

Continuum mechanics and fluid-structure interaction problems: mathematical modelling and numerical approximation

deal.II LAB — Error, hanging nodes, boundary conditions

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How to measure the Error?

- Method of Manufactured Solutions
 - Take the “u” you want as a solution, plug in the equations, get the boundary conditions and the right hand side that force the given “u”
 - Integrate (with a fine quadrature formula) the difference between the exact solution and the computed one
(VectorTools::integrate_difference, or helper classes)
 - Possibly integrate the difference between the gradients of the exact and computed solutions



Error Estimates

Local Estimate:

$$\|u - \Pi u\|_{s, T_m} \lesssim \rho_m^{-s} h_m^{k+1} |u|_{k+1, T_m}$$

Global Estimate (for quasi uniform triangulations):

$$\sum_m \left(\|u - \Pi u\|_{s, T_m} \right) \lesssim h^{k+1-s} |u|_{k+1, \Omega}$$





Error Estimates

Local Estimate:

$$\|u - \Pi u\|_{s, T_m} \lesssim \rho_m^{-s} h_m^{k+1} |u|_{k+1, T_m}$$

If $V_h \subset H^s(\Omega)$

$$\|u - \Pi u\|_{s, \Omega} \lesssim h^{k+1-s} |u|_{k+1, \Omega}$$





To Reduce the Error:

- Globally, the error is dominated by *largest* element of the mesh and the $H^{k+1}(\Omega)$ norm of the exact solution
- Reduce the overall size of the mesh h (**global refinement**), when we don't know the $H^{k+1}(\Omega)$ norm of the exact solution
- Reduce the size of the elements where the solution has large $H^{k+1}(\Omega)$ norm, or where we estimate that $H^{k+1}(\Omega)$ norm of the solution would be large (**local refinement**)



Estimate the rate of convergence

- Once you have computed the error, how do we measure if we get the correct *convergence ratio*?
- Consider Poisson Problem. $V := H^1(\Omega)$

$$\|u - u_h\|_1 \lesssim \|u - \Pi u\|_1 \lesssim h^1 |u|_{2,\Omega}$$

$$\|u - \Pi u\|_0 \lesssim h^2 |u|_{2,\Omega}$$

Note: one needs to prove that we can use u_h in the last estimate!



Estimate the rate of convergence

- Compute two successive solutions, on half the size of the mesh (i.e., after one global refinement):

$$\| u - u_{2h} \| \sim \tilde{C}(2h)^p$$

$$\| u - u_h \| \sim \tilde{C}(h)^p$$

$$\frac{\| u - u_{2h} \|}{\| u - u_h \|} \sim 2^p$$

$$p \sim \log_2 \left(\frac{\| u - u_{2h} \|}{\| u - u_h \|} \right)$$





Back to C++

- Today's program:
 - Poisson for general coefficients, boundary data, and rhs
 - Work on successively refined grids
 - Estimate $L^2(\Omega)$ and $H^1(\Omega)$ errors

**The devil is in the details:
boundary conditions and constraints??**



Poisson problem revisited

Homogeneous Dirichlet case, constant coefficient equal to 1:

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega \end{aligned}$$

$$\gamma_{\Gamma} : H^1(\Omega) \mapsto H^{\frac{1}{2}}(\Gamma) \quad \text{Trace operator}$$

$$V := H_0^1(\Omega) := \{v \mid v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\partial\Omega} v = 0\}$$

Weak form: given $f \in V^*$, find $u \in V$ such that

$$(\nabla u, \nabla v) = (f, v) \quad \forall v \in V$$



Poisson problem revisited

Non-homogeneous Dirichlet case, constant coefficient equal to 1:

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega \\ u &= g && \text{on } \partial\Omega \end{aligned}$$

$$V_0 := H_0^1(\Omega) := \{v \mid v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\partial\Omega} v = 0\}$$

$$V_g := V_0 + u_D \quad \text{Where } \gamma_{\partial\Omega} u_D = g$$

Weak form: given $f \in V^*$, find $u \in V_g$ such that

$$(\nabla u, \nabla v) = (f, v) \quad \forall v \in V_0$$



Poisson problem revisited

Mixed boundary conditions, non-constant coefficients

$$\begin{aligned} -\nabla \cdot (a \nabla u) &= f && \text{in } \Omega \\ u &= g_D && \text{on } \Gamma_D \\ n \cdot (a \nabla u) &= g_N && \text{on } \Gamma_N \end{aligned}$$

$$V_{0,\Gamma_D} := H_0^1(\Omega) := \{v \mid v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\Gamma_D} v = 0\}$$

$$V_{g_D,\Gamma_D} := V_{0,\Gamma_D} + u_D \quad \text{Where } \gamma_{\Gamma_D} u_D = g_D$$

Weak form: given $f \in V_{0,\Gamma_D}^*$, find $u \in V_{g_D,\Gamma_D}$ such that

$$(a \nabla u, \nabla v) = (f, v) + \int_{\Gamma_N} g_N v \quad \forall v \in V_{0,\Gamma_D}$$



Trial spaces VS test spaces

$$V_{0,\Gamma_D} := H_0^1(\Omega) := \{v \mid v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\Gamma_D} v = 0\}$$

$$V_{g_D,\Gamma_D} := V_{0,\Gamma_D} + u_D$$

$$\text{Where } \gamma_{\Gamma_D} u_D = g_D$$

Weak form: given $f \in V_{0,\Gamma_D}^*$, find $u \in V_{g_D,\Gamma_D}$ such that

$$(a \nabla u, \nabla v) = (f, v) + \int_{\Gamma_N} g_N v \quad \forall v \in V_{0,\Gamma_D}$$

CANNOT apply Lax-Milgram: $V_{0,\Gamma_D} \neq V_{g_D,\Gamma_D}$



Trial spaces VS test spaces

$$V_{0,\Gamma_D} := H_0^1(\Omega) := \{v \mid v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\Gamma_D} v = 0\}$$

$$V_{g_D,\Gamma_D} := V_{0,\Gamma_D} + u_D$$

$$\text{Where } \gamma_{\Gamma_D} u_D = g_D$$

Weak form: given $f \in V_{0,\Gamma_D}^*$, find $u_0 \in V_{0,\Gamma_D}$ such that

$$(a \nabla u_0, \nabla v) = (f, v) + \int_{\Gamma_N} (g_N - n \cdot (a \nabla u_D)) v - (a \nabla u_D, \nabla v) \quad \forall v \in V_{0,\Gamma_D}$$

Write $u = u_0 + u_D$ (now we can apply Lax-Milgram)

where u_D is arbitrary, and such that $\gamma_{\Gamma_D} u_D = g_D$



How to implement V_{g_D, Γ_D} , V_{0, Γ_D} ?

