Finite Difference Discretization of Elliptic Equations: FD Formulas and Multidimensional Problems

Lecture 4

Finite Difference Formulas

Problem Definition

Given $l + r + 1$ distinct points $(x_{-l}, x_{-l+1}, \ldots, x_0, \ldots, x_r)$, find the weights δ_j^m such that

$$\left.\frac{d^m v}{dx^m}\right|_{x=x_0} \approx \sum_{j=-l}^{r} \delta_j^m v_j$$

is of optimal order of accuracy.

N1

Two approaches:

- **Lagrange interpolation**
- **Undetermined coefficients**

Finite Difference Formulas

Lagrange interpolation

Lagrange polynomials

$$L_j(x) = \frac{(x - x_{-l}) \cdots (x - x_{j-1})(x - x_{j+1}) \cdots (x - x_r)}{(x_j - x_{-l}) \cdots (x_j - x_{j-1})(x_j - x_{j+1}) \cdots (x_j - x_r)}$$

Lagrange interpolant

$$\hat{v}(x) = \sum_{j=-l}^{r} L_j(x) v_j$$

Finite Difference Formulas

Lagrange interpolation

Approximate

$$\left.\frac{d^m v}{dx^m}\right|_{x=x_0} \approx \left.\frac{d^m \hat{v}}{dx^m}\right|_{x=x_0} = \sum_{j=-l}^{r} \left.\frac{d^m L_j}{dx^m}\right|_{x=x_0} v_j$$

Therefore,

$$\boxed{\delta_j^m = \left.\frac{d^m L_j}{dx^m}\right|_{x=x_0} .}$$

Finite Difference Formulas

Lagrange interpolation

Example...

Set $l = r = 1$, (x_{j-1}, x_j, x_{j+1})

Second order Lagrange interpolant

$$\hat{v}(x) = \frac{(x-x_j)(x-x_{j+1})}{(x_{j-1}-x_j)(x_{j-1}-x_{j+1})}\, v_{j-1} + \frac{(x-x_{j-1})(x-x_{j+1})}{(x_j-x_{j-1})(x_j-x_{j+1})}\, v_j +$$

$$\frac{(x-x_{j-1})(x-x_j)}{(x_{j+1}-x_{j-1})(x_{j+1}-x_j)}\, v_{j+1}$$

Finite Difference Formulas

Lagrange interpolation

...Example...

Assuming a uniform grid

$m = 1$ (First derivative)

	δ^1_{j-1}	δ^1_j	δ^1_{j+1}	
$i = j - 1$	$-\frac{3}{2\Delta x}$	$\frac{2}{\Delta x}$	$-\frac{1}{2\Delta x}$	Forward
$i = j$	$-\frac{1}{2\Delta x}$	0	$\frac{1}{2\Delta x}$	Centered
$i = j + 1$	$\frac{1}{2\Delta x}$	$-\frac{2}{\Delta x}$	$\frac{3}{2\Delta x}$	Backward

Finite Difference Formulas

Lagrange interpolation

...Example

$m = 2$ (Second derivative)

δ^2_{j-1}	δ^2_j	δ^2_{j+1}	
$\frac{1}{\Delta x^2}$	$-\frac{2}{\Delta x^2}$	$\frac{1}{\Delta x^2}$	Centered

N2

Finite Difference Formulas

Undetermined coefficients

Start from

$$\left.\frac{d^m v}{dx^m}\right|_{x=x_i} \approx \sum_{j=-l}^{r} \delta_j^m v_j \,.$$

Insert Taylor expansions for v_j about $x = x_i$

$$v_j = v_0 + v_0'(x_j - x_i) + \frac{1}{2}v_0''(x_j - x_i)^2 + \ldots,$$

determine coefficients δ_j^m to maximize accuracy.

Finite Difference Formulas

Undetermined coefficients

Example...

