

# Algorithms for Scientific Computing

## Finite Element Methods

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*TUM Uhrenturm*

# Part I

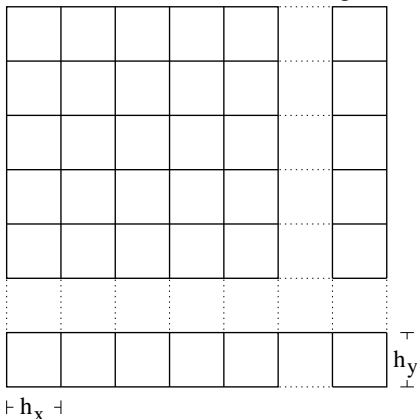
## Looking Back: Discrete Models for Heat Transfer and the Poisson Equation

### Modelling of Heat Transfer

- objective: compute the temperature distribution of some object
- under certain prerequisites:
  - temperature  $T$  at object boundaries given
  - heat sources
  - material parameters  $k, \dots$
- observation from physical experiments:  $q \approx k \cdot \delta T$   
(heat flow proportional to temperature differences)

# A Finite Volume Model

- object: a rectangular metal plate (again)
- model as a collection of small connected rectangular cells



- examine the heat flow across the cell edges

## Heat Flow Across the Cell Boundaries

- Heat flow across a given edge is proportional to
  - temperature difference ( $T_1 - T_0$ ) between the adjacent cells
  - length  $h$  of the edge
- e.g.: heat flow across the left edge:

$$q_{ij}^{(\text{left})} = k_x (T_{ij} - T_{i-1,j}) h_y$$

$k_x$  depends on material

- heat flow across all edges determines change of heat energy:

$$\begin{aligned} q_{ij} &= k_x (T_{ij} - T_{i-1,j}) h_y + k_x (T_{ij} - T_{i+1,j}) h_y \\ &+ k_y (T_{ij} - T_{i,j-1}) h_x + k_y (T_{ij} - T_{i,j+1}) h_x \end{aligned}$$

- equilibrium with source term  $F_{ij} = f_{ij} h_x h_y$  ( $f_{ij}$  heat flow per area) requires  $q_{ij} + F_{ij} = 0$ :

$$\begin{aligned} f_{ij} h_x h_y &= -k_x h_y (2T_{ij} - T_{i-1,j} - T_{i+1,j}) \\ &\quad -k_y h_x (2T_{ij} - T_{i,j-1} - T_{i,j+1}) \end{aligned}$$

## Discrete and Continuous Model

- system of equations derived from the discrete model:

$$f_{ij} = -\frac{k_x}{h_x} (2T_{ij} - T_{i-1,j} - T_{i+1,j}) \\ -\frac{k_y}{h_y} (2T_{ij} - T_{i,j-1} - T_{i,j+1})$$

- **result: average temperature in each cell**
- corresponds to *partial differential equation* (PDE):

$$-k \left( \frac{\partial^2 T(x, y)}{\partial x^2} + \frac{\partial^2 T(x, y)}{\partial y^2} \right) = f(x, y)$$

- **wanted: approximate  $T(x, y)$  as a function!**  
→ solution possible using “coefficients and basis functions”?

## Part II

# Outlook: Finite Element Methods

For *Model Problem*:

- 2D Poisson equation:

$$\frac{\partial^2 T(x, y)}{\partial x^2} + \frac{\partial^2 T(x, y)}{\partial y^2} = f(x, y)$$

- first, however, we consider the 1D case:

$$u''(x) = f(x) \quad \text{for } x \in (0, 1)$$

with  $u(0) = u(1) = 0$ .