- Option 1 (**not implemented in deal.II**):
encode in DoFHandler (n_{dofs} of $H_{0, \Gamma_D}^1(\Omega) < n_{\text{dofs}}$ of $H^1(\Omega)$)
and in basis functions (i.e., $\gamma_{\Gamma_D} v_i = 0 \quad \forall v_i \in V_h$)
- Option 2 (Penalty methods, Lagrange multipliers):
impose boundary conditions weakly (maybe later in this course)
- Option 3 (Algebraic approach: strong imposition):
post-process Linear systems, solution vectors, and rhs vectors to
set to g_D degrees of freedom with support points on Γ_D





Algebraic approach

- Main idea: assemble matrix $\tilde{A}_{ij} := (a \nabla v_j, \nabla v_i)$

and right-hand-side

$$\tilde{F}_i := (f, v_i) + \int_{\Gamma_N} g_N v_i$$

- split dofs

$$u = \begin{pmatrix} u_{\Omega \cup \Gamma_N} \equiv u_O \\ u_C \end{pmatrix} \quad \tilde{F} = \begin{pmatrix} F_O \\ F_C \end{pmatrix}$$

- and matrix

$$\tilde{A} = \begin{pmatrix} A_{OO} & A_{OC} \\ A_{CO} & A_{CC} \end{pmatrix}$$

- where “C” stands for “constrained”



Mimic continuous approach

- compute g_D , using `VectorTools::interpolate_boundary_values`

- eliminate row “C” from \tilde{A} , and set rhs $\tilde{F}_C \mapsto g_D$:
$$\begin{pmatrix} A_{oo} & A_{oc} \\ 0 & I_{cc} \end{pmatrix} \begin{pmatrix} u_o \\ u_D \end{pmatrix} = \begin{pmatrix} \tilde{F}_o \\ g_D \end{pmatrix}$$

- “move” A_{oc} to rhs to restore symmetry in matrix:
$$\begin{pmatrix} A_{oo} & 0 \\ 0 & I_{cc} \end{pmatrix} \begin{pmatrix} u_o \\ u_D \end{pmatrix} = \begin{pmatrix} \tilde{F}_o - A_{oc}g_D \\ g_D \end{pmatrix}$$

- rescale I_{cc} for conditioning:
$$\begin{pmatrix} A_{oo} & 0 \\ 0 & \alpha I_{cc} \end{pmatrix} \begin{pmatrix} u_o \\ u_D \end{pmatrix} = \begin{pmatrix} \tilde{F}_o - A_{oc}g_D \\ \alpha g_D \end{pmatrix}$$

`MatrixTools::apply_boundary_values` $\tilde{A} \mapsto \begin{pmatrix} A_{oo} & 0 \\ 0 & \alpha I_{cc} \end{pmatrix}$ $u \mapsto \begin{pmatrix} u_o \\ u_D \end{pmatrix}$ $\tilde{F} \mapsto \begin{pmatrix} \tilde{F}_o - A_{oc}g_D \\ \alpha g_D \end{pmatrix}$



Special case of AffineConstraints

- General case: constrained dofs are a subset of all dofs $\mathcal{N}_C \subset \mathcal{N}$
- AffineConstraints: $x_i = \sum_{j \in \mathcal{N} \setminus \mathcal{N}_C} C_{ij} x_j + b_i \quad \forall i \in \mathcal{N}_C$
- Algebraic solution can be performed efficiently as a three-step process:
 - Condense
 - Solve
 - Distribute (only needed if $C \neq 0$)

