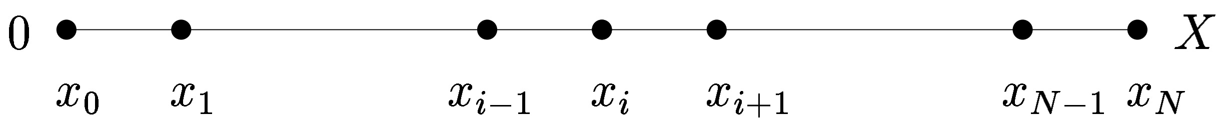
Finite difference method

Principle: derivatives in the partial differential equation are approximated by linear combinations of function values at the grid points

1D: $\Omega = (0, X)$, $u_i \approx u(x_i)$, $i = 0, 1, \ldots, N$

grid points $x_i = i\Delta x$ mesh size $\Delta x = \frac{X}{N}$

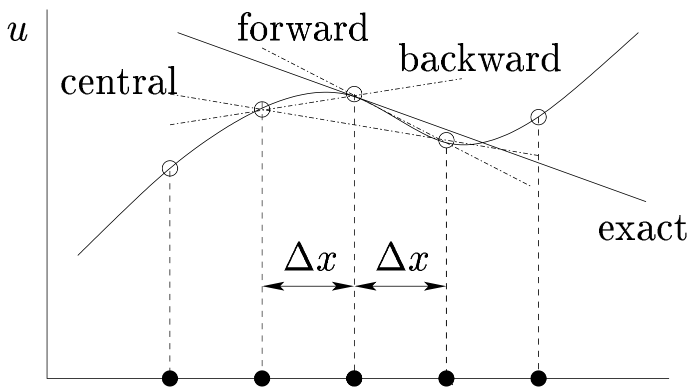


First-order derivatives

$$\begin{aligned}
\frac{\partial u}{\partial x}(\bar{x}) &= \lim_{\Delta x \to 0} \frac{u(\bar{x} + \Delta x) - u(\bar{x})}{\Delta x} = \lim_{\Delta x \to 0} \frac{u(\bar{x}) - u(\bar{x} - \Delta x)}{\Delta x} \\
&= \lim_{\Delta x \to 0} \frac{u(\bar{x} + \Delta x) - u(\bar{x} - \Delta x)}{2\Delta x} \qquad \text{(by definition)}
\end{aligned}$$

Approximation of first-order derivatives

Geometric interpretation



$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1}-u_i}{\Delta x}$ forward difference

$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_i-u_{i-1}}{\Delta x}$ backward difference

$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1}-u_{i-1}}{2\Delta x}$ central difference

Taylor series expansion $\quad u(x) = \sum_{n=0}^{\infty} \frac{(x-x_i)^n}{n!} \left(\frac{\partial^n u}{\partial x^n}\right)_i, \qquad u \in C^\infty([0,X])$

$$T_1: \qquad u_{i+1} = u_i + \Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{(\Delta x)^2}{2} \left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(\Delta x)^3}{6} \left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

$$T_2: \qquad u_{i-1} = u_i - \Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{(\Delta x)^2}{2} \left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^3}{6} \left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

Analysis of truncation errors

Accuracy of finite difference approximations

$$T_1 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

forward difference truncation error $\mathcal{O}(\Delta x)$

$$T_2 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

backward difference truncation error $\mathcal{O}(\Delta x)$

$$T_1 - T_2 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

central difference truncation error $\mathcal{O}(\Delta x)^2$

Leading truncation error

$$\epsilon_\tau = \alpha_m(\Delta x)^m + \alpha_{m+1}(\Delta x)^{m+1} + \ldots \approx \alpha_m(\Delta x)^m$$

Approximation of second-order derivatives

Central difference scheme

$$T_1 + T_2 \quad \Rightarrow \quad \left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2$$

Alternative derivation

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \left[\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right)\right]_i = \lim_{\Delta x \to 0} \frac{\left(\frac{\partial u}{\partial x}\right)_{i+1/2} - \left(\frac{\partial u}{\partial x}\right)_{i-1/2}}{\Delta x}$$

$$\approx \frac{\frac{u_{i+1}-u_i}{\Delta x} - \frac{u_i - u_{i-1}}{\Delta x}}{\Delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$