$m = 2, l = r = 1, i = 0$, (uniform spacing Δx)

$$v_0'' = \delta^2_{-1}\left(v_0 - \Delta x v_0' + \frac{\Delta x^2}{2} v_0'' - \frac{\Delta x^3}{6} v_0''' + \frac{\Delta x^4}{24} v_0^{(4)} + \ldots\right)$$
$$+ \delta^2_0 \quad v_0$$
$$+ \delta^2_1\left(v_0 + \Delta x v_0' + \frac{\Delta x^2}{2} v_0'' + \frac{\Delta x^3}{6} v_0''' + \frac{\Delta x^4}{24} v_0^{(4)} + \ldots\right)$$

Finite Difference Formulas

Undetermined coefficients

...Example

Equating coefficients of $v_0^{(k)}$

$$k = 0 \Rightarrow \quad \delta_{-1}^2 + \delta_0^2 + \delta_1^2 = 0$$

$$k = 1 \Rightarrow \quad \Delta x(\delta_1^2 - \delta_{-1}^2) = 0$$

$$k = 2 \Rightarrow \quad \frac{\Delta x^2}{2}(\delta_1^2 + \delta_{-1}^2) = 1$$

Solve,

$$\delta_{-1}^2 = \frac{1}{\Delta x^2}, \quad \delta_0^2 = -\frac{2}{\Delta x^2}, \quad \delta_1^2 = \frac{1}{\Delta x^2}$$

N3 N4

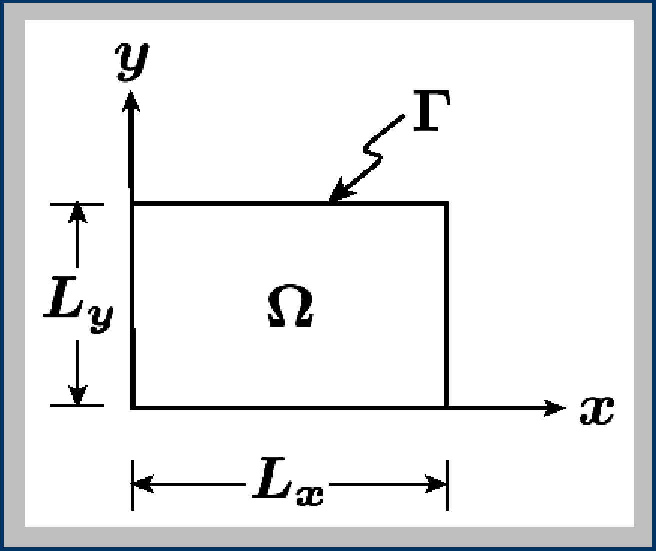
Poisson Equation in 2D

Definition

$$-\nabla^2 u(x,y) = f(x,y) \quad \text{in} \quad \Omega$$

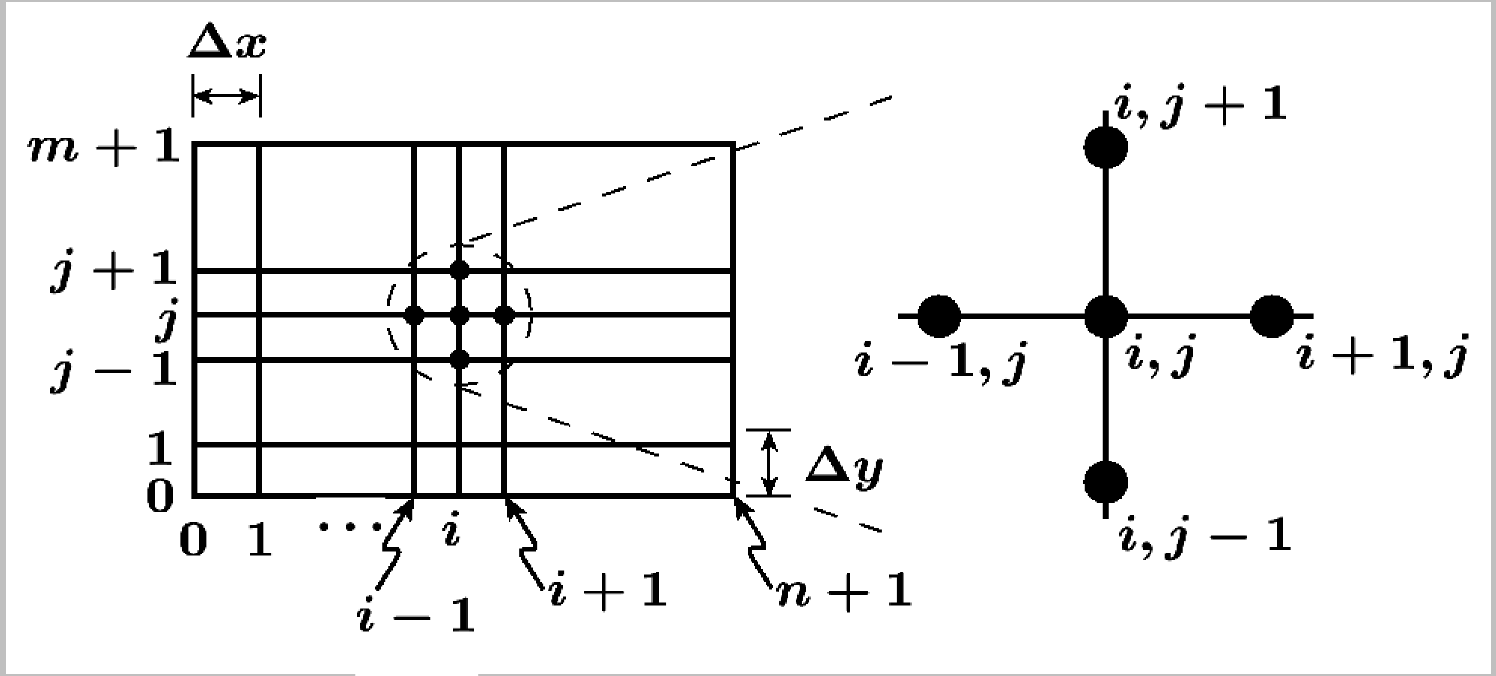
$$u = 0 \quad \text{on} \quad \Gamma$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}, \qquad f \in C^0$$