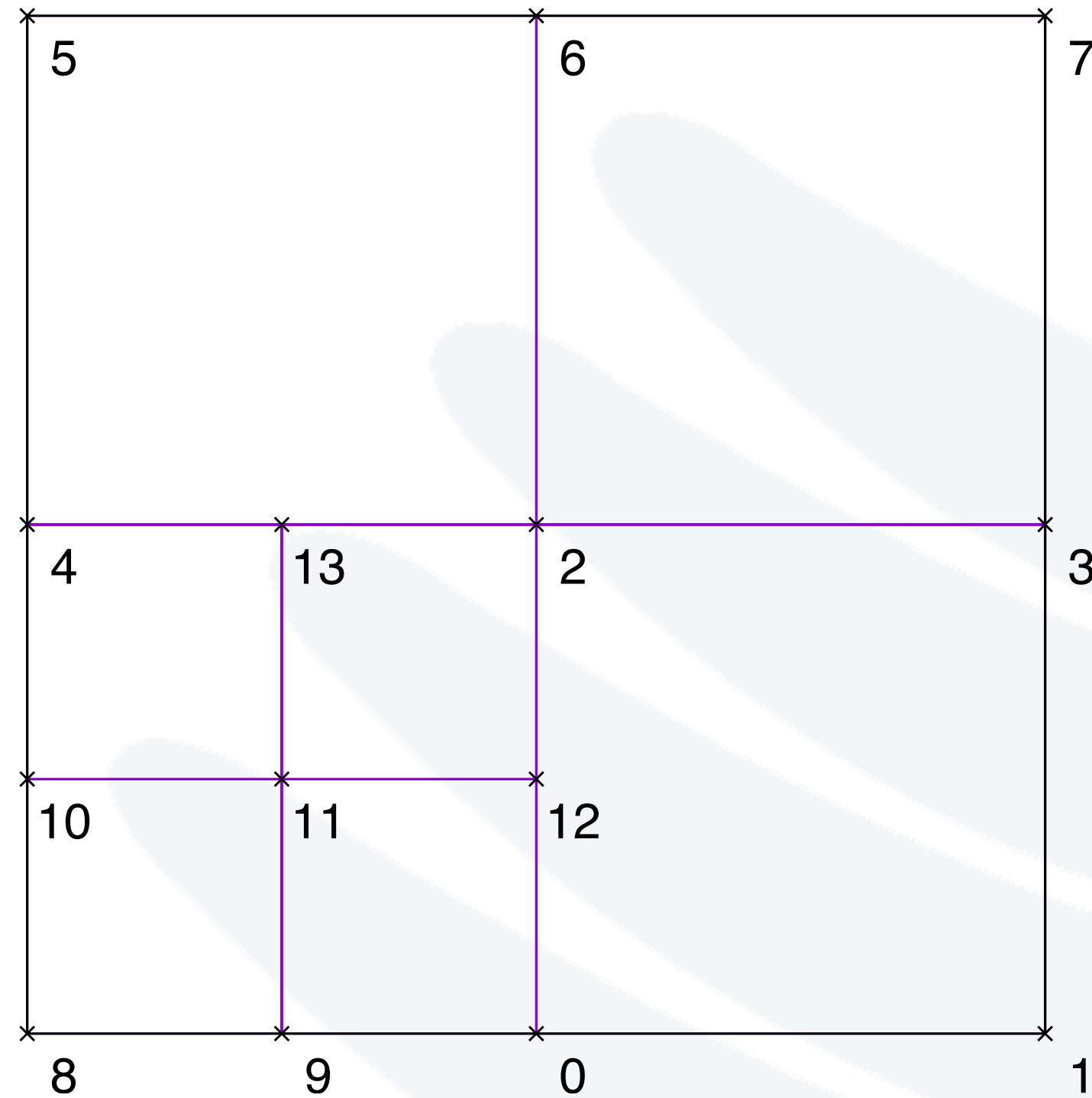


Condense-Solve-Distribute

- Given, $\tilde{A} = \begin{pmatrix} A_{oo} & A_{oc} \\ A_{co} & A_{cc} \end{pmatrix}$, $\tilde{F} = \begin{pmatrix} F_o \\ F_c \end{pmatrix}$, and constraints $u_c = Cu_o + b$
- Take constraints into accounts in “O”: $A_{oo}u_o + A_{oc}u_c = (A_{oo} + A_{oc}C)u_o + A_{oc}b = F_o$
- Ignore rows “C” in matrix and rhs and solve $Au = F$ where
 - $\tilde{A} = \begin{pmatrix} A_{oo} & A_{oc} \\ A_{co} & A_{cc} \end{pmatrix} \mapsto A = \begin{pmatrix} A_{oo} + A_{oc}C & 0 \\ 0 & \alpha I_{cc} \end{pmatrix}$
 - $\tilde{F} = \begin{pmatrix} F_o \\ F_c \end{pmatrix} \mapsto F = \begin{pmatrix} F_o - A_{oc}b \\ \alpha b \end{pmatrix}$
- Distribute constraints: $u = \begin{pmatrix} u_o \\ b \end{pmatrix} \mapsto u = \begin{pmatrix} u_o \\ Cu_o + b \end{pmatrix}$



Hanging nodes

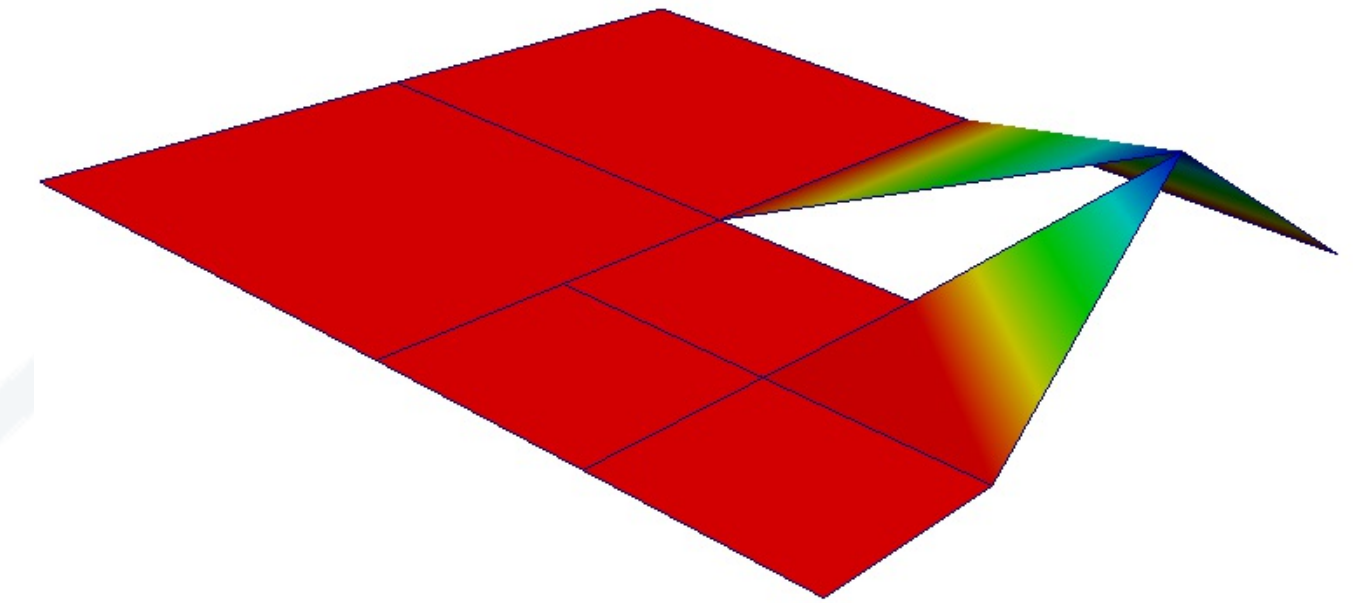


Discontinuous FE space!