Variable coefficients $\qquad f(x) = d(x)\frac{\partial u}{\partial x} \qquad$ *diffusive flux*

$$\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x} = \frac{d_{i+1/2}\frac{u_{i+1}-u_i}{\Delta x} - d_{i-1/2}\frac{u_i-u_{i-1}}{\Delta x}}{\Delta x}$$

$$= \frac{d_{i+1/2}u_{i+1} - (d_{i+1/2} + d_{i-1/2})u_i + d_{i-1/2}u_{i-1}}{(\Delta x)^2}$$

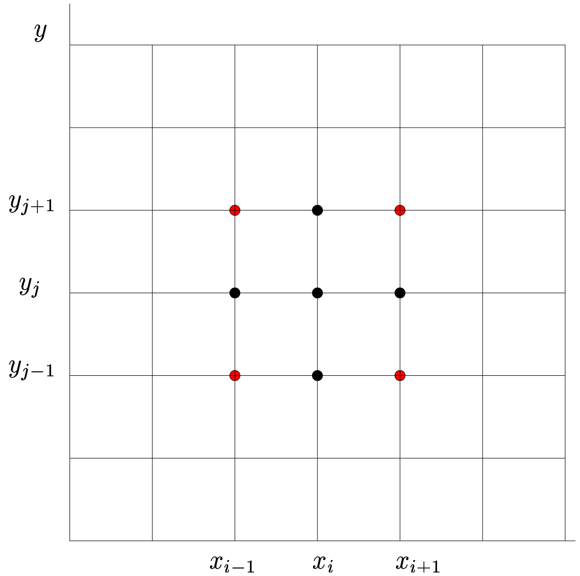
Approximation of mixed derivatives

2D: $\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)$

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j}}{2\Delta x} + \mathcal{O}(\Delta x)^2$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} + \mathcal{O}(\Delta y)^2$$

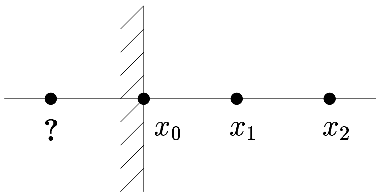
$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y} + \mathcal{O}(\Delta y)^2$$



Second-order difference approximation

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4\Delta x \Delta y} + \mathcal{O}[(\Delta x)^2, (\Delta y)^2]$$

One-sided finite differences



$$\left(\frac{\partial u}{\partial x}\right)_0 = \frac{u_1 - u_0}{\Delta x} + \mathcal{O}(\Delta x) \quad \text{forward difference}$$

backward/central difference approximations would need u_{-1} which is not available

Polynomial fitting

$$u(x) = u_0 + x\left(\frac{\partial u}{\partial x}\right)_0 + \frac{x^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_0 + \frac{x^3}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_0 + \dots$$

$$u(x) \approx a + bx + cx^2, \qquad \frac{\partial u}{\partial x} \approx b + 2cx, \qquad \left(\frac{\partial u}{\partial x}\right)_0 \approx b$$

approximate u by a polynomial and differentiate it to obtain the derivatives

$$\begin{aligned} u_0 &= a \\ u_1 &= a + b\Delta x + c\Delta x^2 \\ u_2 &= a + 2b\Delta x + 4c\Delta x^2 \end{aligned} \quad \Rightarrow \quad \begin{aligned} c\Delta x^2 &= u_1 - u_0 - b\Delta x \\ b &= \frac{-3u_0 + 4u_1 - u_2}{2\Delta x} \end{aligned}$$

Analysis of the truncation error

One-sided approximation $$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{\alpha u_i + \beta u_{i+1} + \gamma u_{i+2}}{\Delta x}$$

$$u_{i+1} = u_i + \Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(\Delta x)^3}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

$$u_{i+2} = u_i + 2\Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{(2\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(2\Delta x)^3}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

$$\tfrac{\alpha u_i + \beta u_{i+1} + \gamma u_{i+2}}{\Delta x} = \tfrac{\alpha+\beta+\gamma}{\Delta x} u_i + (\beta + 2\gamma)\left(\tfrac{\partial u}{\partial x}\right)_i + \tfrac{\Delta x}{2}(\beta + 4\gamma)\left(\tfrac{\partial^2 u}{\partial x^2}\right)_i + \mathcal{O}(\Delta x^2)$$