## Finite Elements – Main Idea

- we consider the residual of the (1D) PDE:

$$u''(x) = f(x) \quad \rightsquigarrow \quad u''(x) - f(x) = 0$$

- represent the functions  $u$  and  $f$  in our “favorite” form:

$$\left( \sum u_j \phi_j(x) \right)'' - \sum f_j \phi_j(x) = 0$$

- however: we will usually not find  $u_j$  that solve this equation exactly (as solution  $u$  can not be represented as  $\sum u_j \phi_j(x)$ )
- remedy?  
→ find “best approximation”, given by orthogonality:

$$\left\langle w(x), \left( \sum u_j \phi_j(x) \right)'' - \sum f_j \phi_j(x) \right\rangle = 0 \quad \text{“for all } w(x)\text{”}$$

- remember that  $\langle g, f \rangle = \int g \cdot f \, dx$

# Finite Elements – Main Ingredients

1. compute a *function* as numerical solution;  
search in a function space  $W_h$ :

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

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 functions with *local support*, e.g.:

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

(such as the hat functions)



## Choose Test and Ansatz Space

- search for solution functions  $u_h$  of the form

$$u_h = \sum_j u_j \varphi_j(x)$$

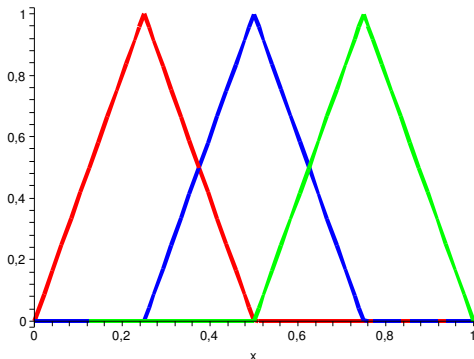
- the basis (“shape”, “ansatz”) functions  $\varphi_j(x)$  build a vector space (or function space)  $W_h$

$$\text{span}\{\varphi_1, \dots, \varphi_J\} = W_h$$

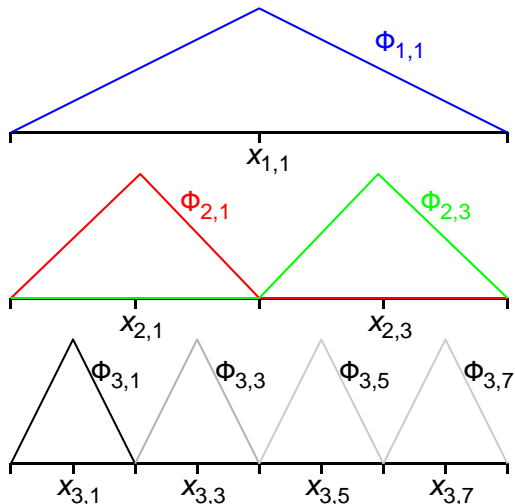
- the “best” solution  $u_h$  in this function space is wanted

## Example: Nodal Basis

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



# Or Better A Hierarchical Basis?



# Weak Forms and Weak Solutions

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

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

$V$  a certain class of functions

- “real solution”  $u$  also solves the weak form  
(but additional, approximate solutions accepted ...)
- motivation for weak form:
  - we cannot test  $Lu(x) = f(x)$  for all  $x \in (0, 1)$  on a computer (infinitely many  $x$ )
  - frequent choice  $V = W_h$ , so check whether  $Lu$  and  $f$  have the “same behaviour” w.r.t. scalar product
  - approximate solution  $\hat{u}$  might not solve PDE:  $L\hat{u} \neq f$   
thus: additional functions need to be “acceptable” as solution  
→ “orthogonality” idea

## Weak Form of the Poisson Equation – 1D

- Poisson equation with Dirichlet conditions:

$$-u''(x) = f(x) \quad \text{in } \Omega = (0, 1), \quad u(0) = u(1) = 0$$

- weak form:

$$-\int_{\Omega} v(x)u''(x) \, dx = \int_{\Omega} v(x)f(x) \, dx \quad \forall v$$

- integration by parts:

$$-\int_{\Omega} v(x)u''(x) \, dx = -v(x) \cdot u'(x) \Big|_0^1 + \int_{\Omega} v'(x) \cdot u'(x) \, dx$$

- choose functions  $v$  such that  $v(0) = v(1) = 0$ :

$$\int_{\Omega} v'(x) \cdot u'(x) \, dx = \int_{\Omega} v(x)f(x) \, dx \quad \forall v$$

## Weak Form of the Poisson Equation – 2D/3D

- Poisson equation with Dirichlet conditions:

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

- weak form:

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

- apply Green's formula:

$$-\int_{\Omega} v \Delta u \, d\Omega = \int_{\Omega} \nabla v \cdot \nabla u \, d\Omega - \int_{\partial\Omega} v \cdot \nabla u \, ds$$

- choose functions  $v$  such that  $v = 0$  on  $\partial\Omega$ :

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

# Weak Form of the Poisson Equation – Summary

- Poisson equation with Dirichlet conditions:

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

- transformed into weak form:

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

- weaker requirements for a solution  $u$ :  
*twice differentiable*  $\rightarrow$  *first derivative integrable*
- remember use of nodal basis: availability of first vs. second derivative!

