

# Scientific Computing I

## Module 8: Discretisation of PDEs

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# The Model Problem

- 2D Poisson Equation on unit square:

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

- Dirichlet boundary conditions:

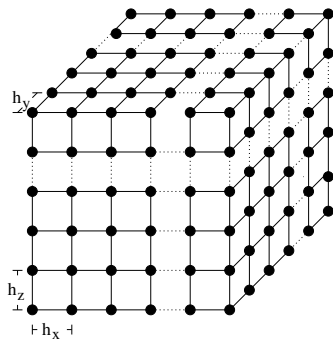
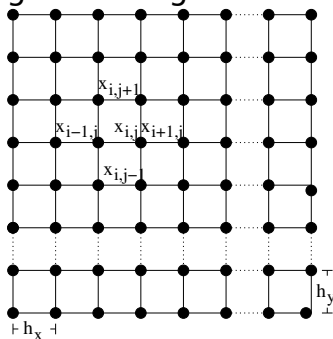
$$u(x,y) = g(x,y) \quad \text{on } \partial\Omega$$

Part I

Finite Differences

# Grid Generation

- generate a grid on the given domain



- Compute values of unknown function  $u$  at each grid point:

$$u_{ij} \approx u(x_{ij})$$

$$u_{ijk} \approx u(x_{ijk})$$

# Finite Difference Discretisation

- Replace derivatives (at each grid point) by difference quotients:

$$\frac{\partial^2 u}{\partial x^2}(x_{i,j}) \approx \frac{u(x_{i+1,j}) - 2u(x_{i,j}) + u(x_{i-1,j}))}{h_x^2}$$

$$\frac{\partial^2 u}{\partial x^2}(x_{i,j}) \approx \frac{u(x_{i+1,j}) - 2u(x_{i,j}) + u(x_{i-1,j}))}{h_x^2}$$

- leads to linear system of equations:

$$\begin{aligned} \frac{1}{h^2} (u_{i+1,j} + u_{i,j+1} - 4u_{i,j} \\ + u_{i,j-1} + u_{i-1,j}) &= f(x_{i,j}) \quad x_{i,j} \in (0, 1)^2 \\ u(x_{i,j}) &= g(x_{i,j}) \quad x_{i,j} \in \partial\Omega \end{aligned}$$

# System of Linear Equations

- write linear system as  $A_h x_h = f_h$
- $A_h$  is a sparse matrix (band structure):

$$A_h = \frac{1}{h^2} \begin{pmatrix} B_h & -I & & & \\ -I & \ddots & \ddots & & \\ & \ddots & \ddots & -I & \\ & & & -I & B_h \end{pmatrix}$$

- $B_h = \text{tridiag}(-1, 4, -1)$
- $A_h$  block-tridiagonal (5-diagonal) matrix
- boundary values to right-hand side



# Stencil Notation

- illustrate matrix structure as a *discretisation stencil*
- represents one line of the matrix
- elements placed according to the geometrical position
- stencils for the Poisson equation:

$$1D: \quad [ 1 \quad -2 \quad 1 ] \quad 2D: \quad \begin{bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{bmatrix}$$

# Accuracy

- for 5-point Poisson stencil;  
order of accuracy:  $\|u_h - u\| = \mathcal{O}(h^2) = \mathcal{O}(N^{-2})$
- *curse of dimension*:  
for that, we need  $\mathcal{O}(N^d)$  points

Possibilities of an improvement:

- use higher-order discretisation
  - via higher order terms of Taylor series
  - leads to larger stencils  
(involving more neighbouring grid points)
- use locally refined (*adaptive*) grids

## Part II

# Finite Element Methods

# Finite Elements – Main Ingredients

- 1 compute a *function* as numerical solution; search in a function space  $V_h$ :

$$u_h = \sum_j u_j \varphi_j(x), \quad \text{span}\{\varphi_1, \dots, \varphi_J\} = V_h$$

- 2 solve *weak form* of PDE to reduce regularity properties

$$u'' = f \quad \longrightarrow \quad \int v' u' dx = \int v f dx$$

- 3 choose basis function with a *local support*, e.g.:

$$\varphi_j(x_i) = \delta_{ij}$$

# Weak Forms and Weak Solutions

- consider a PDE  $Lu = f$  (e.g.  $Lu = \Delta u$ )
- transformation to the *weak form*:

$$\langle Lu, v \rangle = \int vLu \, dx = \int vf \, dx = \langle f, v \rangle \quad \forall v \in V$$

