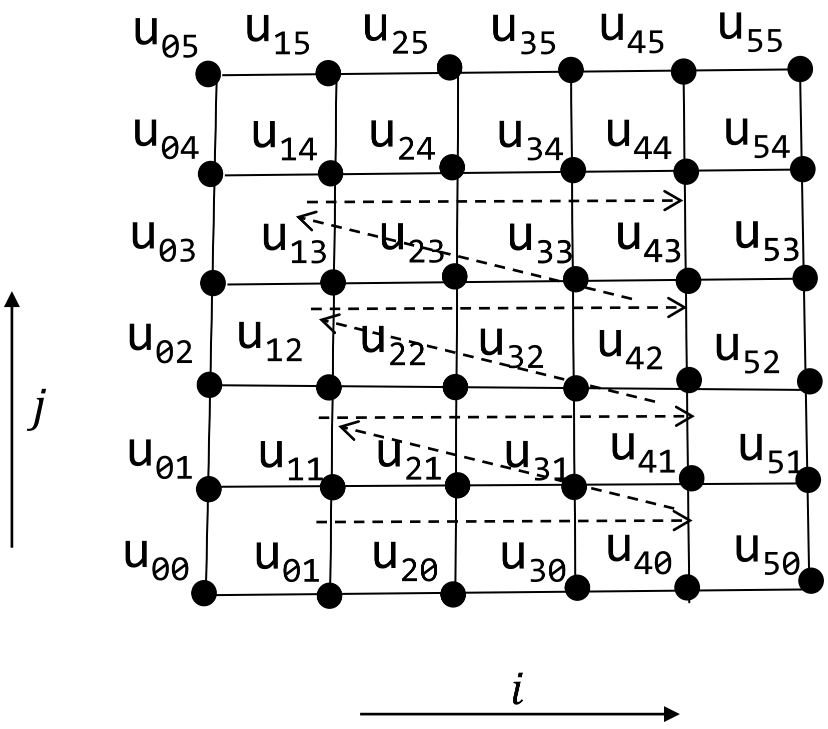
$u_{xx} + u_{yy} = 0$ in the square $0 < x < 1, 0 < y < 1$

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


u_{05} u_{15} u_{25} u_{35} u_{45} u_{55}
u_{04} u_{14} u_{24} u_{34} u_{44} u_{54}
u_{03} u_{13} u_{23} u_{33} u_{43} u_{53}
u_{02} u_{12} u_{22} u_{32} u_{42} u_{52}
u_{01} u_{11} u_{21} u_{31} u_{41} u_{51}
u_{00} u_{01} u_{20} u_{30} u_{40} u_{50}
j
i

Elliptic Equation – Computing Stencil

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



u_{05} u_{15} u_{25} u_{35} u_{45} u_{55}
u_{04} u_{14} u_{24} u_{34} u_{44} u_{54}
u_{03} u_{13} u_{23} u_{33} u_{43} u_{53}
u_{02} u_{12} u_{22} u_{32} u_{42} u_{52}
u_{01} u_{11} u_{21} u_{31} u_{41} u_{51}
u_{00} u_{01} u_{20} u_{30} u_{40} u_{50}
j
i

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

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?