Second-order accurate if $\alpha + \beta + \gamma = 0, \quad \beta + 2\gamma = 1, \quad \beta + 4\gamma = 0$

$$\alpha = -\tfrac{3}{2}, \quad \beta = 2, \quad \gamma = -\tfrac{1}{2} \quad \Rightarrow \quad \left(\tfrac{\partial u}{\partial x}\right)_i = \tfrac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

Application to second-order derivatives

One-sided approximation $$\left(\frac{\partial^2 u}{\partial x^2}\right)_i \approx \frac{\alpha u_i + \beta u_{i+1} + \gamma u_{i+2}}{\Delta x^2}$$

$$u_{i+1} = u_i + \Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(\Delta x)^3}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

$$u_{i+2} = u_i + 2\Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{(2\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{(2\Delta x)^3}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

$$\frac{\alpha u_i + \beta u_{i+1} + \gamma u_{i+2}}{\Delta x^2} = \frac{\alpha+\beta+\gamma}{\Delta x^2} u_i + \frac{\beta+2\gamma}{\Delta x}\left(\frac{\partial u}{\partial x}\right)_i + \frac{\beta+4\gamma}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \mathcal{O}(\Delta x)$$

First-order accurate if $\alpha+\beta+\gamma = 0, \quad \beta + 2\gamma = 0, \quad \beta + 4\gamma = 2$

$$\alpha = 1, \quad \beta = -2, \quad \gamma = 1 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - 2u_{i+1} + u_{i+2}}{\Delta x^2} + \mathcal{O}(\Delta x)$$

High-order approximations

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{2u_{i+1} + 3u_i - 6u_{i-1} + u_{i-2}}{6\Delta x} + \mathcal{O}(\Delta x)^3 \qquad \text{backward difference}$$

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 6u_{i+1} - 3u_i - 2u_{i-1}}{6\Delta x} + \mathcal{O}(\Delta x)^3 \qquad \text{forward difference}$$

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x} + \mathcal{O}(\Delta x)^4 \qquad \text{central difference}$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12(\Delta x)^2} + \mathcal{O}(\Delta x)^4 \qquad \text{central difference}$$

Pros and cons of high-order difference schemes

$\ominus$ more grid points, fill-in, considerable overhead cost

$\oplus$ high resolution, reasonable accuracy on coarse grids

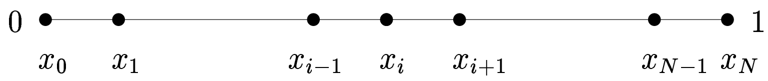
Criterion: total computational cost to achieve a prescribed accuracy

Example: 1D Poisson equation

Boundary value problem

$$-\frac{\partial^2 u}{\partial x^2} = f \quad \text{in } \Omega = (0,1), \qquad u(0) = u(1) = 0$$

One-dimensional mesh



$$u_i \approx u(x_i), \quad f_i = f(x_i) \qquad x_i = i\Delta x, \quad \Delta x = \frac{1}{N}, \quad i = 0, 1, \ldots, N$$

Central difference approximation $\qquad \mathcal{O}(\Delta x)^2$

$$\begin{cases} -\frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} = f_i, & \forall i = 1, \ldots, N-1 \\ u_0 = u_N = 0 & \text{Dirichlet boundary conditions} \end{cases}$$

Result: the original PDE is replaced by a linear system for nodal values

Example: 1D Poisson equation

Linear system for the central difference scheme

$$\begin{cases} i=1 & -\frac{u_0-2u_1+u_2}{(\Delta x)^2} & = f_1 \\ i=2 & -\frac{u_1-2u_2+u_3}{(\Delta x)^2} & = f_2 \\ i=3 & -\frac{u_2-2u_3+u_4}{(\Delta x)^2} & = f_3 \\ & \dots & \\ i=N-1 & \frac{u_{N-2}-2u_{N-1}+u_N}{(\Delta x)^2} & = f_{N-1} \end{cases}$$

Matrix form $\boxed{Au=F}$ $\quad A \in \mathbb{R}^{N-1\times N-1} \quad u, F \in \mathbb{R}^{N-1}$

$$A = \frac{1}{(\Delta x)^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \dots & \\ & & & -1 & 2 \end{bmatrix}, \qquad u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ u_{N-1} \end{bmatrix}, \qquad F = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \cdot \\ f_{N-1} \end{bmatrix}$$

The matrix A is tridiagonal and symmetric positive definite $\Rightarrow$ invertible.