$V$  a certain class of functions

- “real solution”  $u$  also solves the weak form
- $\langle Lu, v \rangle$  a *bilinear form*; often written as:

$$a(Lu, v) = \langle f, v \rangle \quad \forall v \in V$$

# Weak Form of the Poisson Equation

- Poisson equation with Dirichlet conditions:

$$-\Delta u = f \quad \text{in } \Omega, u = 0 \quad \text{on } \delta\Omega$$

- weak form:

$$-\int_{\Omega} v \Delta u \, d\Omega = \int_{\Omega} v f \, d\Omega \quad \forall v$$

apply Green's formula (and boundary conditions):

$$\int_{\Omega} \nabla v \cdot \nabla u \, d\Omega = \int_{\Omega} v f \, d\Omega \quad \forall v$$

- weaker requirements for a solution  $u$ :  
*twice differentiable*  $\rightarrow$  *first derivative integrable*

# Choose Test and Ansatz Space

- search for weak solutions  $u$  in a certain function space  $W$

$$\int vL\left(\sum_j u_j\varphi_j(x)\right) dx = \int vf dx \quad \forall v \in V$$

where  $\text{span}\{\varphi_j\} = W$  ("ansatz space")

- choose a basis  $\{\psi_i\}$  of the test space  $V$ ;  
then:

$$\int \psi_iL\left(\sum_j u_j\varphi_j(x)\right) dx = \int \psi_if dx \quad \forall \psi_i$$

- leads to system of equations for unknowns  $u_j$
- usually  $V$  and  $W$  chosen identically (Ritz-Galerkin method)

# Discretisation – Finite Elements

- $L$  linear  $\Rightarrow$  system of linear equations

$$\sum_j \left( \underbrace{\int \psi_i L \varphi_j(x) dx}_{=: A_{ij}} \right) u_j = \int \psi_i f dx \quad \forall \psi_i$$

- aim: make matrix  $A$  *sparse*  $\rightarrow$  most  $A_{ij} = 0$
- approach: local basis functions on a discretisation grid
- $\psi_j, \varphi_j$  zero everywhere except in grid cells adjacent to grid point  $x_j$
- $A_{ij} = 0$ , if  $\psi_i$  and  $\varphi_j$  don't overlap



# A Road to Theory

- weak formulation is equivalent to variational approach:  
solution  $u$  minimises an energy functional
- *best approximation* property:

$$\left\| u - u_h^{FE} \right\|_a \leq \inf_{u_h \in V} \|u - u_h\|_a$$

in terms of the norm induced by the bilinear form  $a$   
(energy norm)

- thus: error bounded by interpolation error  
(in energy norm)

# Example Problem: Poisson 1D

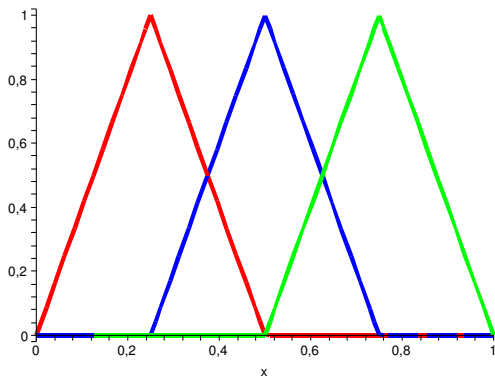
- 1D Poisson's equation on  $\Omega = [0, 1]$ , homogeneous Dirichlet boundary conditions
- weak form:

$$\int_0^1 \nabla v \cdot \nabla u \, dx = \int_0^1 v f \, dx \quad \forall v$$

- computational grid:  
 $x_i = ih$ , (for  $i = 1, \dots, n-1$ ); mesh size  $h = 1/n$
- $V = W$ : piecewise linear functions  
(on intervals  $[x_i, x_{i+1}]$ )

# Nodal Basis

$$\varphi_i(x) := \begin{cases} \frac{1}{h}(x - x_{i-1}) & x_{i-1} < x < x_i \\ \frac{1}{h}(x_{i+1} - x) & x_i < x < x_{i+1} \\ 0 & \text{otherwise} \end{cases}$$