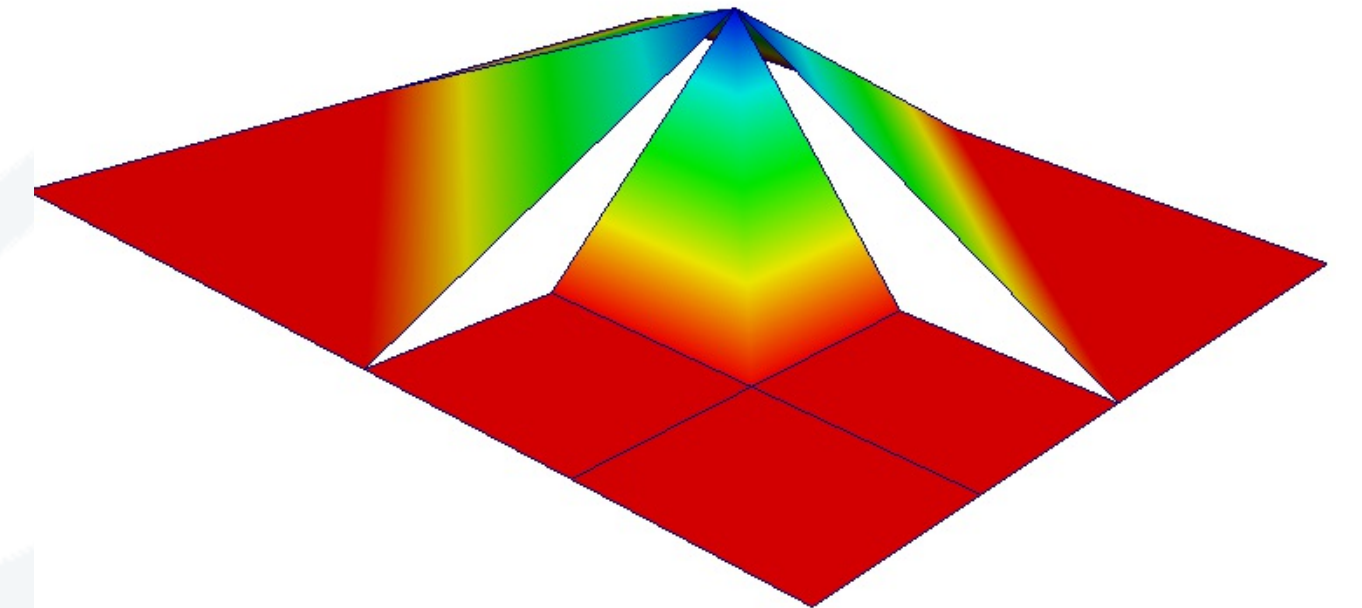
Not a subspace of H^1

Bilinear forms would
require special treatment
as gradients are not
defined everywhere

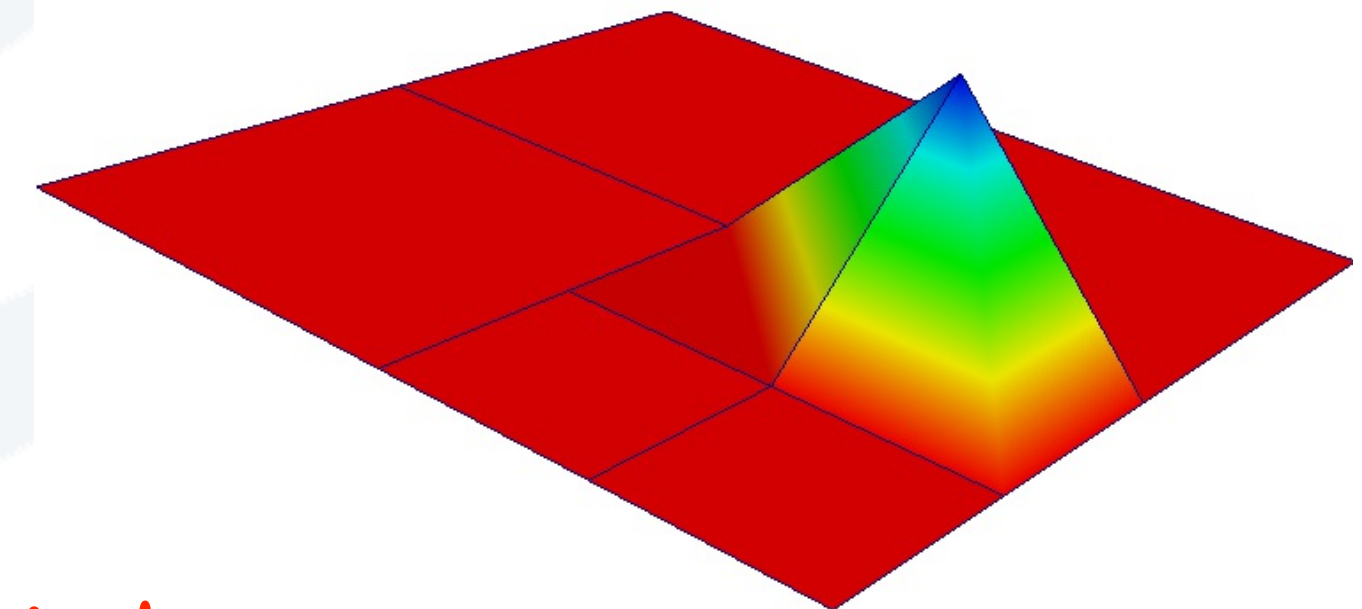
$N_0(\mathbf{x})$:



$N_2(\mathbf{x})$:



$N_{12}(\mathbf{x})$:



Solution: introduce constraints to require continuity!



Hanging nodes

Use standard (possibly globally discontinuous) shape functions, but require continuity of their linear combination

$$\mathcal{S}^h = \{u^h = \sum_i u_i N_i(\mathbf{x}) : u^h(\mathbf{x}) \in C^0\}$$

Note, that we encounter discontinuities along edges 0-12-2 and 2-13-4.

We can make the function continuous by making it continuous at vertices 12 and 13:

$$u_{12} = \frac{1}{2}u_0 + \frac{1}{2}u_2$$

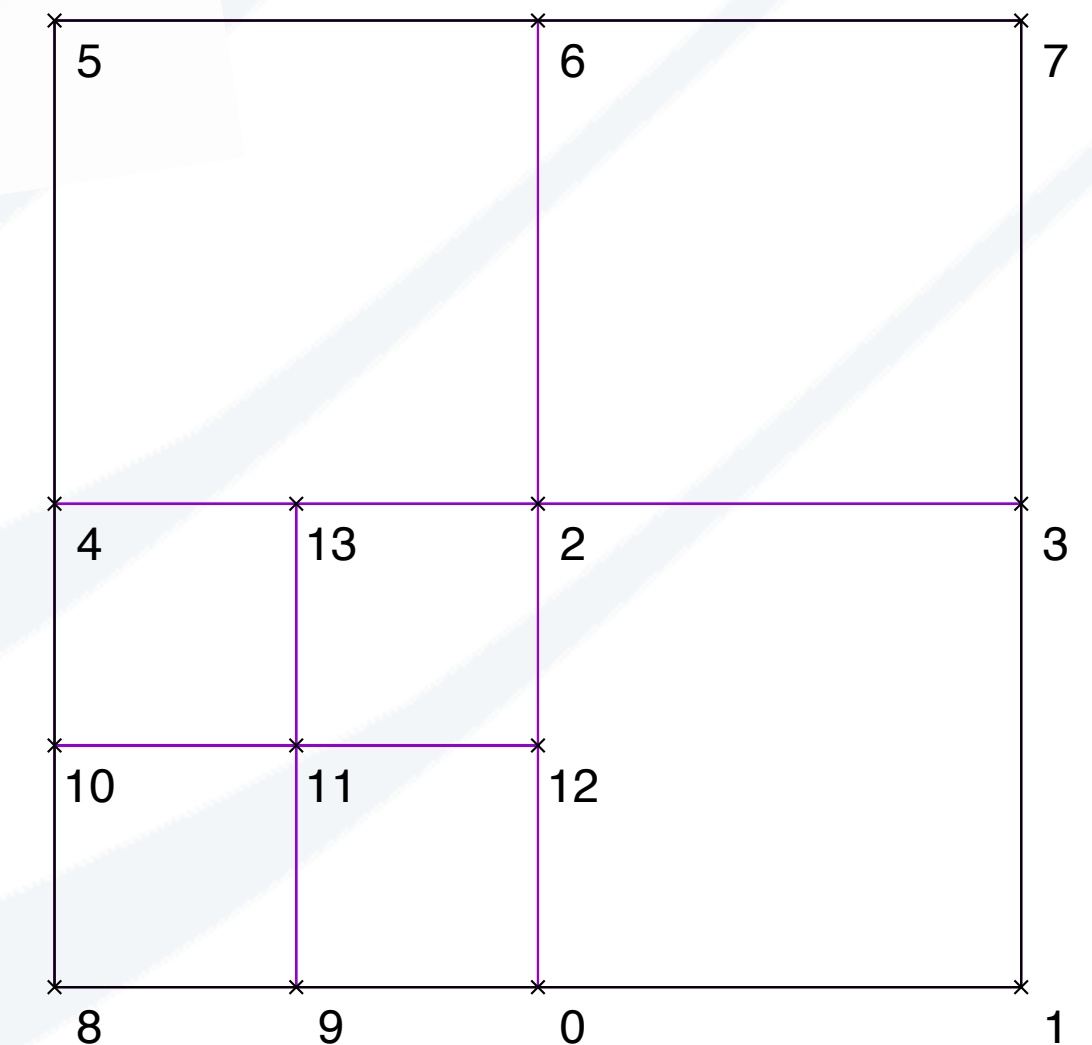
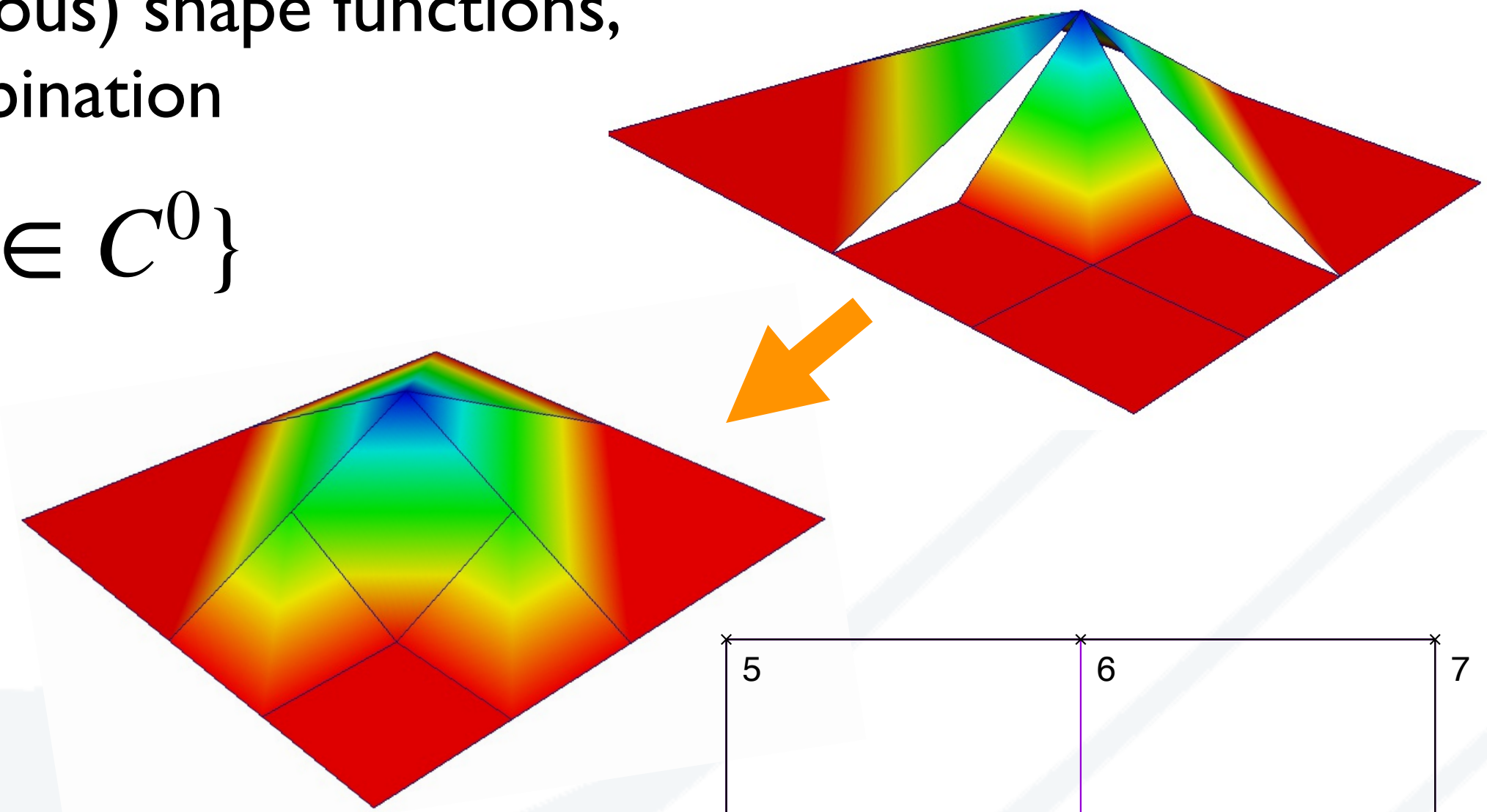
$$u_{13} = \frac{1}{2}u_2 + \frac{1}{2}u_4$$

The general form:

$$u_i = \sum_{j \in \mathcal{N}} c_{ij} u_j + b_i \quad \forall i \in \mathcal{N}_C$$

define a subset of all DoFs to be constrained

$$\mathcal{N}_C \subset \mathcal{N}$$



similar constraints arise from boundary conditions (normal/tangential component) or hp-adaptive FE