## Choose Test and Ansatz Space

- search for solutions  $u_h$  in a function space  $W_h$ :

$$u_h = \sum_j u_j \varphi_j(x)$$

where  $\text{span}\{\varphi_j\} = W_h$  (“ansatz space”)

- insert into weak solution

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



## Choose Test and Ansatz Space (2)

- choose a basis  $\{\psi_i\}$  of the *test* space  $V$
- then: if all basis functions  $\psi_i$  satisfy

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

then all  $v \in V$  satisfy the equation

- leads to system of equations for unknowns  $u_j$   
(one equation per test basis function  $\psi_i$ )
- $V$  is often chosen to be identical to  $W_h$  (Ritz-Galerkin method)

## Discretisation – Finite Elements

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

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

- aim: make system of equations easy to solve!  
 $\rightarrow$  thus, make matrix  $A$  *sparse*  $\rightarrow$  most  $A_{ij} = 0$
- approach: local basis functions on a discretisation grid
- consider hat functions, e.g.:  $\psi_j, \varphi_j$  zero everywhere, except in grid cells adjacent to grid point  $x_j$
- then  $A_{ij} = 0$ , if  $\psi_i$  and  $\varphi_j$  don't overlap

## Example Problem: Poisson 1D

- in 1D:  $u''(x) = f(x)$  on  $\Omega = (0, 1)$ ,  
hom. Dirichlet boundary cond.:  $u(0) = u(1) = 0$

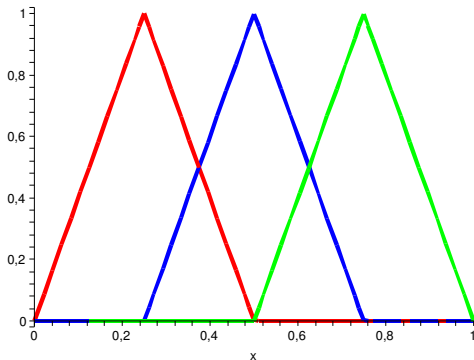
- weak form:

$$\int_0^1 v'(x) \cdot u'(x) dx = \int_0^1 v(x) f(x) dx \quad \forall v$$

- 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:

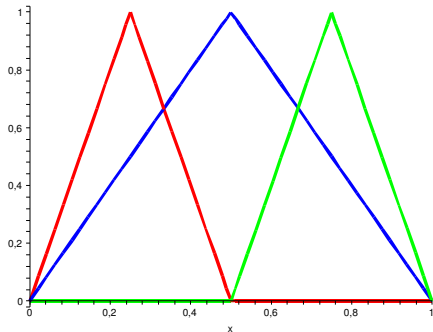
$$\frac{1}{h} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 2 \\ & & & & -1 & 2 \end{pmatrix}$$

- 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)

## Part III

# Finite Element Methods – Basis Functions for 2D

### Hierarchical Basis in 2D

#### Quadtrees and Hierarchical Bases

Quadtrees to Represent Objects

Hierarchical Basis vs. Quadtree

## 2D Hierarchical Basis – Tensor Product<sup>+</sup>

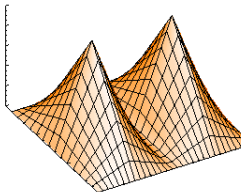
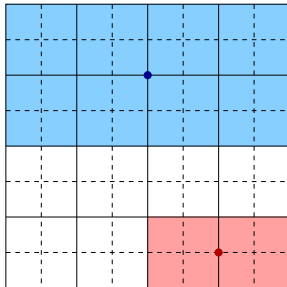
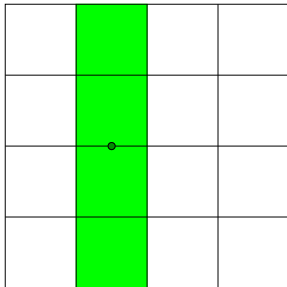
- define 2D basis functions via tensor product:

$$\phi_{i,j}(x, y) := \phi_i(x) \cdot \phi_j(y)$$

- remember multi-index for 2D hierarchical basis:

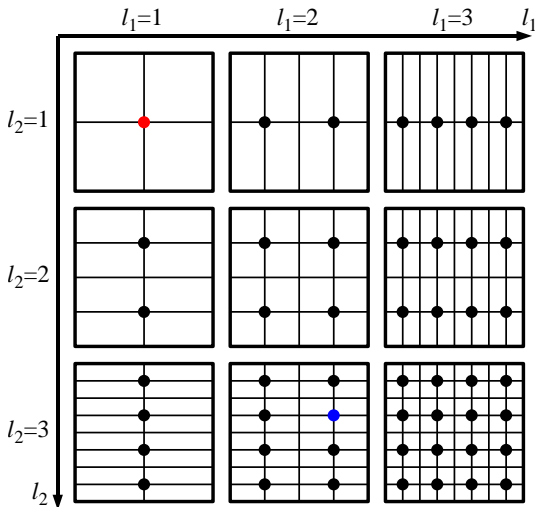
$$\phi_{\vec{l}, \vec{k}}(x_1, x_2) := \phi_{l_1, l_2, k_1, k_2}(x_1, x_2) := \phi_{l_1, k_1}(x_1) \cdot \phi_{l_2, k_2}(x_2)$$

- illustrate via support of the basis functions:

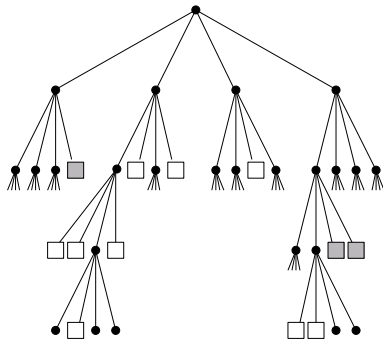
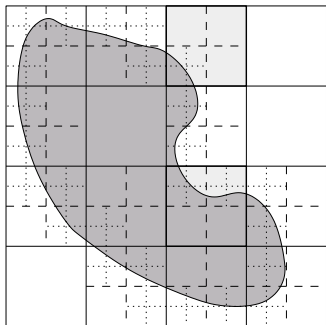




# Illustrate via Location of Hat Functions



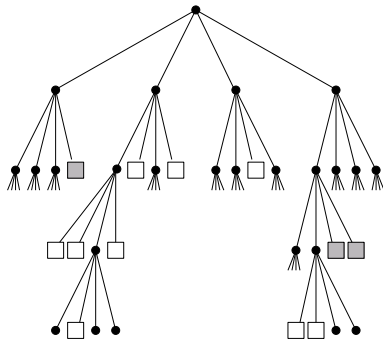
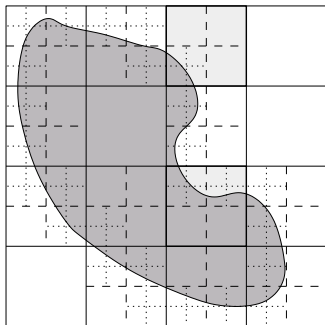
## Adding Adaptivity: Quadrees



### Quadtrees to Represent Objects:

- start with an initial square (covering the entire domain)
- recursive substructuring into four subsquares
- adaptive refinement?

# Quadrees for Adaptive Simulations

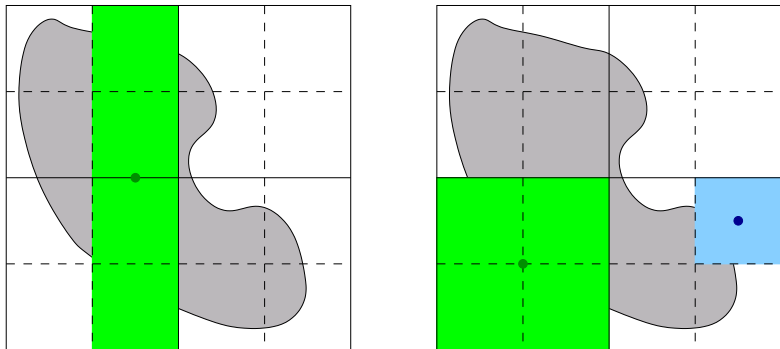


## Adaptively Refined Meshes for Finite Elements:

- refine, unless squares entirely within or outside domain
- also: refine, if solution not exact enough!
- question: can we build a hierarchical basis on such a quadtree?