Other types of boundary conditions

Dirichlet-Neumann BC $\quad u(0) = \frac{\partial u}{\partial x}(1) = 0$

$$u_0 = 0, \qquad \frac{u_{N+1} - u_{N-1}}{2\Delta x} = 0 \quad \Rightarrow \quad u_{N+1} = u_{N-1} \qquad \text{central difference}$$

Extra equation for the last node

$$-\frac{u_{N-1} - 2u_N + u_{N+1}}{(\Delta x)^2} = f_N \qquad \longrightarrow \qquad \frac{-u_{N-1} + u_N}{(\Delta x)^2} = \frac{1}{2} f_N$$

Extended linear system $\quad \boxed{Au = F} \qquad A \in \mathbb{R}^{N \times N} \quad u, F \in \mathbb{R}^N$

$$A = \frac{1}{(\Delta x)^2} \begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & & \cdots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}, \qquad u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ u_{N-1} \\ u_N \end{bmatrix}, \qquad F = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \cdot \\ f_{N-1} \\ \frac{1}{2} f_N \end{bmatrix}$$

The matrix A remains tridiagonal and symmetric positive definite.

Other types of boundary conditions

Non-homogeneous Dirichlet BC $\quad u(0) = g_0 \quad$ only F changes

$$u_0 = g_0 \quad \Rightarrow \quad \frac{2u_1 - u_2}{(\Delta x)^2} = f_1 + \frac{g_0}{(\Delta x)^2} \qquad \text{first equation}$$

Non-homogeneous Neumann BC $\quad \frac{\partial u}{\partial x}(1) = g_1 \quad$ only F changes

$$\frac{u_{N+1} - u_{N-1}}{2\Delta x} = g_1 \quad \Rightarrow \quad u_{N+1} = u_{N-1} + 2\Delta x g_1$$

$$-\frac{u_{N-1} - 2u_N + u_{N+1}}{(\Delta x)^2} = f_N \qquad \longrightarrow \qquad \frac{-u_{N-1} + u_N}{(\Delta x)^2} = \frac{1}{2} f_N + \frac{g_1}{\Delta x}$$

Non-homogeneous Robin BC $\quad \frac{\partial u}{\partial x}(1) + \alpha u(1) = g_2 \quad$ A and F change

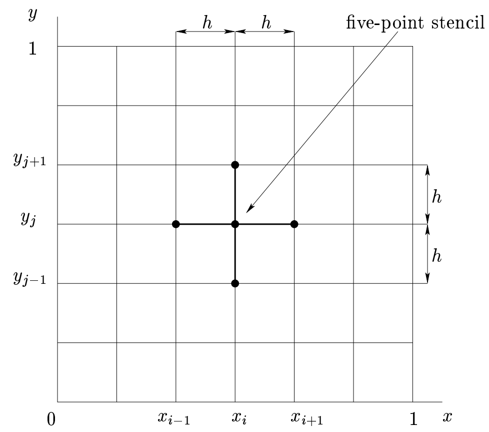
$$\frac{u_{N+1} - u_{N-1}}{2\Delta x} + \alpha u_N = g_2 \quad \Rightarrow \quad u_{N+1} = u_{N-1} - 2\Delta x \alpha u_N + 2\Delta x g_2$$

$$-\frac{u_{N-1} - 2u_N + u_{N+1}}{(\Delta x)^2} = f_N \qquad \longrightarrow \qquad \frac{-u_{N-1} + (1 + \alpha\Delta x) u_N}{(\Delta x)^2} = \frac{1}{2} f_N + \frac{g_2}{\Delta x}$$

