Scientific Computing

Lecture 2

Delft University of Technology

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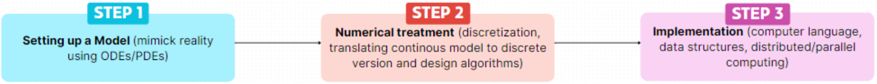
Recap Last Week

- Model problem
- Uniqueness
- Real-world Applications
- Setting up the Numerical Model (Ch. 3)

Sources of Errors



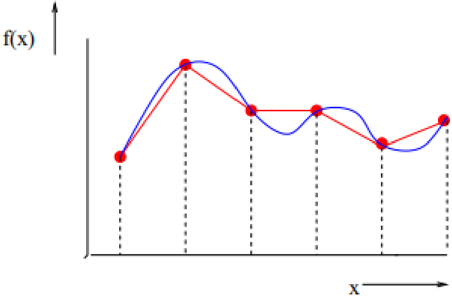
- Modelling error
- Error in data

- Discretization error
- Truncation error
- Round-off error

- Programming errors

Sources of Errors - Discretization

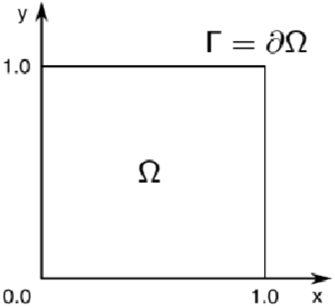
Discretization error



Only n values are obtained: gives an approximate solution curve.

§ 3.4: Model Problem (MP) - 2D Poisson

- Continuous Poisson operator: $-\triangle u := -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f$ with $u(x, y), f(x, y) \in \mathbb{R}$
- Continuous Domain



- Boundary conditions:
  - Dirichlet: $u(x, y) = b(x, y)$
  - Neumann: $\frac{\partial u}{\partial n} = c(x, y)$

§ 3.4: Continuous 1D Poisson MP

Given the domain $\Omega = (0, 1)$ with boundary $\Gamma = \partial\Omega$ and outward normal $\mathbf{n}$, solve for $u(x)$

$$-\frac{d^2 u(x)}{dx^2} = f(x) \text{ on } \Omega$$

with either Dirichlet BCs

$$u(x) = b(x) \text{ on } \Gamma$$

or Neumann BCs

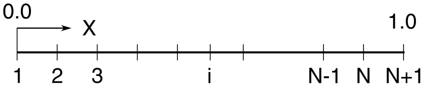
$$\frac{\partial u(x)}{\partial n} = \nabla u(x) \cdot \mathbf{n} = c(x) \text{ on } \Gamma$$

Continuous eigenfunction and eigenvalues with homog. Dirichlet

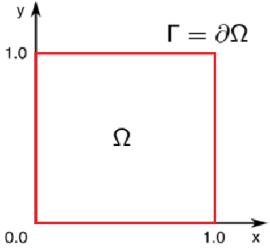
$$u^{[k]}(x) = \sin(k\pi x), \lambda_k = k^2\pi^2 \text{ for } k \in \mathbb{N}, k \neq 0$$

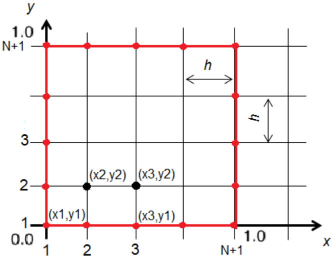
§ 3.5: Grid Construction

- 1D Discrete Grid G_h
  $x_i = (i-1)h$, $i = 1, \ldots, N+1$ where $h = \frac{1}{N}$ st $x_1 = 0, x_{N+1} = 1$



- 2D Discrete Grid G_h
  $x_i = (i-1)h, y_j = (j-1)h$, $i, j = 1, 2, \ldots N+1$
  $(x_1, y_1) = (0, 0), (x_1, y_{N+1}) = (0, 1)$, etc.





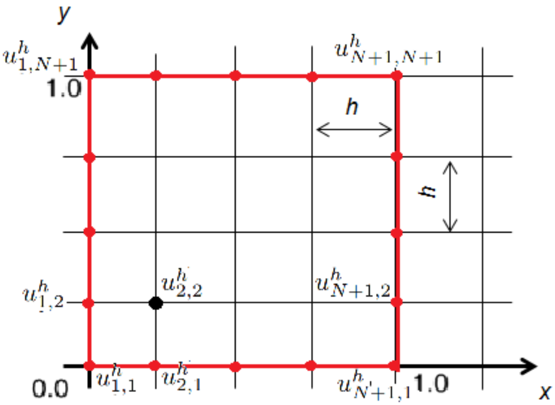
§ 3.5: Finite Differences (FD)

How can we represent continuous differential operators on a discrete grid? Finite Differences!