Poisson Equation in 2D

Discretization



$$\Delta x = \frac{L_x}{n+1}, \quad \Delta y = \frac{L_y}{m+1}, \qquad x_i = i\Delta x, \quad y_j = j\Delta y$$

Poisson Equation in 2D

Approximation

For example . . .

$$\left.\frac{\partial^2 v}{\partial x^2}\right|_{i,j} \approx \frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{\Delta x^2}$$

$$\left.\frac{\partial^2 v}{\partial y^2}\right|_{i,j} \approx \frac{v_{i,j+1} - 2v_{i,j} + v_{i,j-1}}{\Delta y^2}$$

for Δx, Δy small

Poisson Equation in 2D

Equations

$-u_{xx} - u_{yy} = f$ suggests ...

$$-\frac{\hat{u}_{i+1,j} - 2\hat{u}_{i,j} + \hat{u}_{i-1,j}}{\Delta x^2} - \frac{\hat{u}_{i,j+1} - 2\hat{u}_{i,j} + \hat{u}_{i,j-1}}{\Delta y^2} = \hat{f}_{i,j}$$

$$\hat{u}_{0,j} = \hat{u}_{n,j} = 0 \qquad 1 \le j \le m$$
$$\hat{u}_{i,0} = \hat{u}_{i,m} = 0 \qquad 1 \le i \le n$$

$$\Rightarrow \quad \boxed{A\underline{\hat{u}} = \underline{\hat{f}}}$$

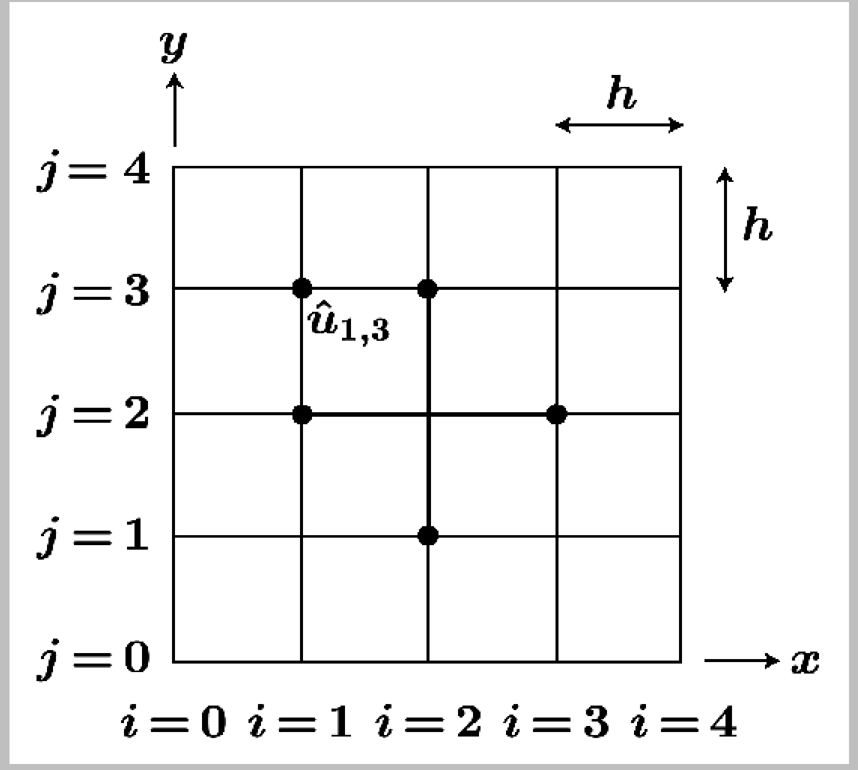
Poisson Equation in 2D

Equations

Example...