Example: 2D Poisson equation

Boundary value problem

$$\begin{cases} -\dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial^2 u}{\partial y^2} = f & \text{in } \Omega = (0,1) \times (0,1) \\ u = 0 & \text{on } \Gamma = \partial\Omega \end{cases}$$



Uniform mesh: $\Delta x = \Delta y = h, \quad N = \frac{1}{h}$

$$u_{i,j} \approx u(x_i, y_j), \quad f_{i,j} = f(x_i, y_j), \qquad (x_i, y_j) = (ih, jh), \quad i, j = 0, 1, \ldots, N$$

Central difference approximation $\qquad \mathcal{O}(h^2)$

$$\begin{cases} -\dfrac{u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i+1,j} + u_{i,j+1}}{h^2} = f_{i,j}, & \forall i, j = 1, \ldots, N-1 \\ u_{i,0} = u_{i,N} = u_{0,j} = u_{N,j} = 0 & \forall i, j = 0, 1, \ldots, N \end{cases}$$

Example: 2D Poisson equation

Linear system $\boxed{Au = F}$ $A \in \mathbb{R}^{(N-1)^2 \times (N-1)^2}$ $u, F \in \mathbb{R}^{(N-1)^2}$

row-by-row node numbering

$$u = [u_{1,1} \dots u_{N-1,1} \; u_{1,2} \dots u_{N-1,2} \; u_{1,3} \dots u_{N-1,N-1}]^T$$

$$F = [f_{1,1} \dots f_{N-1,1} \; f_{1,2} \dots f_{N-1,2} \; f_{1,3} \dots f_{N-1,N-1}]^T$$

$$A = \begin{bmatrix} B & -I & & & & \\ -I & B & -I & & & \\ & & \dots & \dots & & \\ & & & -I & B & -I \\ & & & & -I & B \end{bmatrix}, \qquad B = \begin{bmatrix} 4 & -1 & & & & \\ -1 & 4 & -1 & & & \\ & & \dots & \dots & & \\ & & & -1 & 4 & -1 \\ & & & & -1 & 4 \end{bmatrix}$$

$$I = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & \cdot & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}$$

The matrix A is sparse, block-tridiagonal (for the above numbering) and SPD.

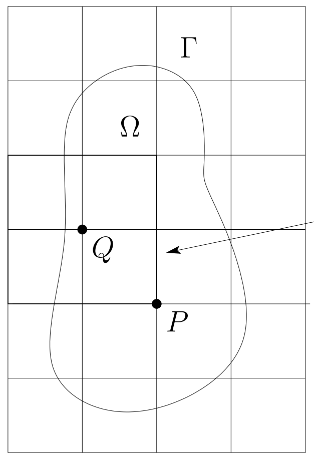
$$\mathrm{cond}_2(A) = \frac{|\lambda_{\max}|}{|\lambda_{\min}|} = \mathcal{O}(h^{-2})$$

Caution: convergence of iterative solvers deteriorates as the mesh is refined

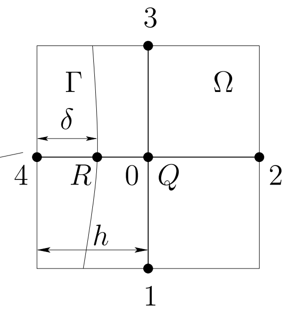
Treatment of complex geometries

2D Poisson equation

$$\begin{cases} -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f & \text{in } \Omega \\ u = g_0 & \text{on } \Gamma \end{cases}$$



