Algorithms for Scientific Computing

Finite Element Methods

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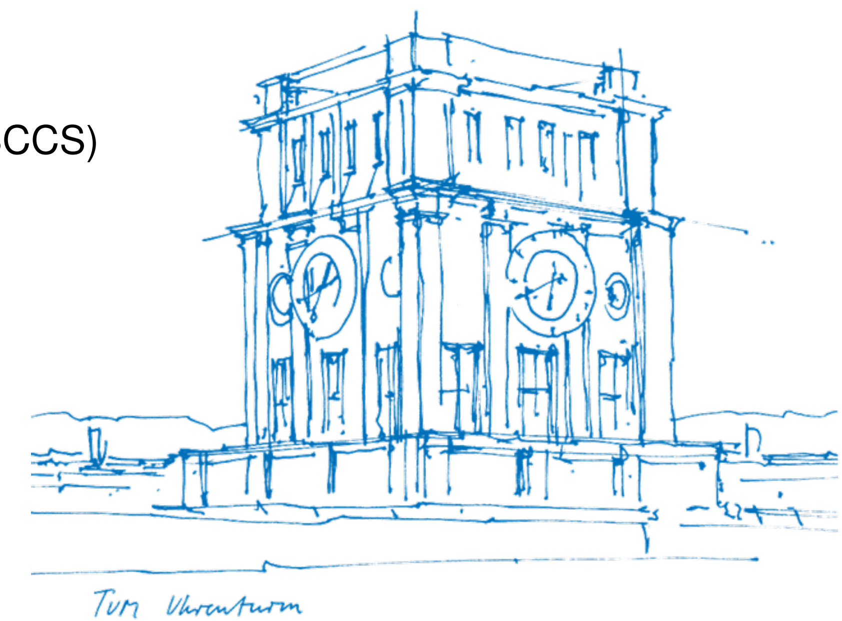


Part I

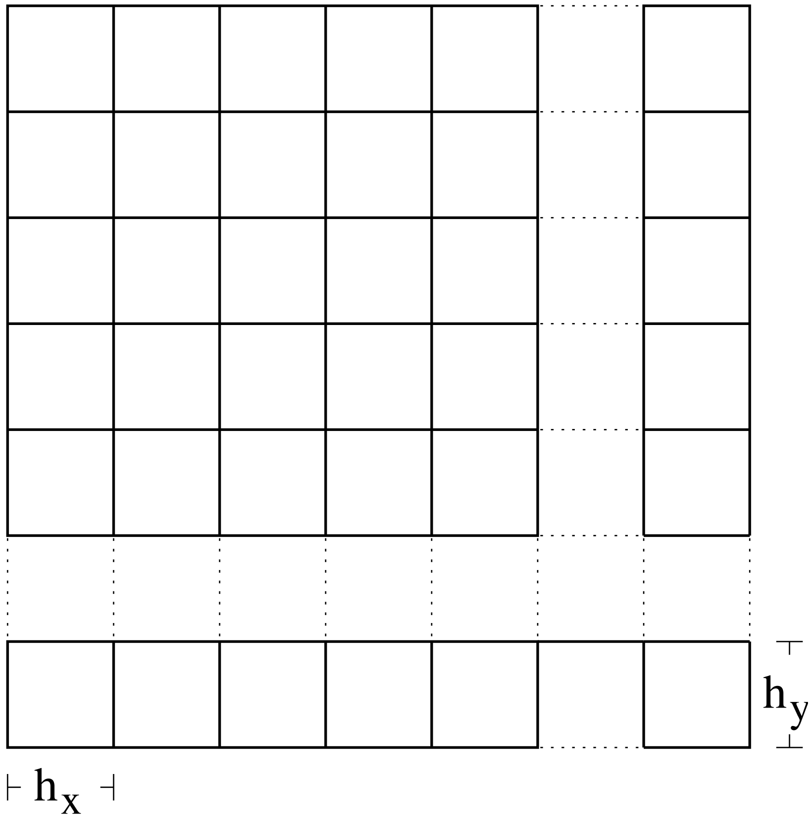
Discrete Models for Heat Transfer and the Poisson Equation

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 $k, \ldots$
- 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
- 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:

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

  k_x depends on material

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

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

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

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

Discrete and Continuous Model

- system of equations derived from the discrete model:

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

- **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!**

  $\rightarrow$ 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:

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

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 the solution u cannot be represented as $\sum u_j \phi_j(x)$)
- remedy?

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- remedy?
  $\rightarrow$ 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 $< g, f >= \int g(x) \cdot f(x) \, \mathrm{dx}$

Finite Elements – Main Ingredients

1. compute a *function* as numerical solution;
   search in a function space W_h:
   $$u_h = \sum_j u_j \varphi_j(x), \qquad \mathrm{span}\{\varphi_1, \ldots, \varphi_J\} = W_h$$
2. solve *weak form* of PDE to reduce regularity properties
   $$-u'' = f \quad \longrightarrow \quad \int v' u' \,\mathrm{d}x = \int v f \,\mathrm{d}x$$
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

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

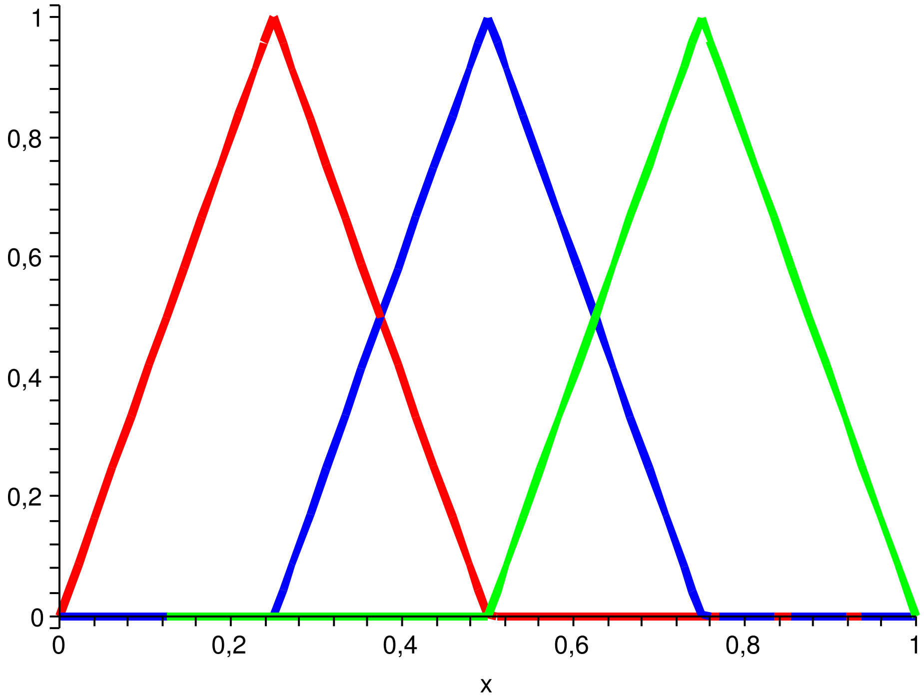
- the basis ("shape", "ansatz") functions $\varphi_j(x)$ build a vector space (or function space) W_h