$$n = m = 3$$

$$\Delta x = \Delta y = h$$



Poisson Equation in 2D

Equations

...Example

$$A = \frac{1}{h^2} \left[\begin{array}{ccc|ccc|ccc}
4 & -1 & & -1 & & & & & \\
-1 & 4 & -1 & & -1 & & & & \\
& -1 & 4 & & & -1 & & & \\
\hline
-1 & & & 4 & -1 & & -1 & & \\
& -1 & & -1 & 4 & -1 & & -1 & \\
& & -1 & & -1 & 4 & & & -1 \\
\hline
& & & -1 & & & 4 & -1 & \\
& & & & -1 & & -1 & 4 & -1 \\
& & & & & -1 & & -1 & 4
\end{array} \right]$$

Poisson Equation in 2D

Equations

Numbering

$$\underline{\hat{u}} = \begin{pmatrix} \hat{u}_{11} \\ \vdots \\ \hat{u}_{n1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \hat{u}_{nm} \end{pmatrix}, \qquad \underline{\hat{f}} = \begin{pmatrix} \hat{f}_{11} \\ \vdots \\ \hat{f}_{n1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \hat{f}_{nm} \end{pmatrix}$$

(i, j) becomes component $(jm + i)$

Poisson Equation in 2D

Equations

Block Matrix...

$$A = \begin{pmatrix} A_x + 2I_y & -I_y & 0 & \cdots & 0 \\ -I_y & A_x + 2I_y & -I_y & \ddots & \vdots \\ 0 & \ddots & \ddots & \vdots & 0 \\ \vdots & \ddots & -I_y & A_x + 2I_y & -I_y \\ 0 & \cdots & 0 & -I_y & A_x + 2I_y \end{pmatrix}$$

Block $(m \times m)$ tridiagonal matrix

$$A_x, I_y : (n \times n), \quad \boxed{A : (nm \times nm)}$$

Poisson Equation in 2D

Equations

...Block Matrix

Block Definitions

$$A_x = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \vdots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}, \quad I_y = \frac{1}{\Delta y^2}\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \ddots & \vdots \\ 0 & \ddots & \ddots & \vdots & 0 \\ \vdots & \ddots & 0 & 1 & 0 \\ 0 & \cdots & 0 & 0 & 1 \end{pmatrix}$$

A has a banded structure

Bandwidth : $2n + 1$

Poisson Equation in 2D

Equations

SPD Property

$$\underline{v}^T A \underline{v} = \sum_{i=1}^{n+1} \sum_{j=1}^{m+1} [\frac{1}{\Delta x^2}(v_{ij} - v_{i-1,j})^2 + \frac{1}{\Delta y^2}(v_{ij} - v_{i,j-1})^2]$$

Hence $\boxed{\underline{v}^T A \underline{v} \geq 0, \text{ for any } \underline{v} \neq 0}$ (A is **SPD**)

$A\underline{\hat{u}} = \underline{\hat{f}}$: $\underline{\hat{u}}$ **exists** and is **unique**

Poisson Equation in 2D

Error Analysis

Truncation Error

$$-\frac{u(x_{i+1},y_j)-2u(x_i,y_j)+u(x_{i-1},y_j)}{\Delta x^2}$$

$$-\frac{u(x_i,y_{j+1})-2u(x_i,y_j)+u(x_i,y_{j-1})}{\Delta y^2}=f(x_i,y_j)$$

$$\underbrace{-\frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4}(x_i+\theta_i^x\Delta x,y_j)-\frac{\Delta y^2}{12}\frac{\partial^4 u}{\partial y^4}(x_i,y_j+\theta_j^y\Delta y)}_{\tau_{i,j}}$$

For $u \in \mathcal{C}^4$ $\quad \boxed{\tau_{i,j} \sim \mathcal{O}(\Delta x^2, \Delta y^2)}$ $\quad$ for all i,j