curvilinear boundary



stencil of Q

Difference equation

$$-\frac{u_1 + u_2 - 4u_0 + u_3 + u_4}{h^2} = f_0$$

Linear interpolation

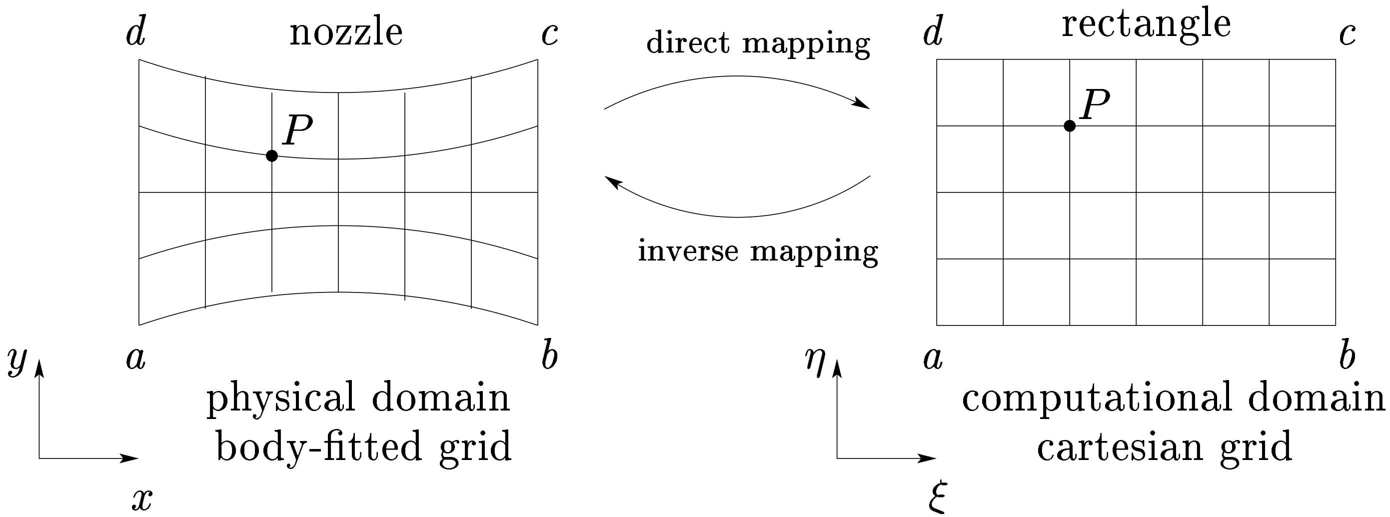
$$u(R) = \frac{u_4(h-\delta) + u_0\delta}{h} = g_0(R) \quad \Rightarrow \quad u_4 = -u_0\frac{\delta}{h-\delta} + g_0(R)\frac{h}{h-\delta}$$

Substitution yields $\quad -u_1 + u_2 - \left(4 + \frac{\delta}{h-\delta}\right)u_0 + u_3 = h^2 f_0 + g_0(R)\frac{h}{h-\delta}$

Neumann and Robin BC are even more difficult to implement

Grid transformations

Purpose: to provide a simple treatment of curvilinear boundaries



The original PDE must be rewritten in terms of (ξ, η) instead of (x, y) and discretized in the computational domain rather than the physical one.

Derivative transformations $\qquad \underbrace{\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \dots}_{\text{difficult to compute}} \longrightarrow \underbrace{\frac{\partial u}{\partial \xi}, \frac{\partial u}{\partial \eta}, \dots}_{\text{easy to compute}}$

PDE transformations for a direct mapping

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

Chain rule $$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial x}, \qquad \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial y} + \frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial y}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial \xi}\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial u}{\partial \eta}\frac{\partial^2 \eta}{\partial x^2} + 2\frac{\partial^2 u}{\partial \xi \partial \eta}\frac{\partial \xi}{\partial x}\frac{\partial \eta}{\partial x} + \frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2 + \frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{\partial u}{\partial \xi}\frac{\partial^2 \xi}{\partial y^2} + \frac{\partial u}{\partial \eta}\frac{\partial^2 \eta}{\partial y^2} + 2\frac{\partial^2 u}{\partial \xi \partial \eta}\frac{\partial \xi}{\partial y}\frac{\partial \eta}{\partial y} + \frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial y}\right)^2 + \frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial y}\right)^2$$

Example: 2D Poisson equation $\boxed{-\Delta u = f}$ turns into

$$-\frac{\partial^2 u}{\partial \xi^2}\left[\left(\frac{\partial \xi}{\partial x}\right)^2 + \left(\frac{\partial \xi}{\partial y}\right)^2\right] - \frac{\partial^2 u}{\partial \eta^2}\left[\left(\frac{\partial \eta}{\partial x}\right)^2 + \left(\frac{\partial \eta}{\partial y}\right)^2\right] - 2\frac{\partial^2 u}{\partial \xi \partial \eta}\left[\frac{\partial \xi}{\partial x}\frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y}\frac{\partial \eta}{\partial y}\right]$$

$$-\frac{\partial u}{\partial \xi}\left[\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2}\right] - \frac{\partial u}{\partial \eta}\left[\frac{\partial^2 \eta}{\partial x^2} + \frac{\partial^2 \eta}{\partial y^2}\right] = f$$

transformed equations
contain many more terms

The *metrics* need to be determined (approximated by finite differences)