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

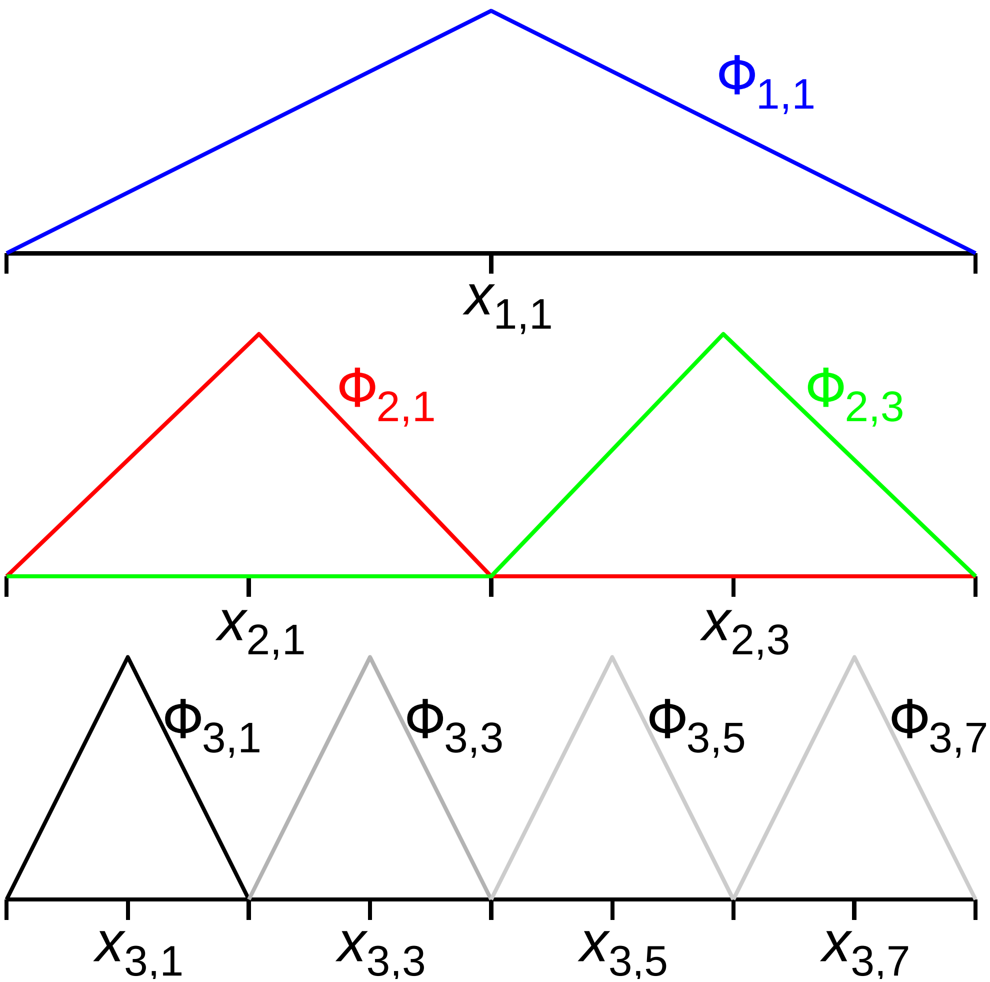
- the "best" solution u_h in this function space is wanted

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*:

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

  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 $\hat{u} \in W_h$ will very likely not solve PDE: $L\hat{u} \neq f$
    thus: additional functions need to be “acceptable” as solution
    $\rightarrow$ follow “orthogonal projection” motif

Weak Form of the Poisson Equation – 1D

- Poisson equation with Dirichlet conditions:

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

- weak form:

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

- integration by parts:

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

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

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

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

- Poisson equation with Dirichlet conditions:

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

- weak form:

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

- apply Green's formula:

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

- 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 differentiabale $\rightarrow$ *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

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

Choose Test and Ansatz Space (2)

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

$$\int \psi_i L\Big(\sum_j u_j \varphi_j(x)\Big)\,\mathrm{dx} = \int \psi_i f\,\mathrm{dx} \quad \forall \psi_i$$

  then all $v \in V$ satisfy the equation
- leads to system of equations for unknowns u_j
  (one equation per test basis function ψ_i)
- V is often chosen to be identical to W_h (Ritz-Galerkin method)

Discretisation – Finite Elements

- L linear $\Rightarrow$ system of linear equations

$$\sum_j \Bigg(\underbrace{\int \psi_i L \varphi_j(x)\,\mathrm{d}x}_{=:A_{ij}} \Bigg) u_j = \int \psi_i f\,\mathrm{d}x \quad \forall \psi_i$$

- aim: make system of equations easy to solve!

Typically: make matrix A *sparse* $\Rightarrow$ most $A_{ij} = 0$

- build **local** basis functions on a discretisation grid
- consider hat functions, e.g.:
  ψ_j, φ_j zero everywhere, except in grid cells adjacent to grid point x_j
- then $A_{ij} = 0$, if ψ_i and φ_j don't overlap

Ideally: make matrix A *diagonal* $\Rightarrow$ requires "orthogonal" basis ψ_i

Example Problem: Poisson 1D

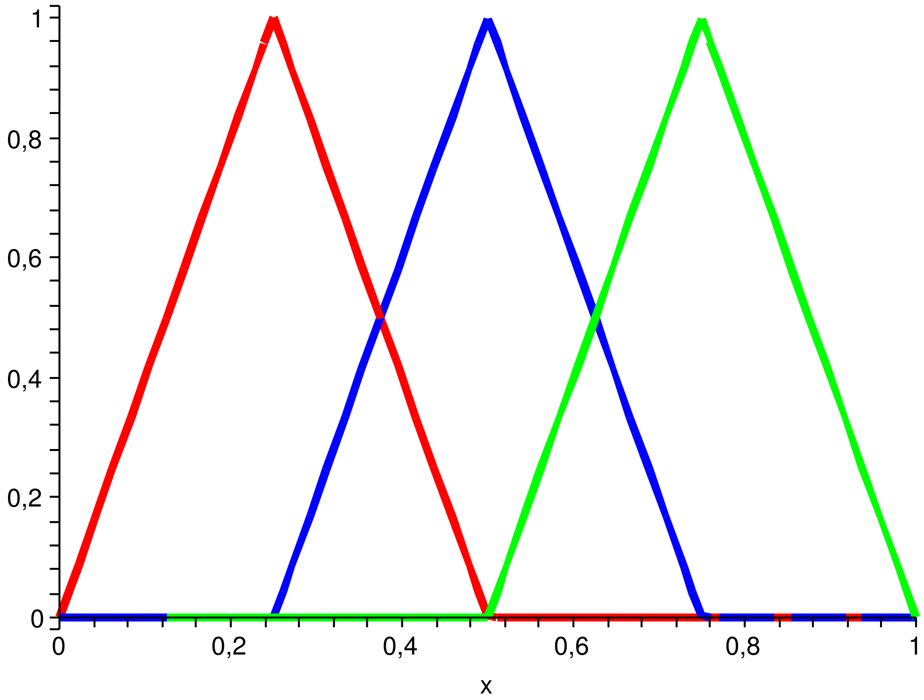
- in 1D: $-u''(x) = f(x)$ on $\Omega = (0,1)$,
  hom. Dirichlet boundary cond.: $u(0) = u(1) = 0$
- weak form:

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

- computational grid:
  $x_i = ih$, (for $i = 1, \ldots, n-1$); 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:

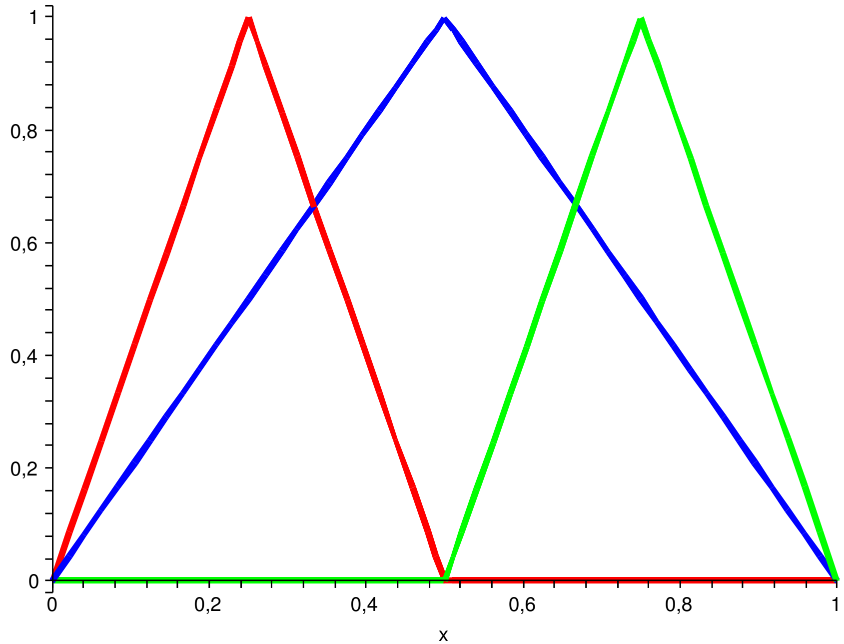
$$\frac{1}{h}\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}$$

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

$$\int_0^1 \varphi_i(x) f(x)\,\mathrm{dx} = \int_0^1 \varphi_i(x)\alpha\,\mathrm{dx} = \alpha h$$

- system of equations very similar to finite differences

Hierarchical Basis

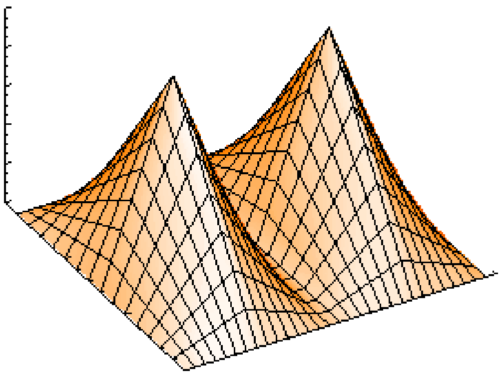


- leads to diagonal stiffness matrix!
  (for 1D Poisson)
- solution function identical to that with nodal basis (same function space)

Part III

Finite Element Methods – Basis Functions for 2D

2D Hierarchical Basis – Tensor Product



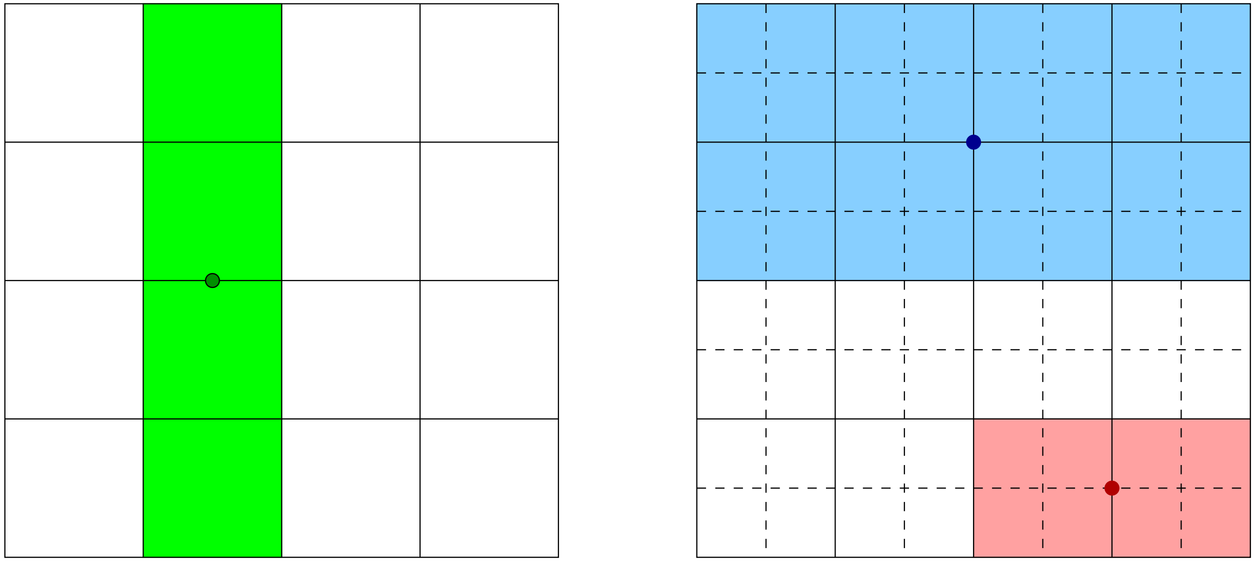
- define 2D basis functions via tensor product:

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

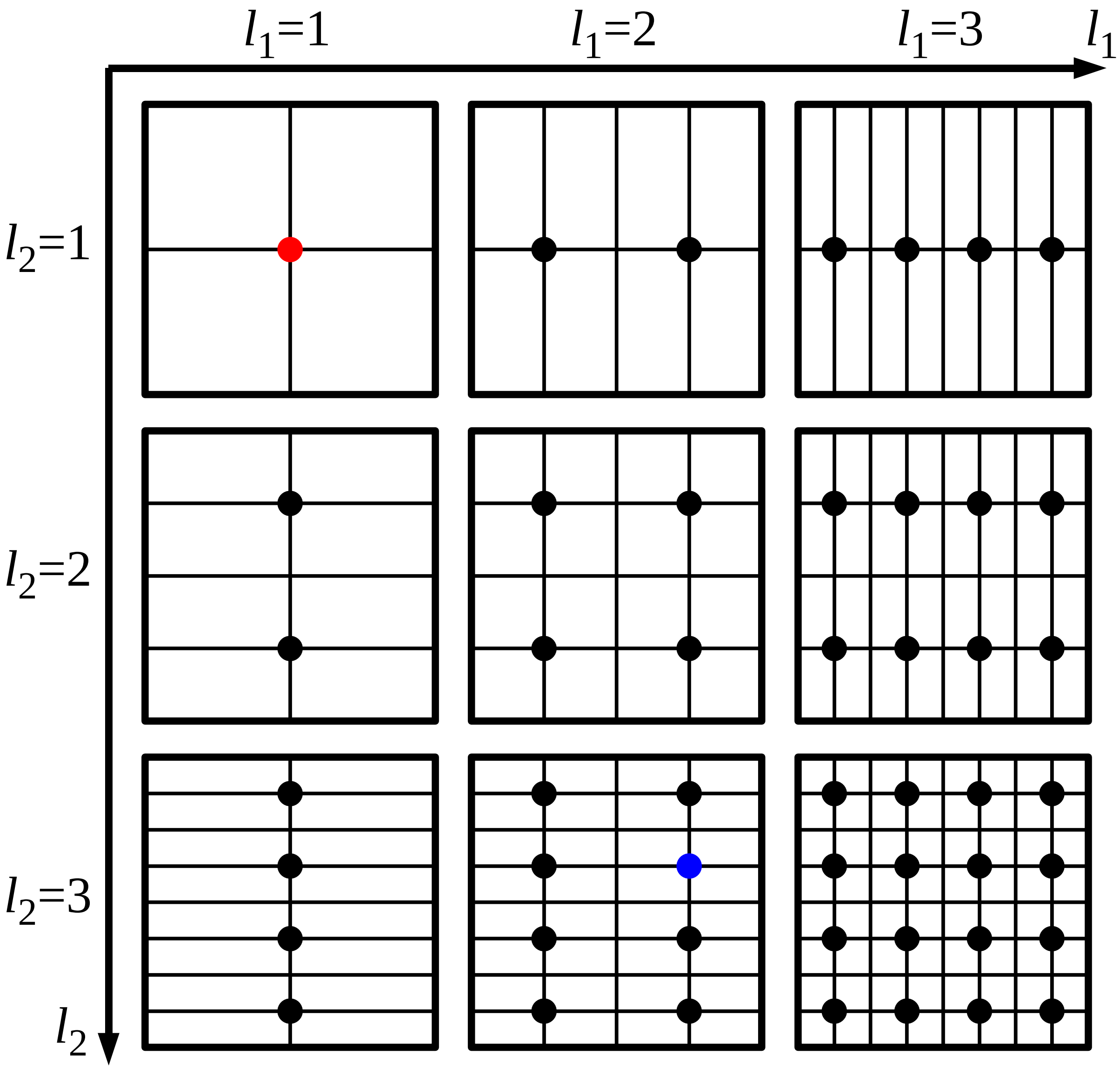
- remember multi-index for 2D hierarchical basis:

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

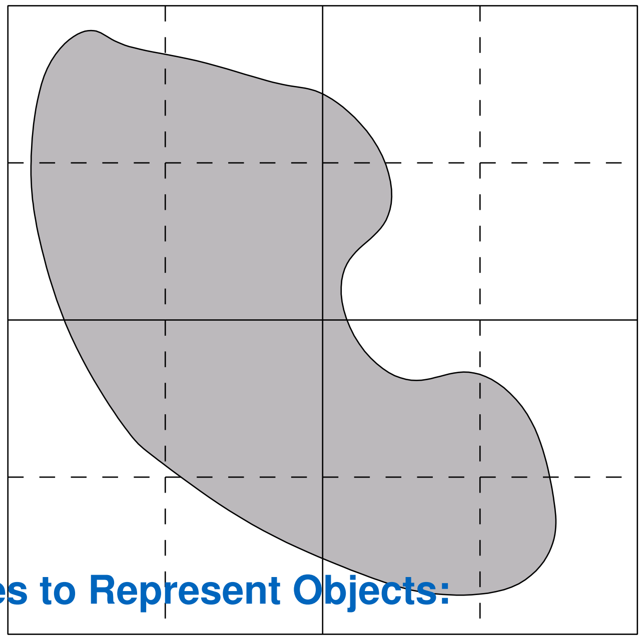
- illustrate via support of the basis functions:

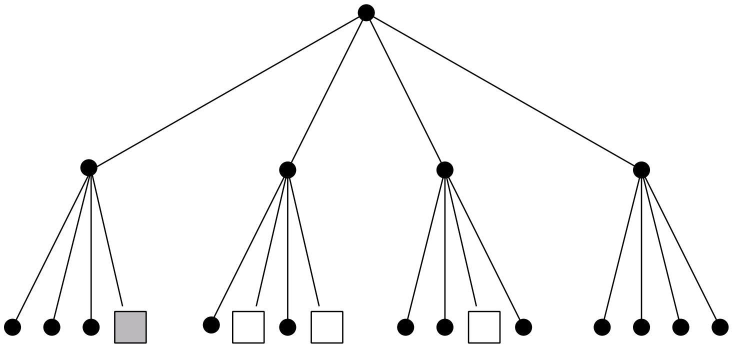


Illustrate via Location of Hat Functions



Adding Adaptivity: Quadtrees

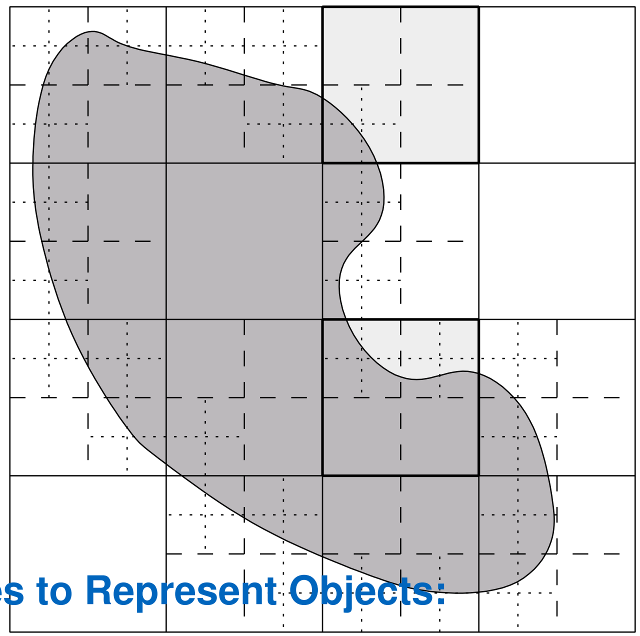


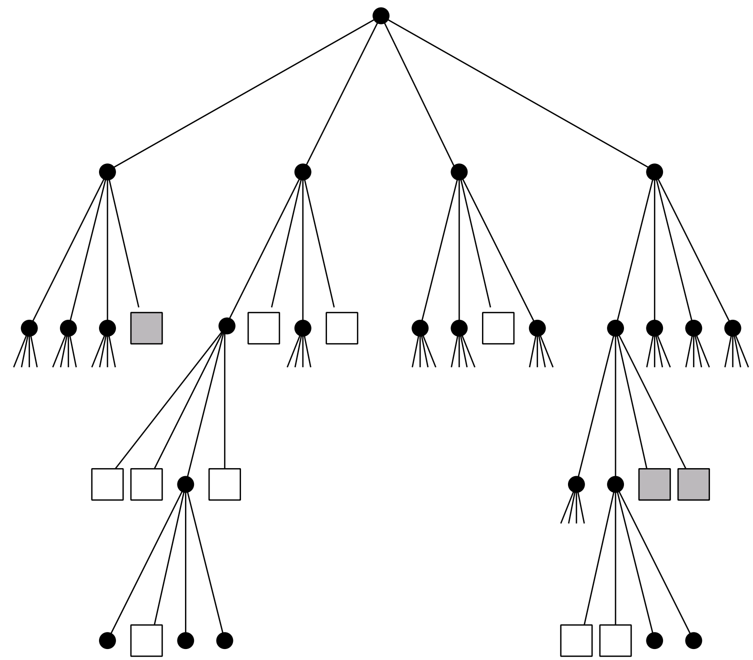


Quadtrees to Represent Objects:

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

Adding Adaptivity: Quadtrees





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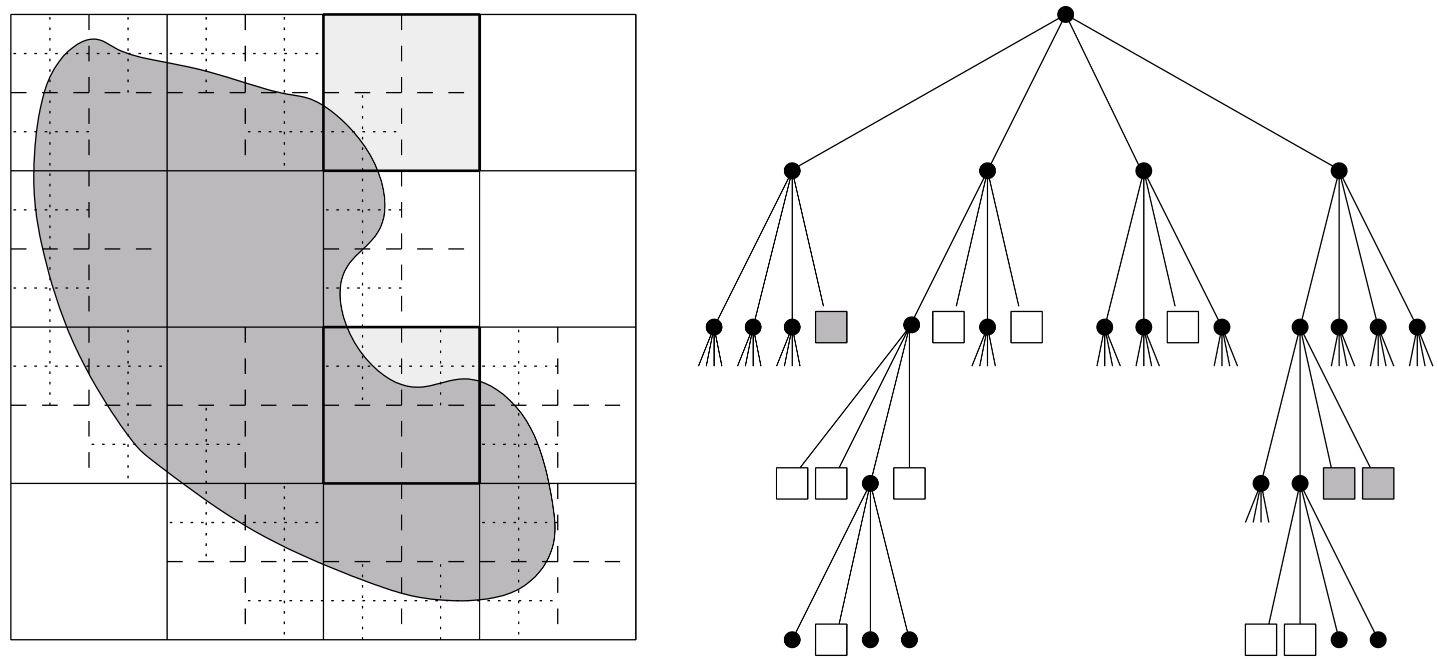
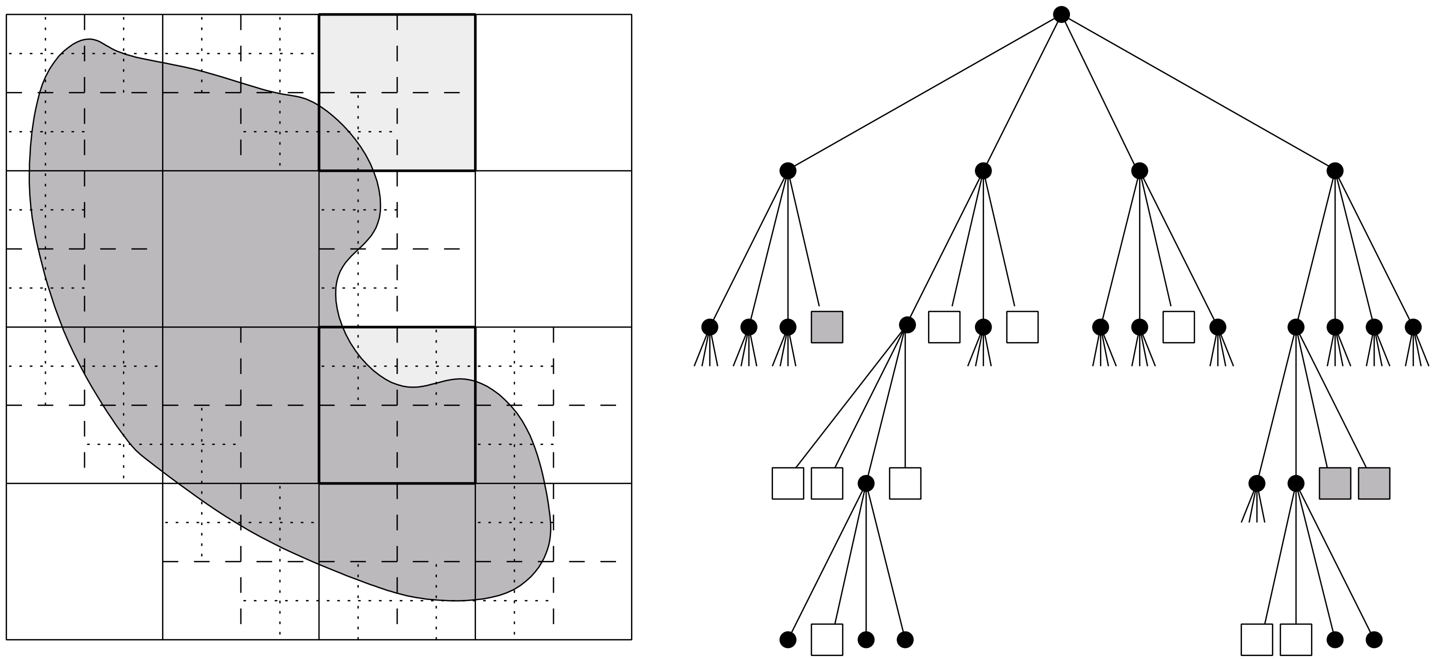
Quadtrees for Adaptive Simulations



Adaptively Refined Meshes for Finite Elements:

- refine, unless squares entirely within or outside domain

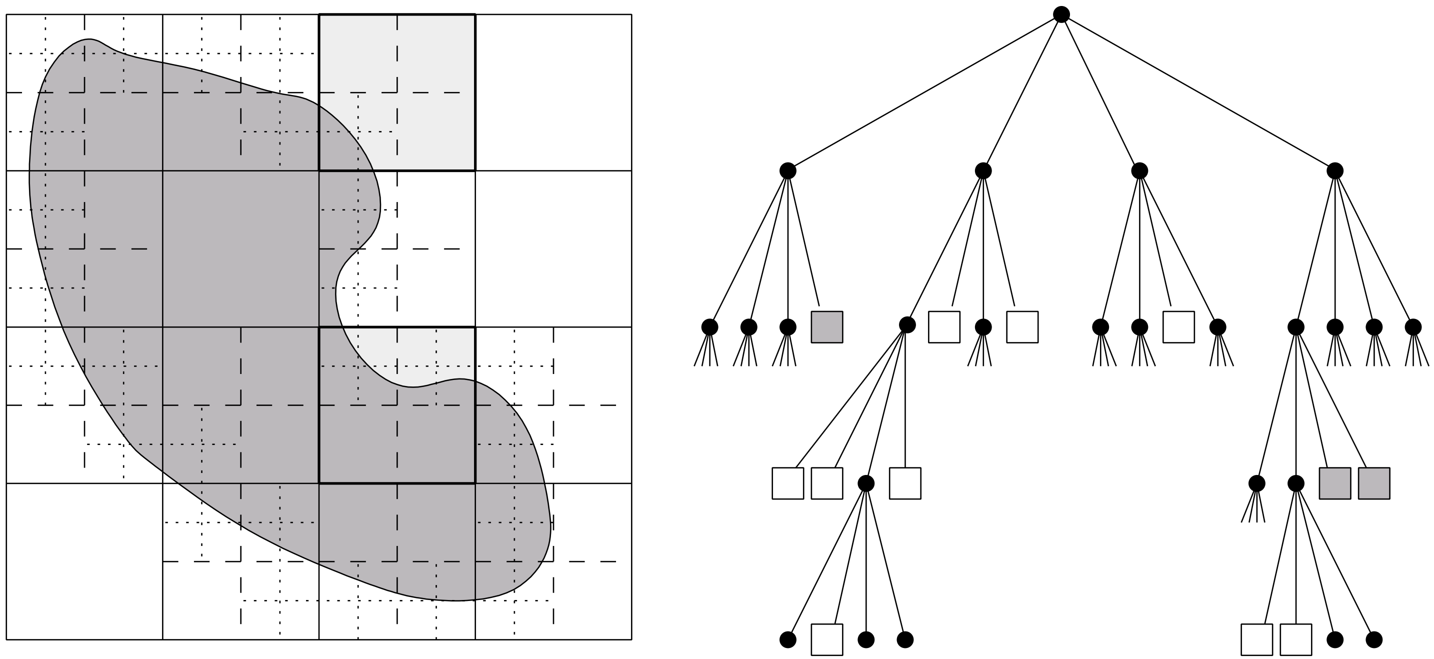
Quadtrees for Adaptive Simulations



Adaptively Refined Meshes for Finite Elements:

- refine, unless squares entirely within or outside domain
- also: refine, if solution not exact enough!

Quadtrees for Adaptive Simulations

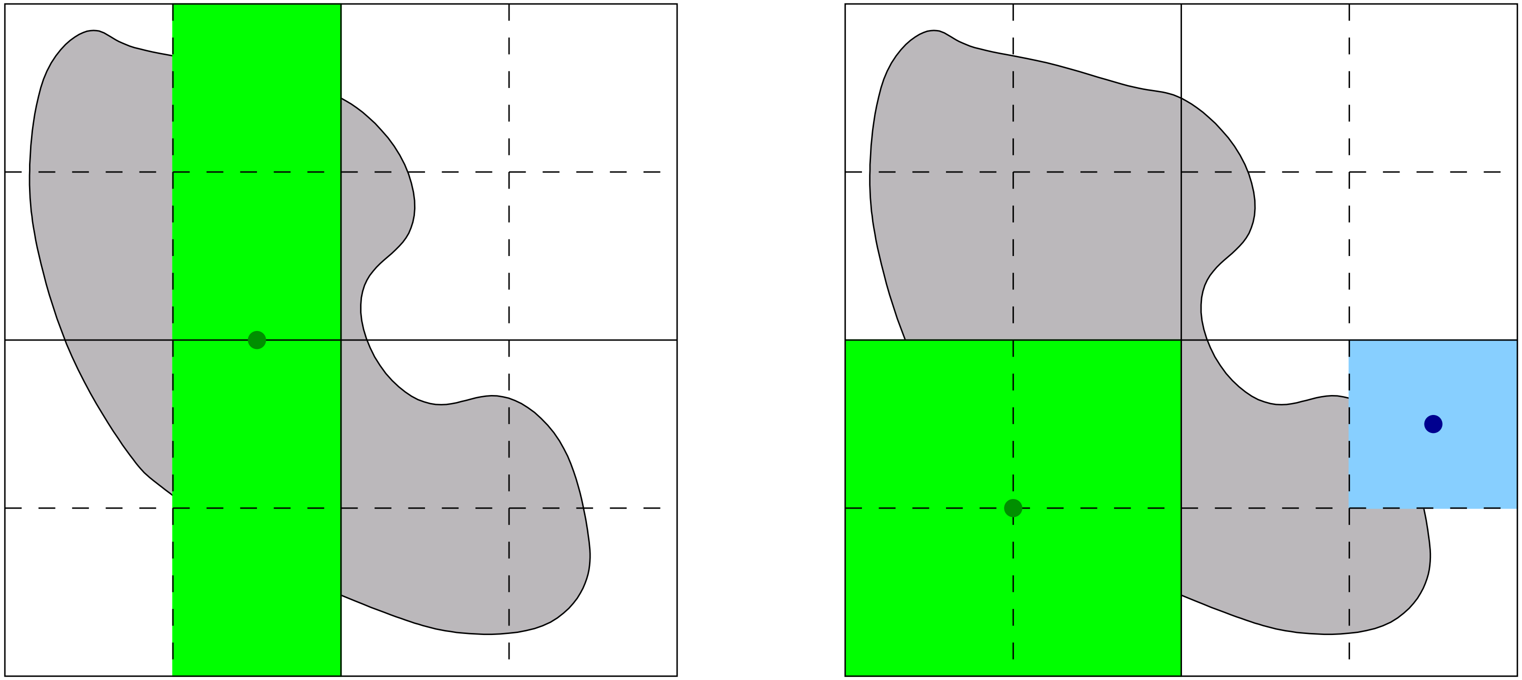


Adaptively Refined Meshes for Finite Elements:

- 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?