Poisson Equation in 2D

Error Analysis

$\|\cdot\|_\infty$ Stability

It can be shown that

$$\|A^{-1}\|_\infty \leq \frac{1}{8}$$

Ingredients:

- Positivity of the coefficients of A^{-1}
- Bound on the maximum row sum

Poisson Equation in 2D

Error Analysis

$\|\cdot\|_\infty$ Convergence

Error equation $A\underline{e} = \underline{\tau} \quad \Rightarrow \quad \boxed{\underline{e} = A^{-1}\underline{\tau}}$

$$\|\underline{e}\|_\infty = \|A^{-1}\underline{\tau}\|_\infty \leq \|A^{-1}\|_\infty \, \|\underline{\tau}\|_\infty \leq \frac{1}{8}\|\underline{\tau}\|_\infty$$

$$\leq \frac{1}{96}\left(\Delta x^2 \max_{(x,y)\in\Omega} |u_x^{(4)}| + \Delta y^2 \max_{(x,y)\in\Omega} |u_y^{(4)}|\right)$$

If $u \in \mathcal{C}^4 \quad \|\underline{e}\|_\infty \sim \mathcal{O}(\Delta x^2, \Delta y^2)$

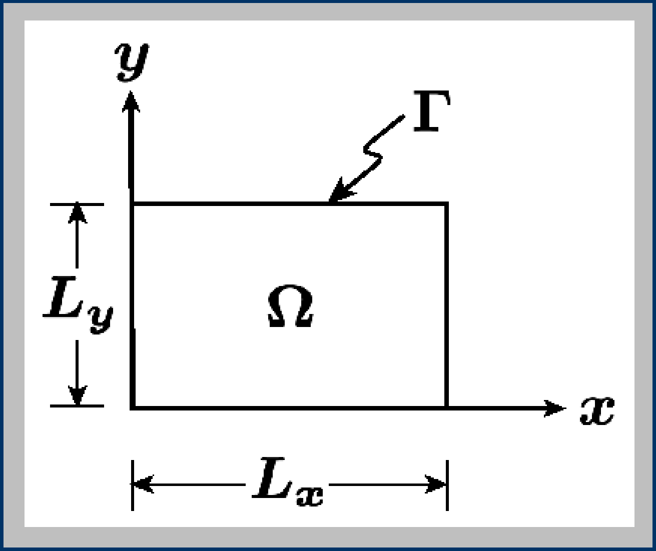
Eigenvalue Problem in 2D

Statement

$$-\nabla^2 u = \lambda u \quad \text{in} \quad \Omega$$

$$u = 0 \qquad \text{on} \quad \Gamma$$

Assume (for simplicity)
$L_x = L_y = 1$



Solutions $(u(x, y), \ \lambda)$

Eigenvalue Problem in 2D

Exact Solution

Eigenvalues

$$u^{k,l}(x,y) = \sin(k\pi x)\sin(l\pi y)$$

$$-\nabla^2 u^{k,l} = (k^2\pi^2 + l^2\pi^2)\, u^{k,l}$$

Eigenvectors

$$\lambda^{k,l} = k^2\pi^2 + l^2\pi^2, \qquad k,l = 1,\ldots$$

Eigenvalue Problem in 2D

Discrete Problem

Eigenvectors

$$\boxed{A\underline{\hat{u}} = \hat{\lambda}\underline{\hat{u}}} \quad \Rightarrow \quad (\underline{u}^{k,l}, \hat{\lambda}^{k,l})$$

$$u_{i,j}^{k,l} = \sin(k\pi x_i)\ \sin(l\pi y_j)$$

$$= \sin(k\pi i \Delta x)\ \sin(l\pi j \Delta y)$$

$$= \sin(\frac{k\pi i}{n+1})\ \sin(\frac{l\pi j}{m+1})$$

$$k, i = 1, \ldots, n \quad l, j = 1, \ldots, m$$

Eigenvalue Problem in 2D

Discrete Problem

Eigenvalues

$$\hat{\lambda}^{k,l} = \frac{2}{\Delta x}\{1 - \cos(k\pi\Delta x)\} + \frac{2}{\Delta y}\{1 - \cos(l\pi\Delta y)\}$$

Low Modes

$\Delta x, \Delta y \rightarrow 0$ (k, l fixed)

$$\hat{\lambda}^{k,l} = k^2\pi^2 + l^2\pi^2 + \mathcal{O}(\Delta x^2, \Delta y^2)$$

High Modes

$k \approx n$, $l \approx m$

$$\hat{\lambda}^{k,l} = 4(n+1)^2 + 4(m+1)^2$$

as $\Delta x, \Delta y \rightarrow 0$

Eigenvalue Problem in 2D

Condition Number of A

$$\kappa_A \rightarrow \frac{4n^2 + 4m^2}{2\pi^2} \quad \text{as} \quad \Delta x, \Delta y \rightarrow 0$$

If $m \approx n$

$$\kappa_A \rightarrow \frac{4n^2}{\pi^2}$$

grows (in $\mathbb{R}^2$) as number of grid points.
(better than in 1D, relatively speaking !!)