Condensed shape functions

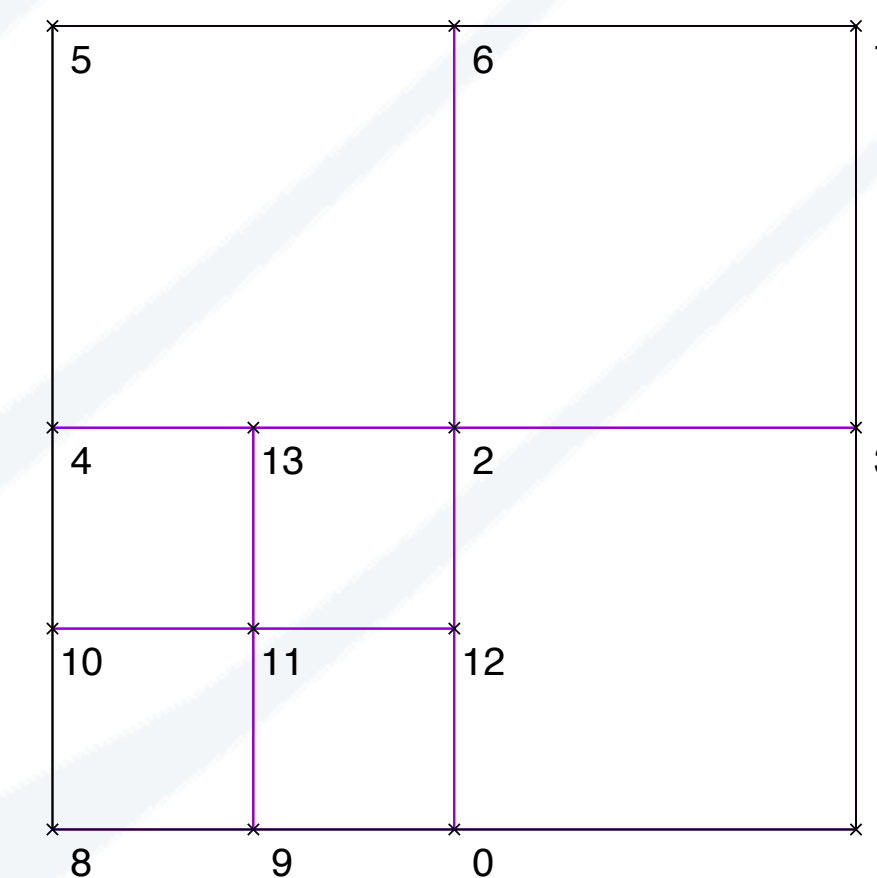
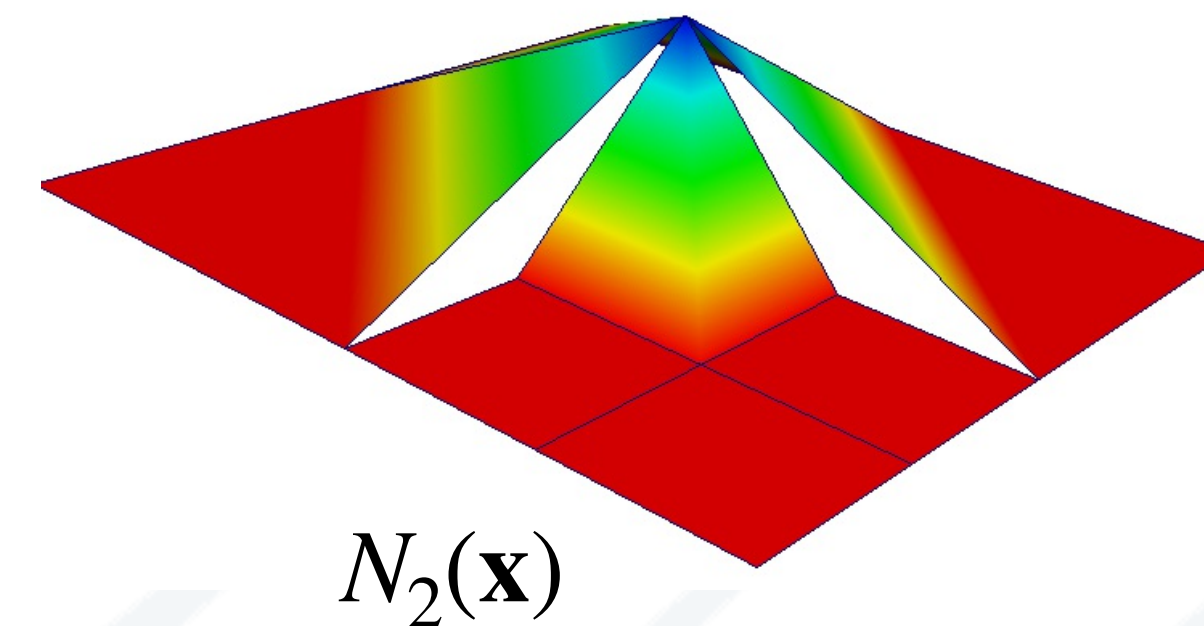
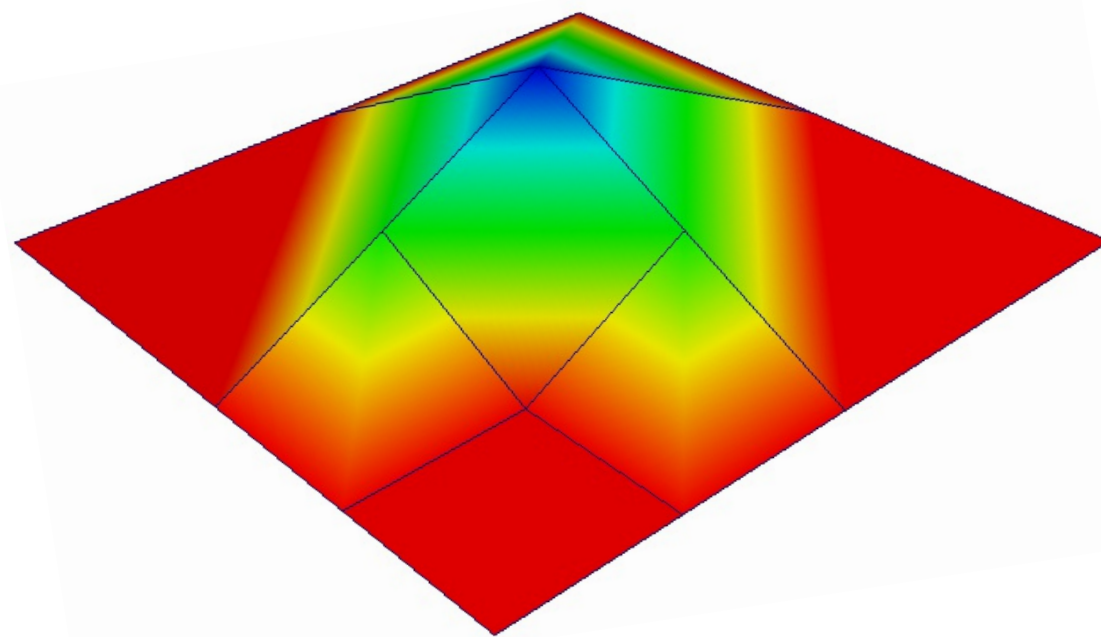
The alternative viewpoint is to construct a set of conforming shape functions:

$$\widetilde{N}_2 := N_2 + \frac{1}{2}N_{13} + \frac{1}{2}N_{12}$$

$$\mathcal{S}^h = \{u^h = \sum_{i \in \mathcal{N} \setminus \mathcal{N}_c} u_i \widetilde{N}_i(\mathbf{x})\}$$

$$[\mathbf{K}]_{ij} = \begin{cases} a(\widetilde{N}_i, \widetilde{N}_j) & \text{if } i \in \mathcal{N} \setminus \mathcal{N}_c \text{ and } j \in \mathcal{N} \setminus \mathcal{N}_c \\ 1 & \text{if } i \equiv j \text{ and } j \in \mathcal{N}_c \\ 0 & \text{otherwise} \end{cases}$$

$$[\mathbf{F}]_i = \begin{cases} (f, \widetilde{N}_i) & \text{if } i \in \mathcal{N} \setminus \mathcal{N}_c \\ 0 & \text{otherwise} \end{cases}$$



The beauty of the approach is that we can assemble local matrix and RHS as usual and then obtain condensed forms in a separate step, i.e

$$\forall i \in \mathcal{N} \setminus \mathcal{N}_c : [\mathbf{F}]_i = (f, \widetilde{N}_i) = (f, N_i + \sum_{j \in \mathcal{N}_c} c_{ji} N_j) = (f, N_i) + \sum_{j \in \mathcal{N}_c} c_{ji} (f, N_j) = [\widetilde{\mathbf{F}}]_i + \sum_{j \in \mathcal{N}_c} c_{ji} [\mathbf{F}]_j$$





Using constraints:

- The beauty of the FEM is that we do exactly the same thing on every cell
- In other words: assembly on cells with hanging nodes should work exactly as on cells without



Approach 1:

$$\widetilde{\mathcal{S}}^h = \{u^h = \sum_i u_i N_i(x)\}$$

this is not a continuous space, but we may still use it as an intermediate step for matrices!

$$\mathcal{S}^h = \{u^h = \sum_i u_i N_i(x) : u^h(x) \in C^0\}$$

Step 1: Build matrix/rhs $\widetilde{\mathbf{K}}, \widetilde{\mathbf{F}}$ with all DoFs as if there were no constraints.

Step 2: Modify $\widetilde{\mathbf{K}}, \widetilde{\mathbf{F}}$ to get \mathbf{K}, \mathbf{F}

i.e. eliminate the rows and columns of the matrix that correspond to constrained degrees of freedom

Step 3: Solve $\mathbf{K} \cdot \mathbf{u} = \mathbf{F}$

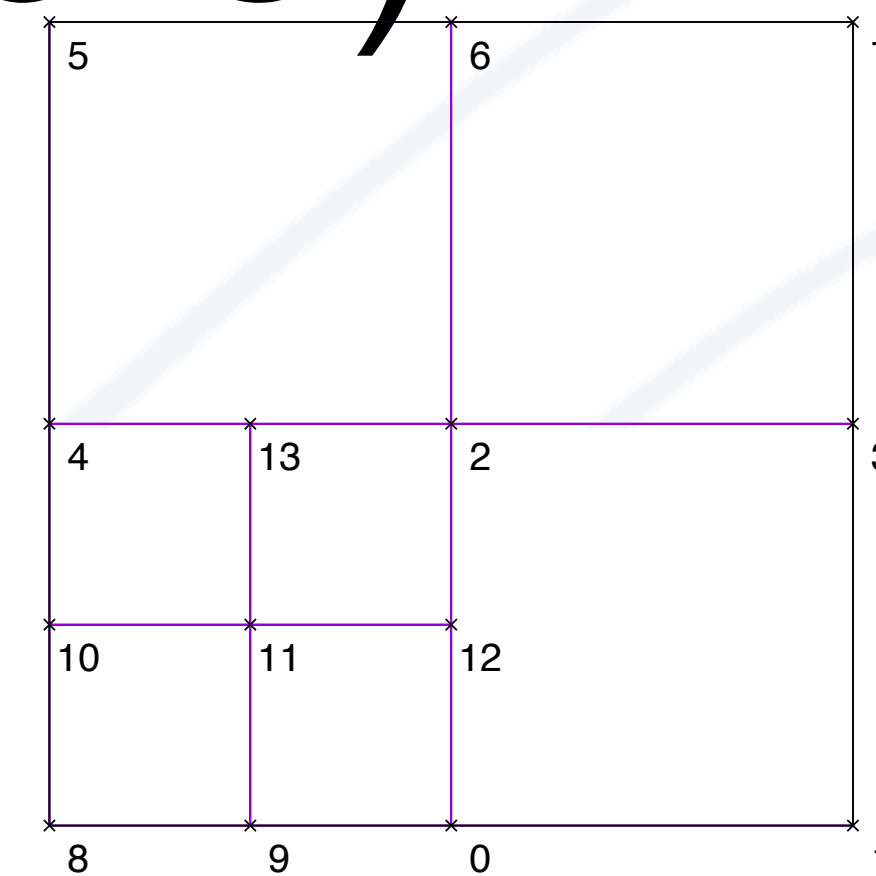
Step 4: Fill in the constrained components of \mathbf{u} to use $\widetilde{\mathcal{S}}^h$ for evaluation of the field.

Disadvantages: (i) bottleneck for 3d or higher order/hp FEM; (ii) hard to implement in parallel where a process may not have access to all elements of the matrix; (iii) two matrices may have different sparsity pattern.