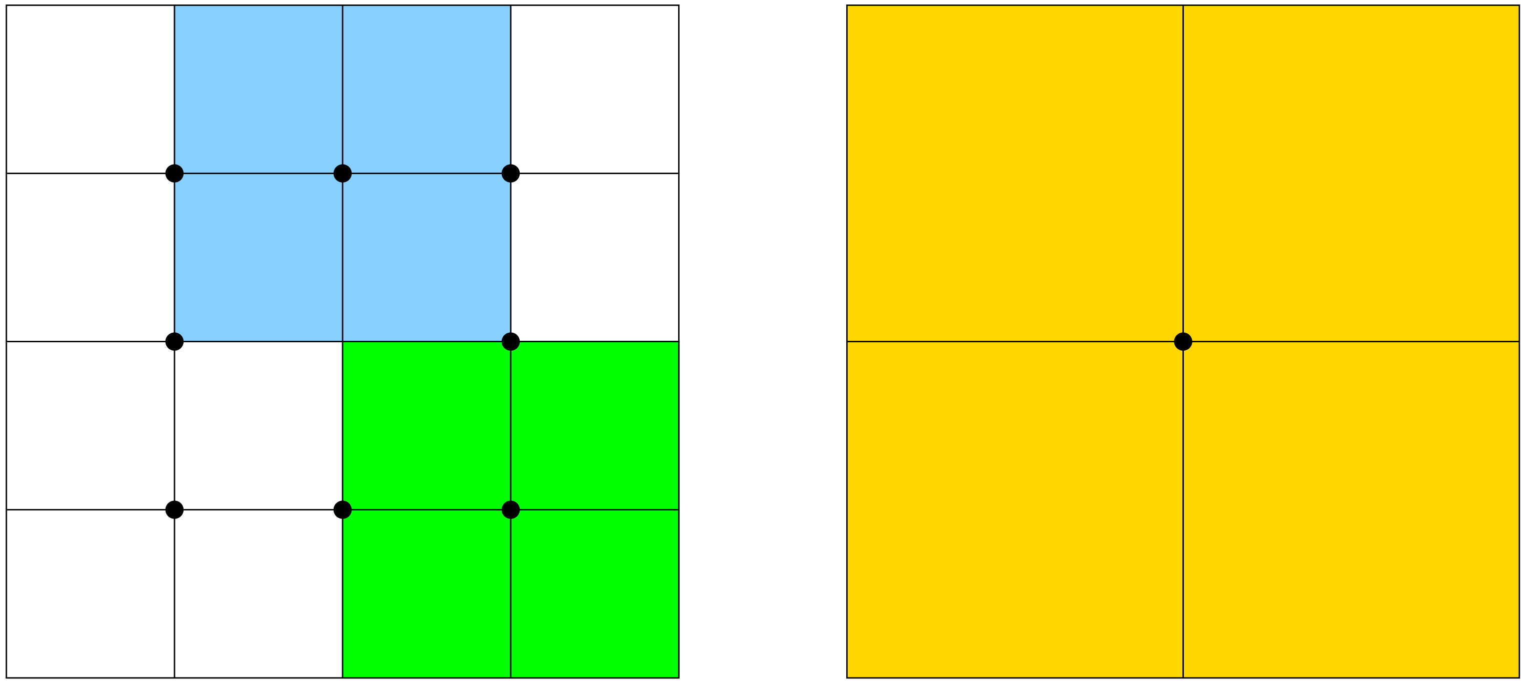


⇒ stretched tensor basis functions do not match quadtree cells

⇒ use basis functions with “square” domain (cover 4 siblings → to solve)

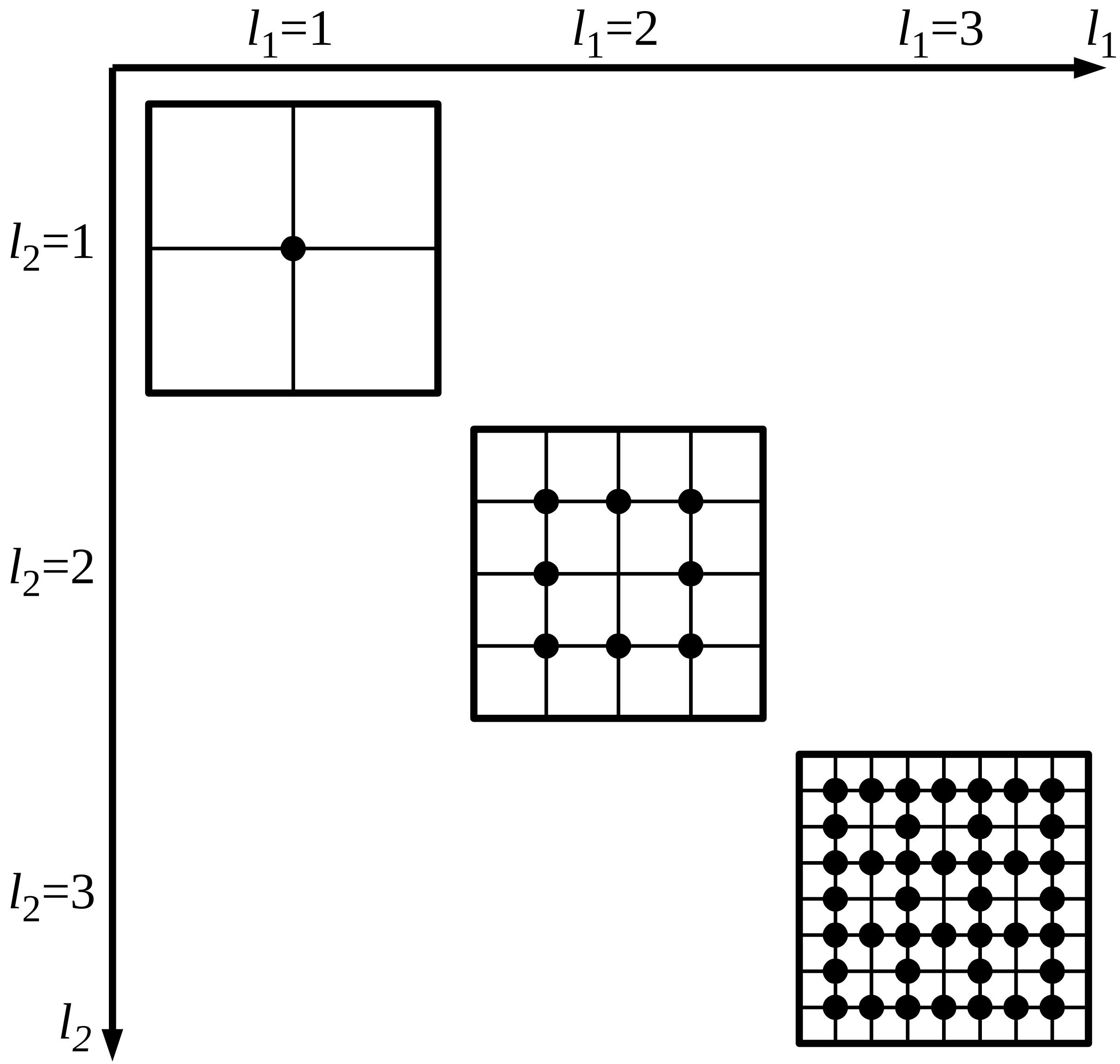
Hierarchical Basis for Quadtrees

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

Similar to tensor-product basis:

- Level-wise hierarchical increments

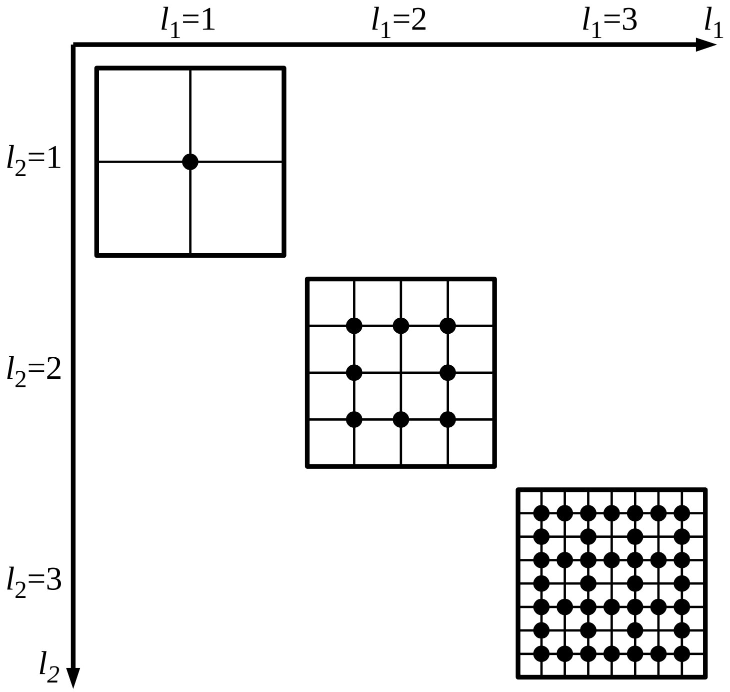
$$W_{\vec{l}} := \text{span}\{\phi_{\vec{l},\vec{i}}\}_{\vec{i} \in \hat{\mathscr{I}}_{\vec{l}}}$$

- Only use "diagonal" levels:

$$\vec{l} := \{l, \ldots, l\}$$

- Omit grid points for which all indices are even:

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



Part IV

Finite Element Methods – Towards Implementation

Project: 2D Adaptive Hierarchical Basis

Consider:

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

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- what do you need to compute, if you add a hierarchical basis function?

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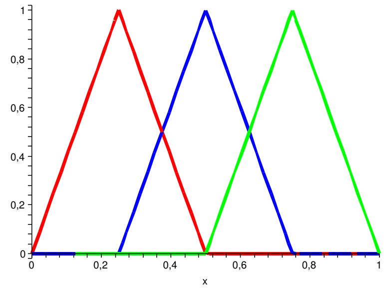
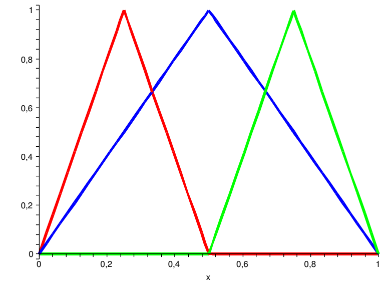
Idea: move from node-oriented to element-oriented approach

Recall: Hierarchical Basis Transformation



$\longrightarrow$



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

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

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

$$\begin{pmatrix} \phi_{2,1}(x) \\ \phi_{1,1}(x) \\ \phi_{2,3}(x) \end{pmatrix} = \begin{pmatrix} \phi_{2,1}(x) \\ \tfrac{1}{2}\phi_{2,1}(x) + \phi_{2,2}(x) + \tfrac{1}{2}\phi_{2,3}(x) \\ \phi_{2,3}(x) \end{pmatrix}$$

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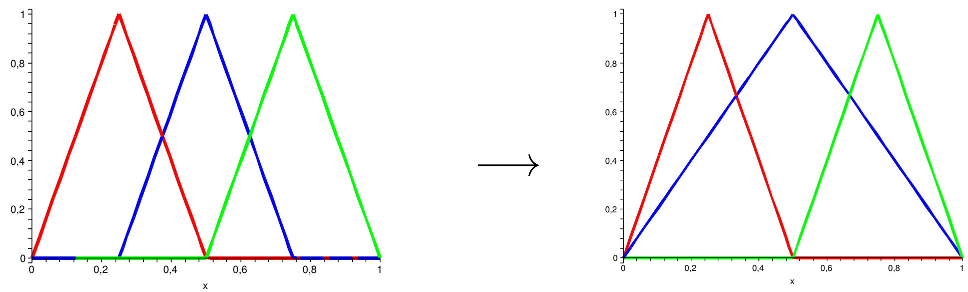

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Recall: Hierarchical Basis Transformation (2)

- 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

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

Recall: Hierarchical Coordinate Transformation

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- 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

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- compare coordinates and get

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

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

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

FEM and Hierarchical Basis Transform

- FEM discretisation with hierarchical test and shape functions:

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

- leads to respective stiffness matrix $A^{\mathrm{HB}}_{i,j}$:

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

$$\int \psi_i(x) L\Big(\sum_j v_j \phi_j(x)\Big)\,\mathrm{dx} = \sum_j v_j \int \psi_i(x) L \phi_j(x)\,\mathrm{dx} = \sum_j v_j A^{*}_{i,j}$$

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

FEM and Hierarchical Basis Transform (2)

- status: FEM with hierarchical test and nodal shape functions

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

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

Element Stiffness Matrices

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

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

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

$$\begin{aligned} \int_\Omega \nabla v \cdot \nabla u \,\mathrm{d}x &= \sum_k \int_{\Omega^{(k)}} \nabla v \cdot \nabla u \,\mathrm{d}x \\ \int_\Omega v f \,\mathrm{d}x &= \sum_i \int_{\Omega^{(i)}} v f \,\mathrm{d}x \end{aligned}$$

Element Stiffness Matrices (2)

- leads to local stiffness matrices for each element:

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

- 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 2×2 elements of $A^{(k)}$ are non-zero
- therefore convention to omit zero columns/rows
  $\Rightarrow$ 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

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

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:

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

Project: Adaptive Hierarchical Basis

Consider:

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

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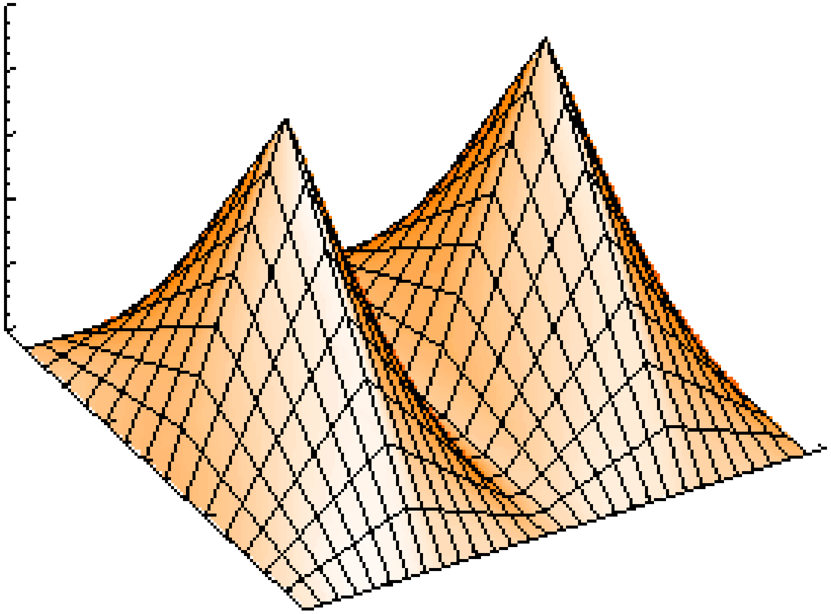
Example: 2D Poisson

- $-\Delta u = f$ 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

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