Eigenvalue Problem in 2D

Link to $-\nabla^2 u = f$

$\|\cdot\|$ Error Estimate

Error equation $\quad A\underline{e} = \underline{\tau} \quad \Rightarrow \quad \boxed{\underline{e} = A^{-1}\underline{\tau}}$

$$\|\underline{e}\|_2 = \|A^{-1}\underline{\tau}\|_2 \le \|A^{-1}\|_2\ \|\tau\|_2 \le \frac{1}{\hat{\lambda}^{1,1}}\|\tau\|_2$$

$$(\Delta x \Delta y)^{1/2}\|\underline{e}\|_2 \le \frac{1}{\hat{\lambda}^{1,1}}(\Delta x \Delta y)^{1/2}\|\underline{\tau}\|_2$$

$$\Rightarrow \qquad \|\underline{e}\| \le \frac{1}{\hat{\lambda}^{1,1}}\|\underline{\tau}\| \sim \mathcal{O}(\Delta x^2, \Delta y^2)$$

Discrete Fourier Solution

A is SPD $\quad \Rightarrow \quad \boxed{A = Z \Lambda Z^T}$

Λ diagonal matrix of eigenvalues $(nm \times nm)$

Z is matrix of eigenvectors $(nm \times nm)$

$$Z = 2\sqrt{\Delta x \Delta y} \begin{pmatrix} \hat{u}^{1,1} & \hat{u}^{2,1} & & \hat{u}^{n,m} \\ \vdots & \vdots & & \vdots \\ \downarrow & \downarrow & & \downarrow \\ \vdots & \vdots & & \vdots \end{pmatrix}$$

Discrete Fourier Solution

Poisson Problem 2D

$$Z \Lambda Z^T \underline{\hat{u}} = \underline{\hat{f}} \quad \Rightarrow \quad Z^T \underline{\hat{u}} = \Lambda^{-1} Z^T \underline{\hat{f}} \quad \boxed{\underline{\hat{u}} = Z \Lambda^{-1} Z^T \underline{\hat{f}}}$$

ALGORITHM

1. $\underline{\hat{f}}^* = Z^T \underline{\hat{f}}$
2. $\underline{\hat{u}}^* = \Lambda^{-1} \underline{\hat{f}}^*$
3. $\underline{\hat{u}} = Z \underline{\hat{u}}^*$

Still cost is $\mathcal{O}(n^4)$ $(n \approx m)$ ... **BUT** ...

Discrete Fourier Solution

- Matrix multiplications can be reorganized (tensor product evaluation) N5 $\Rightarrow \mathcal{O}(n^3)$

- $\underline{\hat{f}}^* = Z^T \underline{\hat{f}}$ $(\underline{\hat{u}} = Z \underline{\hat{u}}^*)$ is a (Inverse) Discrete Fourier Transform

  Using FFT $\Rightarrow \mathcal{O}(n^2 \log n)$

Non-Rectangular Domains

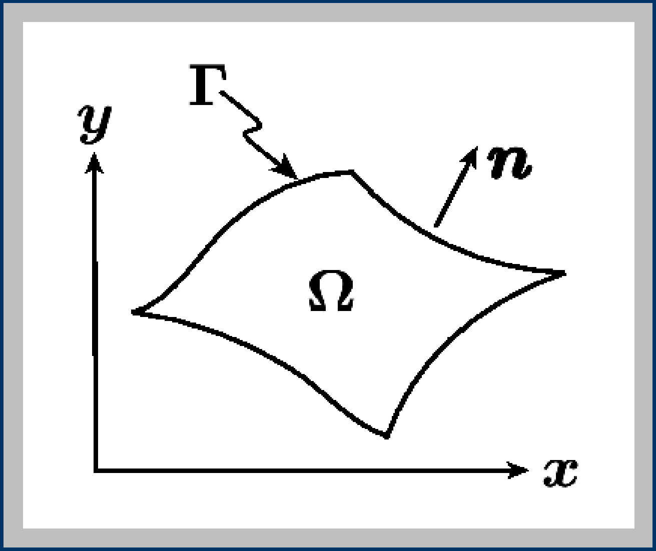
We are interested in solving

$$-\nabla^2 u = f \qquad \text{in } \Omega$$

$$u = g \qquad \text{on } \Gamma_D$$

$$\frac{\partial u}{\partial n} = h \qquad \text{on } \Gamma_N = \Gamma \backslash \Gamma_D$$