# Nodal Basis – System of Equations

- stiffness matrix:

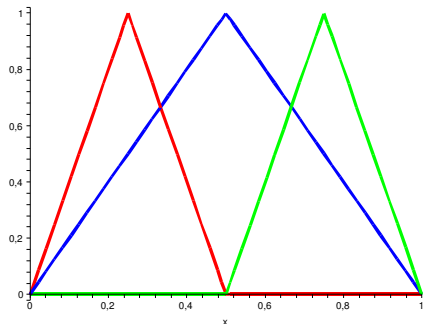
$$\frac{1}{h} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 2 \end{pmatrix}$$

- right hand sides (assume  $f(x) = \alpha \in \mathbb{R}$ ):

$$\int_0^1 \varphi_i(x) f(x) dx = \int_0^1 \varphi_i(x) \alpha dx = \alpha h$$

- system of equations very similar to finite differences

# Hierarchical Basis



- leads to diagonal stiffness matrix!  
(for 1D Poisson)
- solution function identical to that with nodal basis  
(same function space)

# Element Stiffness Matrices

- domain  $\Omega$  splitted into finite elements  $\Omega^{(i)}$
- element-wise evaluation of the integrals:

$$\int_{\Omega} \nabla v \cdot \nabla u \, dx = \sum_i \int_{\Omega^{(i)}} \nabla v \cdot \nabla u \, dx$$

$$\int_{\Omega} v f \, dx = \sum_i \int_{\Omega^{(i)}} v f \, dx$$

- leads to system of equations for each element:

$$A^{(i)} x = b^{(i)}$$

- accumulate to obtain global system:

$$\underbrace{\sum_i A^{(i)}}_{=:A} x = \sum_i b^{(i)}$$

## Example: 1D Poisson

Notation:

- notation: omit zero columns/rows  
(leaves only unknowns that are in  $\Omega^{(i)}$ )

1D Poisson:

- $\Omega = [0, 1]$  splitted into  $\Omega^{(i)} = [x_{i-1}, x_i]$
- nodal basis; leads to element stiffness matrix:

$$A^{(i)} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

- stencil notation:

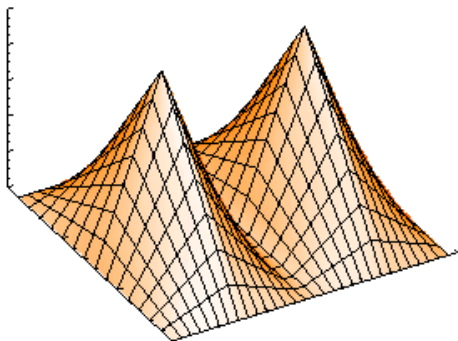
$$[1^* \ -1] + [-1 \ 1^*] \rightarrow [-1 \ 2 \ -1]$$

## Example: 2D Poisson

- $-\Delta u = f$  on domain  $\Omega = [0, 1]^2$
- splitted into  $\Omega^{(ij)} = [x_{i-1}, x_i] \times [x_{j-1}, x_j]$
- bilinear basis functions

$$\varphi_{ij}(x, y) = \varphi_i(x)\varphi_j(y)$$

- “pagoda” functions





## Example: 2D Poisson (2)

- leads to element stiffness matrix:

$$A^{(i)} = \begin{pmatrix} 2 & -\frac{1}{2} & -\frac{1}{2} & -1 \\ -\frac{1}{2} & 2 & -1 & -\frac{1}{2} \\ -\frac{1}{2} & -1 & 2 & -\frac{1}{2} \\ -1 & -\frac{1}{2} & -\frac{1}{2} & 2 \end{pmatrix}$$

- accumulation leads to 9-point stencil

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

# Typical workflow

- 1 choose elements:
  - quadratic or cubic cells
  - triangles (structured, unstructured)
  - tetrahedra, etc.
- 2 set up basis functions for each element  $\Omega_h$ ; at all nodes  $x_i \in \Omega_h$

$$\varphi_i(x_i) = 1$$

$$\varphi_i(x_j) = 0 \quad \text{for all } j \neq i$$

- 3 for element stiffness matrix, compute all

$$A_{ij} = \int_{\Omega_h} \varphi_i \mathcal{L} \varphi_j \, d\Omega$$

- 4 accumulate global stiffness matrix