- Numerical approximation using FD only defined in the grid points
- Grid functions for all $(x_i, y_j) \in G_h$:

  $u(x,y) \approx u(x_i,y_j) \approx u^h_{i,j}, f(x,y) \approx f(x_i,y_j) \approx f^h_{i,j}$

  $b(x_i,y_j) \approx b^h_{i,j}, c(x_i,y_j) \approx c^h_{i,j}$



§ 3.5: Finite Differences (FD)

We now (recall) several finite difference formulas

Forward difference:

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(h)$$

Backward difference:

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{h} + O(h)$$

Central differences:

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} + O\left[(h^2)\right]$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O\left[(h^2)\right]$$

§ 3.5: Finite Differences (FD)

Similar formulas for $\frac{\partial u}{\partial y}$ and $\frac{\partial^2 u}{\partial y^2}$
Forward difference:

$$\left.\frac{\partial u}{\partial y}\right|_{i,j} \simeq \frac{u_{i,j+1} - u_{i,j}}{h}$$

Backward difference:

$$\left.\frac{\partial u}{\partial y}\right|_{i,j} \simeq \frac{u_{i,j} - u_{i,j-1}}{h}$$

Central differences:

$$\left.\frac{\partial u}{\partial y}\right|_{i,j} \simeq \frac{u_{i,j+1} - u_{i,j-1}}{2h}$$

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{i,j} \simeq \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(h)^2}$$

§ 3.5: Finite Differences (FD)

Transformed MP: 2D Poisson (internal nodes)

Grid:

$$G_h = \{(x_i, y_j) \mid x_i = (i-1)h, y_j = (j-1)h; 1 \leq i, j \leq N+1\},$$

Continuous MP:

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f$$

Discretization x-direction:

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j) = \frac{u^h_{i-1,j} - 2u^h_{i,j} + u^h_{i+1,j}}{h^2} + \mathcal{O}\left(h^2\right) \text{ for } 2 \leq i, j \leq N, (x_i, y_j) \in G_h$$

Discretization y-direction:

$$\frac{\partial^2 u}{\partial y^2}(x_i, y_j) = \frac{u^h_{i,j-1} - 2u^h_{i,j} + u^h_{i,j+1}}{h^2} + \mathcal{O}\left(h^2\right) \text{ for } 2 \leq i, j \leq N, (x_i, y_j) \in G_h$$

Transformed MP:

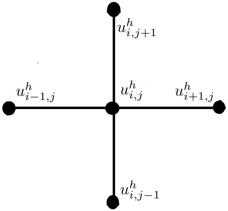
$$\frac{-u^h_{i,j-1} - u^h_{i-1,j} + 4u^h_{i,j} - u^h_{i+1,j} - u^h_{i,j+1}}{h^2} = f^h_{i,j} \text{ for } 2 \leq i, j \leq N$$

§ 3.5: Stencil Notation

On a subset of notes, Transformed MP:

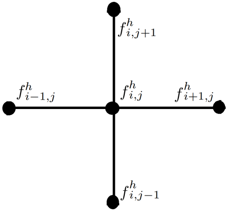
$$\frac{-u^h_{i,j-1}-u^h_{i-1,j}+4u^h_{i,j}-u^h_{i+1,j}-u^h_{i,j+1}}{h^2} = f^h_{i,j} \text{ for } 2 \leq i,j \leq N$$

is represented by a 5-point stencil for each internal $(x_i, y_j) \in G_h$:



with stencil for the LHS

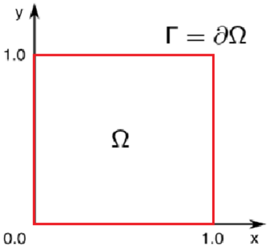
$$\frac{1}{h^2}\begin{bmatrix} 0 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

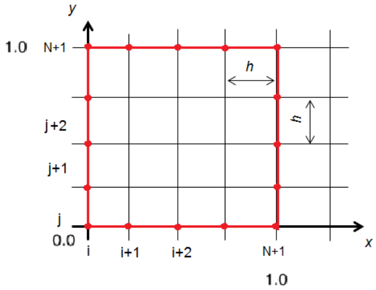


with stencil for the RHS

$$\frac{1}{h^2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

§ 3.5: Boundary Conditions

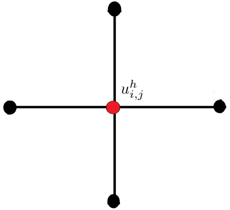




- Set of boundary points in x-direction
  - $y = 0 : \left\{ u^h_{1,1}, u^h_{2,1}, \dots u^h_{N+1,1} \right\}$
  - $y = 1 : \left\{ u^h_{1,N+1}, u^h_{2,N+1}, \dots u^h_{N+1,N+1} \right\}$
- Set of boundary points in y-direction
  - $x = 0 : \left\{ u^h_{1,1}, u^h_{1,2}, \dots u^h_{1,N+1} \right\}$
  - $x = 1 : \left\{ u^h_{N+1,1}, u^h_{N+1,2}, \dots u^h_{N+1,N+1} \right\}$

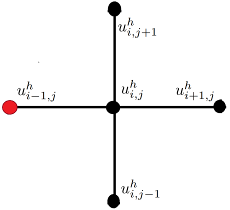
§ 3.5: Boundary Conditions

No elimination: each boundary node becomes an equation for which the RHS $f^h_{i,j}$ is replaced by $b^h_{i,j}$