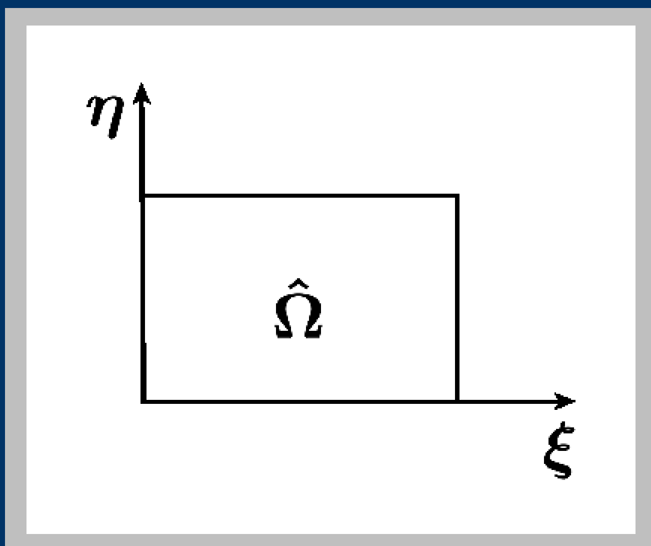
where f, g, and h are given.



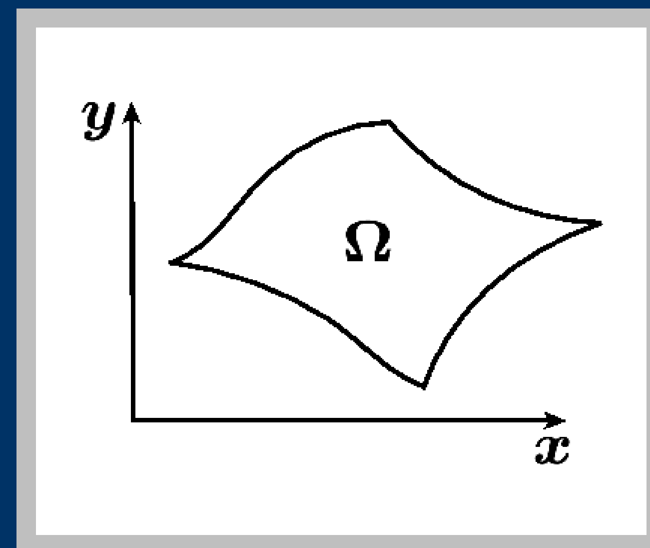
Non-Rectangular Domains

Poisson Problem 2D

Mapping



$$x = x(\xi, \eta)$$
$$y = y(\xi, \eta)$$
$$\longrightarrow$$



? ?

$$-\nabla^2 u = f$$

Can we determine an equivalent problem to be solved on $\hat{\Omega}$?

Non-Rectangular Domains

Poisson Problem 2D

Transformed equations...

$$u(x,y) \equiv \underbrace{u\left(x(\xi,\eta), y(\xi,\eta)\right)}_{u(\xi,\eta)} \quad \Rightarrow \quad \begin{aligned} u_x &= \xi_x u_\xi + \eta_x u_\eta \\ u_y &= \xi_y u_\xi + \eta_y u_\eta \end{aligned}$$

How do we evaluate terms ξ_x, η_x, ξ_y, and η_y?