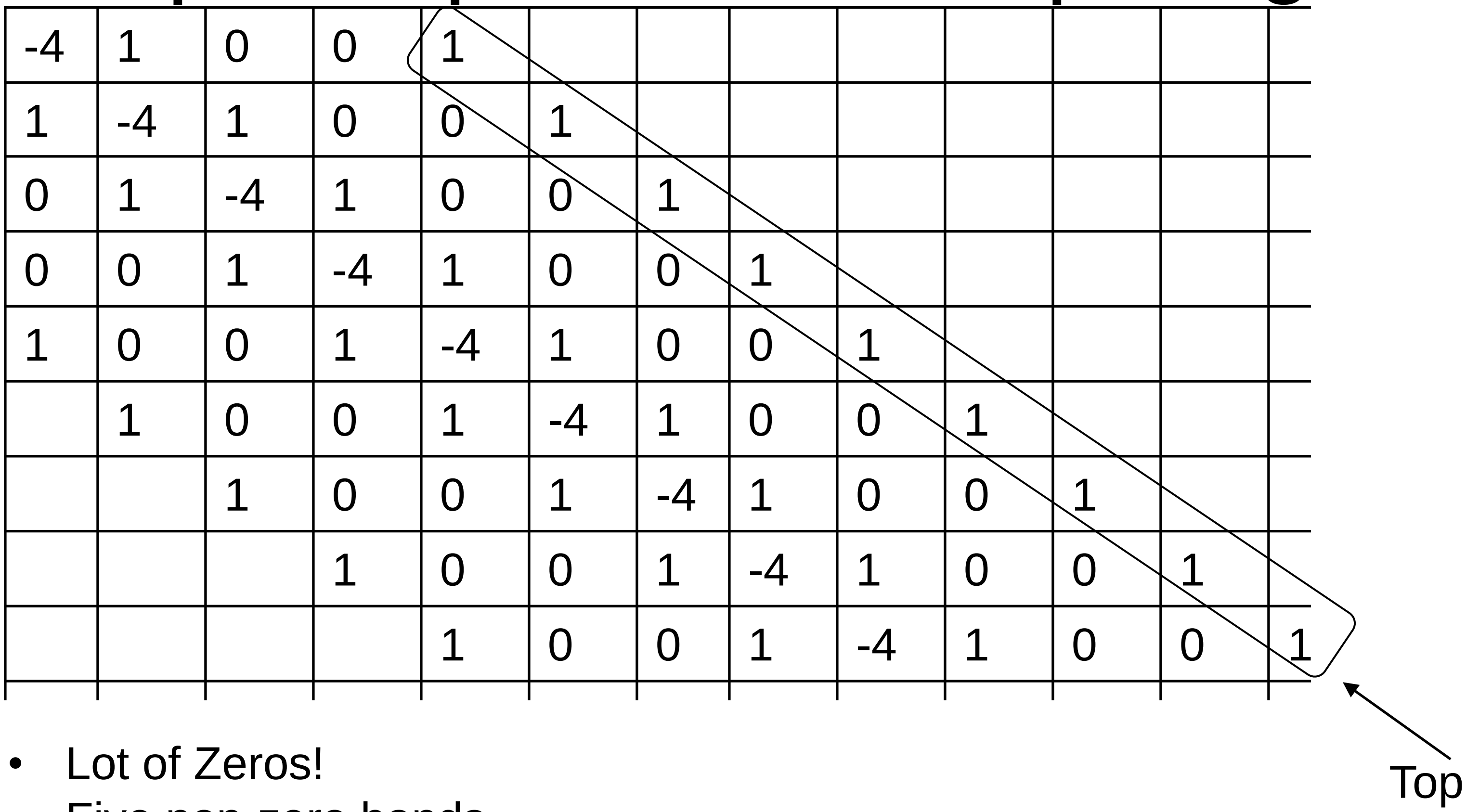
Elliptic Equation – Computing Stencil

-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

- 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.

$$\begin{pmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{pmatrix} = \underset{\underset{L}{\uparrow}}{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}} + \underset{\underset{D}{\uparrow}}{\begin{pmatrix} -4 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & -4 \end{pmatrix}} + \underset{\underset{U}{\uparrow}}{\begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}}$$

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

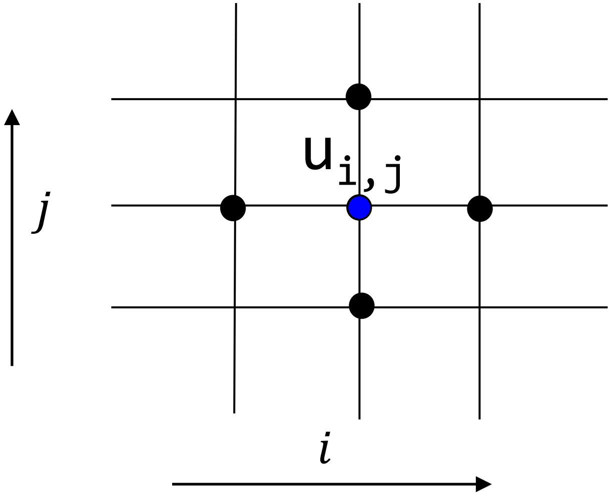
u_{ij} 's value in $(\mathbf{1})^{st}$ iteration is computed based on u_{ij} values computed in $(\mathbf{0})^{th}$ iteration

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 – Recap

- 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)