$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

With elimination: the known boundary values are directly substituted and $b^h_{i-1,j}$ is added to the RHS



$$\frac{1}{h^2}\begin{bmatrix} 0 & -1 & 0 \\ \color{red}{0} & 4 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

§ 3.6: Linear System Formulation

No elimination

- $x-$line lexicographic ordening of internal and boundary nodes node (i,j) is assigned global index $I = i + (j-1)(N+1)$ for $1 \leq i,j \leq N+1$

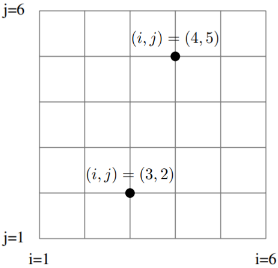


Figure 3.3: grid ordering using (i,j)

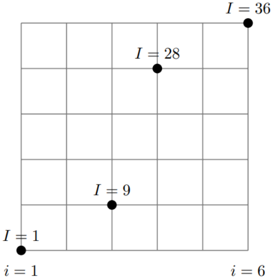


Figure 3.4: x-lexicographic using I

§ 3.6: Linear System Formulation

No elimination

- Group known and unknown grid values $f_{i,j}^h$ and $u_{i,j}^h$ into column vectors $\mathbf{u}^h$ and $\mathbf{f}^h$ of size $(N+1)^2$

Example: 2D Poisson + Dirichlet BCs

Given the domain $\Omega = (0,1)$ with boundary $\Gamma = \partial\Omega$, discretize

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f \text{ on } \Omega$$
$$u(x,y) = b(x,y) \text{ on } \Gamma$$

using second-order FD and write it in the form $A^h u^h = f^h$ using no elimination.
Take $N = 2$ and symmetrize A^h.

§ 3.6: Linear System Formulation

Example: 2D Poisson + Dirichlet BCs

We get system of equations (red: internal node):

$$u_{11} = b_{11}$$
$$u_{21} = b_{21}$$
$$u_{31} = b_{31}$$
$$u_{12} = b_{12}$$
$$\frac{-u_{12} - u_{21} - 4u_{22} - u_{23} - u_{32}}{h^2} = f_{22}$$
$$u_{23} = b_{23}$$
$$u_{13} = b_{13}$$
$$u_{23} = b_{23}$$
$$u_{33} = b_{33}$$

§ 3.6: Linear System Formulation

Example: 2D Poisson + Dirichlet BCs

We get system of equations (red: internal node):

$$\underbrace{\begin{bmatrix} h^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & h^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & h^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & h^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & h^2 \end{bmatrix}}_{A^h} \underbrace{\begin{bmatrix} u_{11} \\ u_{21} \\ u_{31} \\ u_{12} \\ u_{22} \\ u_{23} \\ u_{13} \\ u_{23} \\ u_{33} \end{bmatrix}}_{u^h} = \underbrace{\begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{12} \\ f_{22} \\ b_{23} \\ b_{13} \\ b_{23} \\ b_{33} \end{bmatrix}}_{f^h}$$

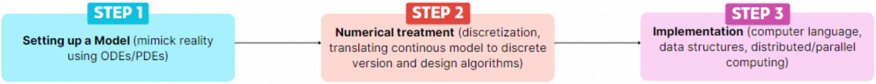
§ 3.6: Linear System Formulation

Example: 2D Poisson + Dirichlet BCs

We get system of equations (red: internal node):

$$\underbrace{\begin{bmatrix} h^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 0 & \mathbf{0} & 4 & \mathbf{0} & 0 & \mathbf{0} & 0 \\ 0 & 0 & 0 & 0 & 0 & h^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & h^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & h^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & h^2 \end{bmatrix}}_{A^h} \underbrace{\begin{bmatrix} u_{11} \\ u_{21} \\ u_{31} \\ u_{12} \\ u_{22} \\ u_{23} \\ u_{13} \\ u_{23} \\ u_{33} \end{bmatrix}}_{u^h} = \underbrace{\begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{12} \\ f_{22} + \frac{b_{21}+b_{12}+b_{23}+b_{32}}{h^2} \\ b_{23} \\ b_{13} \\ b_{23} \\ b_{33} \end{bmatrix}}_{f^h}$$

Sources of Errors



- Modelling error
- Error in data

- Discretization error
- Truncation error
- Round-off error

- Programming errors

Summary and Next Week

1. Transform continuous model to discrete numerical model
   - Transform domain Ω into discrete domain/grid G_h with grid points, i.e. from (x, y) to (x_i, y_j)
   - Discretize solution function $u(x, y)$ to $u(x_i, y_j)$ on the grid points
   - Discretize derivatives of the PDE at grid points using Finite Differences
   - Rewrite system of equations into matrix-vector format
2. Analyze matrix properties (this dictates which numerical algorithm to use (next week))
   - Symmetry
   - Eigenvalues
   - Positive Definiteness
   - Conditioning (remember round-off error example last week!)