PDE transformations for an inverse mapping

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

Metrics transformations $\qquad \underbrace{\frac{\partial \xi}{\partial x}, \frac{\partial \xi}{\partial y}, \frac{\partial \eta}{\partial x}, \frac{\partial \eta}{\partial y}}_{\text{unknown}} \longrightarrow \underbrace{\frac{\partial x}{\partial \xi}, \frac{\partial x}{\partial \eta}, \frac{\partial y}{\partial \xi}, \frac{\partial y}{\partial \eta}}_{\text{known}}$

Chain rule

$$\begin{aligned} \frac{\partial u}{\partial \xi} &= \frac{\partial u}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \xi} \\ \frac{\partial u}{\partial \eta} &= \frac{\partial u}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \eta} \end{aligned} \qquad \Rightarrow \qquad \begin{bmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \end{bmatrix} = \underbrace{\begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix}}_{J} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{bmatrix}$$

where $J = \frac{\partial(x,y)}{\partial(\xi,\eta)}$ is the Jacobian which can be inverted using Cramer's rule

Derivative transformations

$$\frac{\partial u}{\partial x} = \frac{1}{\det J}\left[\frac{\partial u}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial u}{\partial \eta}\frac{\partial y}{\partial \xi}\right], \qquad \frac{\partial u}{\partial y} = \frac{1}{\det J}\left[\frac{\partial u}{\partial \eta}\frac{\partial x}{\partial \xi} - \frac{\partial u}{\partial \xi}\frac{\partial x}{\partial \eta}\right]$$

Direct versus inverse mapping

Total differentials for both coordinate systems

$$\begin{aligned} \xi &= \xi(x,y) \\ \eta &= \eta(x,y) \end{aligned} \quad \Rightarrow \quad \begin{aligned} d\xi &= \tfrac{\partial \xi}{\partial x}dx + \tfrac{\partial \xi}{\partial y}dy \\ d\eta &= \tfrac{\partial \eta}{\partial x}dx + \tfrac{\partial \eta}{\partial y}dy \end{aligned} \qquad \begin{bmatrix} d\xi \\ d\eta \end{bmatrix} = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} \begin{bmatrix} dx \\ dy \end{bmatrix}$$

$$\begin{aligned} x &= x(\xi,\eta) \\ y &= y(\xi,\eta) \end{aligned} \quad \Rightarrow \quad \begin{aligned} dx &= \tfrac{\partial x}{\partial \xi}d\xi + \tfrac{\partial x}{\partial \eta}d\eta \\ dy &= \tfrac{\partial y}{\partial \xi}d\xi + \tfrac{\partial y}{\partial \eta}d\eta \end{aligned} \qquad \begin{bmatrix} dx \\ dy \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{bmatrix} \begin{bmatrix} d\xi \\ d\eta \end{bmatrix}$$

$$\Rightarrow \quad \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{bmatrix}^{-1} = \frac{1}{\det J} \begin{bmatrix} \frac{\partial y}{\partial \eta} & -\frac{\partial x}{\partial \eta} \\ -\frac{\partial y}{\partial \xi} & \frac{\partial x}{\partial \xi} \end{bmatrix}$$

Relationship between the direct and inverse metrics

$$\frac{\partial \xi}{\partial x} = \frac{1}{\det J}\frac{\partial y}{\partial \eta}, \qquad \frac{\partial \eta}{\partial x} = -\frac{1}{\det J}\frac{\partial y}{\partial \xi}, \qquad \frac{\partial \xi}{\partial y} = -\frac{1}{\det J}\frac{\partial x}{\partial \eta}, \qquad \frac{\partial \eta}{\partial y} = \frac{1}{\det J}\frac{\partial x}{\partial \xi}$$