Non-Rectangular Domains

Poisson Problem 2D

...Transformed equations...

$$\xi = \xi(x,y) \qquad x = x(\xi,\eta)$$
$$\eta = \eta(x,y) \qquad y = y(\xi,\eta)$$

$$\begin{pmatrix} d\xi \\ d\eta \end{pmatrix} = \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix} \qquad \begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix} \begin{pmatrix} d\xi \\ d\eta \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \xi_y \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix}^{-1} = \frac{1}{J} \begin{pmatrix} y_\eta & -x_\eta \\ -y_\xi & x_\xi \end{pmatrix}$$

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Non-Rectangular Domains

Poisson Problem 2D

...Transformed equations...

$$u_x = \frac{1}{J}\left(y_\eta u_\xi - y_\xi u_\eta\right)$$

$$u_y = \frac{1}{J}\left(-x_\eta u_\xi + x_\xi u_\eta\right)$$

and

$$u_{xx} = \frac{\partial}{\partial x}(u_x) = \left(\xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta}\right) u_x$$

$$= \frac{1}{J}\left(y_\eta \frac{\partial}{\partial \xi} - y_\xi \frac{\partial}{\partial \eta}\right) u_x$$

$$= \ldots$$

$$u_{yy} = \ldots$$

Non-Rectangular Domains

Poisson Problem 2D

...Transformed equations

Finally, $-(u_{xx} + u_{yy}) = f$, becomes

$$\frac{-1}{J^2}\left(a\, u_{\xi\xi} - 2b\, u_{\xi\eta} + c\, u_{\eta\eta} + d\, u_{\eta} + e\, u_{\xi}\right) = f$$

a, b, c, d, and e depend on the mapping.

$$a = x_\eta^2 + y_\eta^2 \qquad e = \frac{x_\eta \beta - y_\eta \alpha}{J} \qquad \alpha = a x_{\xi\xi} - 2b x_{\xi\eta} + c x_{\eta\eta}$$

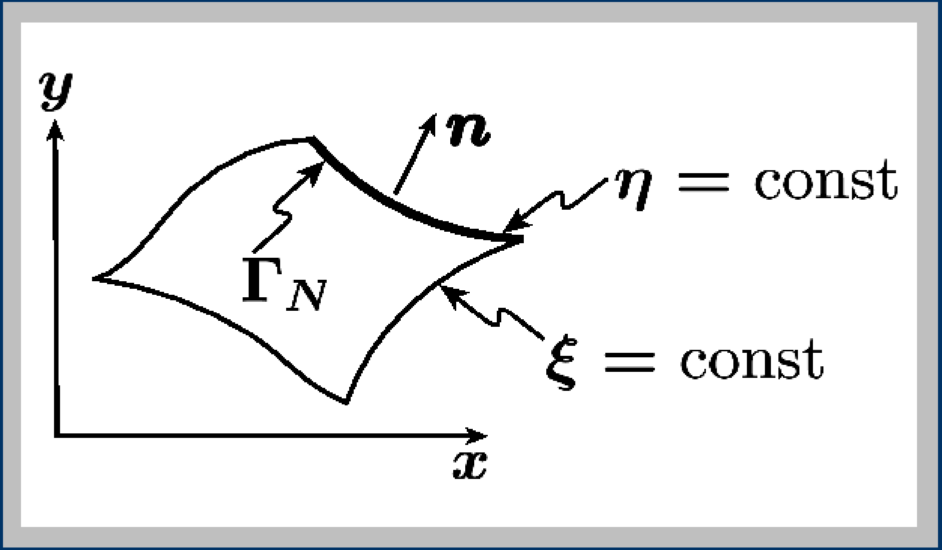
$$b = x_\xi x_\eta + y_\xi y_\eta \qquad d = \frac{y_\xi \alpha - x_\xi \beta}{J} \qquad \beta = a y_{\xi\xi} - 2b y_{\xi\eta} + c y_{\eta\eta}$$

$$c = x_\xi^2 + y_\xi^2$$

Non-Rectangular Domains

Poisson Problem 2D

Normal Derivatives...



$\boldsymbol{n} = (n^x, n^y)$ is parallel to $\nabla\eta$ (or $\nabla\xi$); e.g., on Γ_N

$$\boldsymbol{n} = \frac{1}{\sqrt{\eta_x^2 + \eta_y^2}}(\eta_x, \eta_y) = \frac{1}{\sqrt{x_\xi^2 + y_\xi^2}}(-y_\xi, x_\xi)$$

Non-Rectangular Domains

Poisson Problem 2D

Normal Derivatives...

Thus,

$$\frac{\partial u}{\partial n} = u_x n^x + u_y n^y \; = \; \frac{1}{J} \left[\left(y_\eta n^x - x_\eta n^y \right) u_\xi \right.$$

$$\left. + \left(-y_\xi n^x + x_\xi n^5 y \right) u_\eta \right]$$

with $(n^x, n^y) = \dfrac{1}{\sqrt{x_\xi^2 + y_\xi^2}} (-y_\xi, x_\xi)$.