# Hierarchical Basis vs. Quadtree

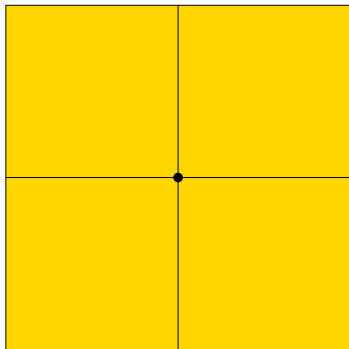
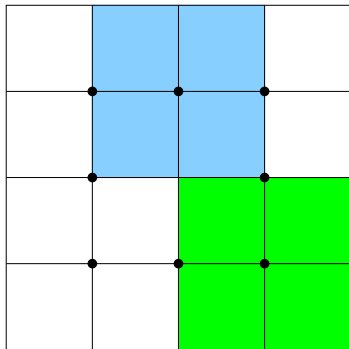
Use hierarchical basis as in 2D sparse grids?



- ⇒ stretched tensor basis functions do not match quadtree cells
- ⇒ use basis functions with “square” domain (cover 4 siblings → to solve)

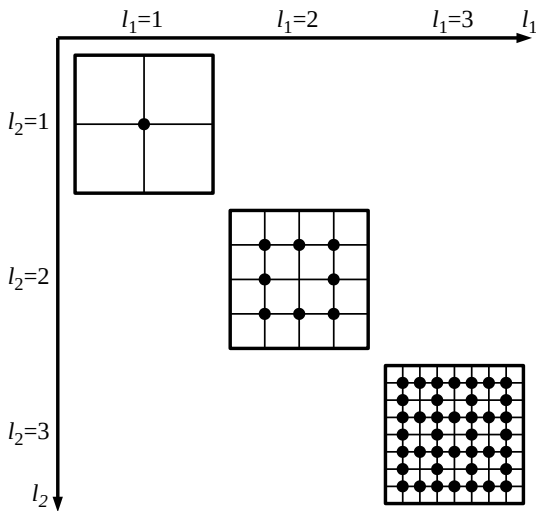
# Hierarchical Basis for Quadrees

Switch to hierarchical “multilevel” basis:



hierarchical concept (again): skip basis functions that exist on previous level!

# Illustrate via Location of Hat Functions



# Quadtree-Compatible Hierarchical Basis

## Basis Functions

Similar to tensor-product basis:

- Level-wise hierarchical increments

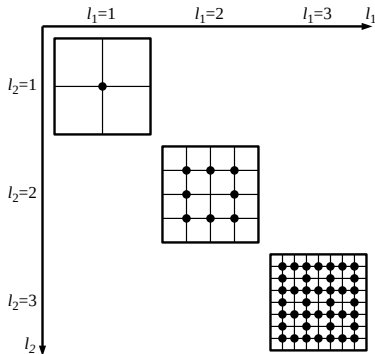
$$W_{\vec{l}} := \text{span}\{\phi_{\vec{l}, \vec{i}}\}_{\vec{i} \in \hat{\mathcal{I}}_{\vec{l}}}$$

- Only use “diagonal” levels:

$$\vec{l} := \{l_1, \dots, l_n\}$$

- Omit grid points for which all indices are even:

$$\hat{\mathcal{I}}_{\vec{l}} := \{\vec{i} : \vec{1} \leq \vec{i} < 2^{\vec{n}}, \text{ any } i_j \text{ odd}\}$$



## Part IV

# Finite Element Methods – Towards Implementation

### **FEM and Hierarchical Basis Transform**

Hierarchical Basis Transformation

FEM and Hierarchical Basis Transform

Element Stiffness Matrices

Workflow



# Project: 2D Adaptive Hierarchical Basis

Consider:

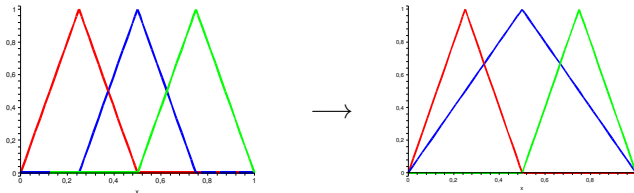
- 2D Poisson problem
- FEM with quadtree-compatible hierarchical basis
- adaptive quadtree-based hierarchical basis

Discuss (again):

- how to compute the stiffness matrix?
- what do you need to compute, if you add a hierarchical basis function?
- how do you know when to add a basis function?

**Idea: move from node-oriented to element-oriented approach**

## Recall: Hierarchical Basis Transformation



- represent “wider” hat function  $\phi_{1,1}(x)$  via basis functions  $\phi_{2,j}(x)$

$$\phi_{1,1}(x) = \frac{1}{2}\phi_{2,1}(x) + \phi_{2,2}(x) + \frac{1}{2}\phi_{2,3}(x)$$

- consider vector of hierarchical/nodal basis functions and write transformation as matrix-vector product:

$$\begin{pmatrix} \psi_{2,1}(x) \\ \psi_{2,2}(x) \\ \psi_{2,3}(x) \end{pmatrix} := \begin{pmatrix} \phi_{2,1}(x) \\ \phi_{1,1}(x) \\ \phi_{2,3}(x) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_{2,1}(x) \\ \phi_{2,2}(x) \\ \phi_{2,3}(x) \end{pmatrix}$$

## Recall: Hierarchical Basis Transformation (2)

- hierarchical basis transformation:  $\psi_{n,i}(x) = \sum_j H_{i,j} \phi_{n,j}(x)$
- written as matrix-vector product:  $\vec{\psi}_n = H_n \vec{\phi}_n$
- $H$  can be written as a sequence of level-wise transforms:

$$H_n = H_n^{(n-1)} H_n^{(n-2)} \dots H_n^{(2)} H_n^{(1)}$$

- where each transform has a shape similar to

$$H_3^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

## Recall: Hierarchical Coordinate Transformation

- consider function  $f(x) \approx \sum_i a_i \psi_{n,i}(x)$  represented via hier. basis
- wanted: corresponding representation in nodal basis

$$\sum_j b_j \phi_{n,j}(x) = \sum_i a_i \psi_{n,i}(x) \approx f(x)$$

- with  $\psi_{n,i}(x) = \sum_j H_{i,j} \phi_{n,j}(x)$  we obtain

$$\sum_j b_j \phi_{n,j}(x) = \sum_i a_i \sum_j H_{i,j} \phi_{n,j}(x) = \sum_j \sum_i a_i H_{i,j} \phi_{n,j}(x)$$

- compare coordinates and get

$$b_j = \sum_i H_{i,j} a_i = \sum_i (H^T)_{j,i} a_i$$

- written in vector notation:  $b = H^T a$

# FEM and Hierarchical Basis Transform

- FEM discretisation with hierarchical test and shape functions:

$$\int \psi_i(x) L \left( \sum_j u_j \psi_j(x) \right) dx = \int \psi_i(x) f(x) dx \quad \forall \psi_i$$

- leads to respective stiffness matrix  $A_{i,j}^{\text{HB}}$ :

$$\int \psi_i(x) L \left( \sum_j u_j \psi_j(x) \right) dx = \sum_j u_j \int \psi_i(x) L \psi_j(x) dx = \sum_j u_j A_{i,j}^{\text{HB}}$$

- vs. stiffness matrix with nodal basis as shape functions:

$$\int \psi_i(x) L \left( \sum_j v_j \phi_j(x) \right) dx = \sum_j v_j \int \psi_i(x) L \phi_j(x) dx = \sum_j v_j A_{i,j}^*$$

- note that  $(A^{\text{HB}} u)_i = \sum_j u_j A_{i,j}^{\text{HB}} = \sum_j v_j A_{i,j}^* = (A^* v)_i$  and  $v = H^T u$

## FEM and Hierarchical Basis Transform (2)

- status: FEM with hierarchical test and nodal shape functions

$$\int \psi_i(x) L\left(\sum_j v_j \phi_j(x)\right) dx = \int \psi_i(x) f(x) dx$$

- represent test functions via nodal basis:

$$\int \sum_k H_{i,k} \phi_k(x) L\left(\sum_j v_j \phi_j(x)\right) dx = \int \sum_k H_{i,k} \phi_k(x) f(x) dx$$

$$\sum_k H_{i,k} \int \phi_k(x) L\left(\sum_j v_j \phi_j(x)\right) dx = \sum_k H_{i,k} \int \phi_k(x) f(x) dx$$

- leads to new system of equations:  $HA^{\text{NB}} v = Hb^{\text{NB}}$   
where  $A^{\text{NB}}$  and  $b^{\text{NB}}$  stem from nodal-basis FEM discretisation!
- with  $v = H^T u$  we obtain  $HA^{\text{NB}} H^T u = Hb$  as system of equations, thus:  
 $A^{\text{HB}} = HA^{\text{NB}} H^T$  ( $\rightsquigarrow$  **Galerkin coarsening**)

# Element Stiffness Matrices

- domain  $\Omega$  splitted into finite elements  $\Omega^{(k)}$ :

$$\Omega = \Omega^{(1)} \cup \Omega^{(2)} \cup \dots \cup \Omega^{(n)}$$

- observation: basis functions are defined element-wise
- use:  $\int_a^b f(x)dx = \int_a^c f(x)dx + \int_c^b f(x)dx$
- element-wise evaluation of the integrals:

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

## Element Stiffness Matrices (2)

- leads to local stiffness matrices for each element:

$$\underbrace{\int_{\Omega^{(k)}} \nabla \phi_i \cdot \nabla \phi_j \, dx}_{=: A_{ij}^{(k)}}$$

- and respective element systems:

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

- accumulate to obtain global system:

$$\underbrace{\sum_k A^{(k)}}_{=: A} x = \sum_k b^{(k)}$$



## Element Stiffness Matrices (3)

Some comments on notation:

- assume: 1D problem,  $n$  elements (i.e. intervals)
- in each element only two basis functions are non-zero!
- hence, almost all  $A_{ij}^{(k)}$  are zero:

$$A_{ij}^{(k)} = \int_{\Omega^{(k)}} \nabla \phi_i \cdot \nabla \phi_j \, dx$$

- only  $2 \times 2$  elements of  $A^{(k)}$  are non-zero
- therefore convention to omit zero columns/rows  
⇒ leaves only unknowns that are in  $\Omega^{(k)}$

# Typical workflow

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

$$\begin{aligned}\varphi_i(x_i) &= 1 \\ \varphi_i(x_j) &= 0 \quad \text{for all } j \neq i\end{aligned}$$

3. for element stiffness matrix, compute all

$$A_{ij}^{(k)} = \int_{\Omega^{(k)}} \varphi_i L \varphi_j \, d\Omega$$

4. accumulate global stiffness matrix

## Example: 1D Poisson

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

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

- consider only two elements:

$$A^{(1)} + A^{(2)} = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

- in stencil notation:

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

# Project: Adaptive Hierarchical Basis

Consider:

- 1D Poisson problem
- FEM with hierarchical basis
- however: not all basis functions used on each grid  
→ adaptive hierarchical basis

Discuss:

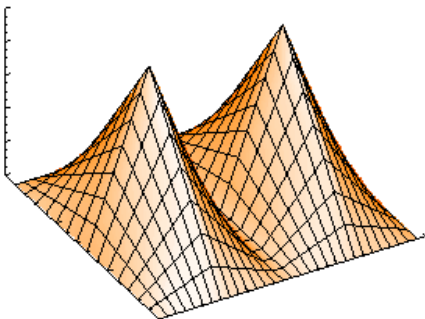
- how to compute the stiffness matrix?
- what do you need to compute, if you add a hierarchical basis function?
- how do you know when to add a basis function?

## Example: 2D Poisson

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

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

- “pagoda” functions



## Example: 2D Poisson (2)

- leads to element stiffness matrix:

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

- accumulation leads to 9-point stencil

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