Approach 1 (example):

$$\begin{bmatrix} u_{12} \\ u_{13} \end{bmatrix} = \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} u_0 \\ u_2 \\ u_4 \end{bmatrix}$$



```
=====
Number of active cells: 7
Number of degrees of freedom: 14
===== constraints =====
12 0: 0.5
12 2: 0.5
13 2: 0.5
13 4: 0.5
```

```
===== un-condensed =====
```

```
===== matrix =====
```

```
1.333e+00 -1.667e-01 -1.667e-01 -3.333e-01 0.000e+00
-1.667e-01 6.667e-01 -3.333e-01 -1.667e-01
-1.667e-01 -3.333e-01 2.667e+00 -3.333e-01 -1.667e-01 -3.333e-01 -3.333e-01 -3.333e-01
-3.333e-01 -1.667e-01 -3.333e-01 1.333e+00
0.000e+00
-1.667e-01
-3.333e-01
-3.333e-01 -3.333e-01 -3.333e-01 -1.667e-01 1.333e+00 -1.667e-01
-3.333e-01 -1.667e-01
-1.667e-01 6.667e-01 -1.667e-01
-1.667e-01 6.667e-01
```

```
-1.667e-01 0.000e+00
0.000e+00 -1.667e-01
-3.333e-01 -3.333e-01 -3.333e-01
-1.667e-01 -1.667e-01 -1.667e-01
```

```
-1.667e-01 -3.333e-01 -1.667e-01
0.000e+00 0.000e+00 -3.333e-01 -1.667e-01 -1.667e-01
-1.667e-01 -3.333e-01 -1.667e-01
6.667e-01 -1.667e-01 -1.667e-01 -3.333e-01
-1.667e-01 1.333e+00 -3.333e-01 -3.333e-01 -3.333e-01
-1.667e-01 -3.333e-01 1.333e+00 -3.333e-01 -3.333e-01
-3.333e-01 -3.333e-01 -3.333e-01 2.667e+00 -3.333e-01 -3.333e-01
-3.333e-01 -3.333e-01 -3.333e-01 1.333e+00 -3.333e-01
-3.333e-01 -3.333e-01 -3.333e-01 1.333e+00
```

```
===== condensed =====
```

```
===== matrix =====
```

```
1.500e+00 -1.667e-01 -8.333e-02 -3.333e-01 -8.333e-02
-1.667e-01 6.667e-01 -3.333e-01 -1.667e-01
-8.333e-02 -3.333e-01 2.833e+00 -3.333e-01 -8.333e-02 -3.333e-01 -3.333e-01 -3.333e-01
-3.333e-01 -1.667e-01 -3.333e-01 1.333e+00
-8.333e-02
-8.333e-02
-3.333e-01
-3.333e-01
-3.333e-01 -3.333e-01 -3.333e-01 -1.667e-01 1.333e+00 -1.667e-01
-3.333e-01 -1.667e-01
-1.667e-01 6.667e-01 -1.667e-01
-1.667e-01 6.667e-01
```

```
-3.333e-01 -1.667e-01
-1.667e-01 -3.333e-01
-5.000e-01 -6.667e-01 -5.000e-01
0.000e+00 0.000e+00 0.000e+00
0.000e+00 0.000e+00
```

```
-3.333e-01 -5.000e-01 0.000e+00
-1.667e-01 -1.667e-01 -6.667e-01 0.000e+00 0.000e+00
-3.333e-01 -5.000e-01 0.000e+00
6.667e-01 -1.667e-01 -1.667e-01 -3.333e-01
-1.667e-01 1.333e+00 -3.333e-01 -3.333e-01 0.000e+00
-1.667e-01 -3.333e-01 1.333e+00 -3.333e-01 0.000e+00
-3.333e-01 -3.333e-01 -3.333e-01 2.667e+00 0.000e+00 0.000e+00
0.000e+00 0.000e+00 1.333e+00 0.000e+00
0.000e+00 0.000e+00 0.000e+00 1.333e+00
```



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Approach 2:

$$\tilde{\mathcal{S}}^h = \{u^h = \sum_i u_i N_i(x)\}$$

$$\mathcal{S}^h = \{u^h = \sum_i u_i N_i(x) : u^h(x) \in C^0\}$$

Step 1: Build local matrix/rhs $\tilde{\mathbf{K}}_K, \tilde{\mathbf{F}}_K$ with all DoFs as if there were no constraints.

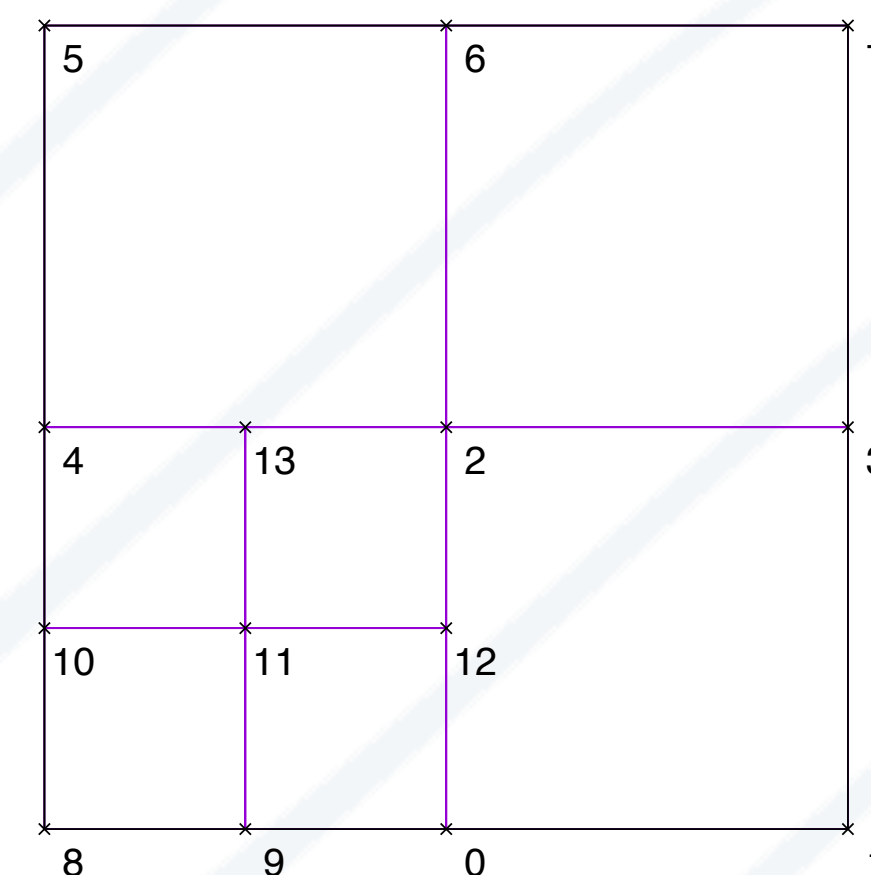
Step 2: Apply constraints during assembly operation (local-to-global) $\mathbf{K}_K, \mathbf{F}_K$

Step 3: Solve $\mathbf{K} \cdot \mathbf{u} = \mathbf{F}$

Step 4: Fill in the constrained components of \mathbf{u} to use $\tilde{\mathcal{S}}^h$ for evaluation of the field.



$$\begin{bmatrix} u_{12} \\ u_{13} \end{bmatrix} = \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} u_0 \\ u_2 \\ u_4 \end{bmatrix}$$



```

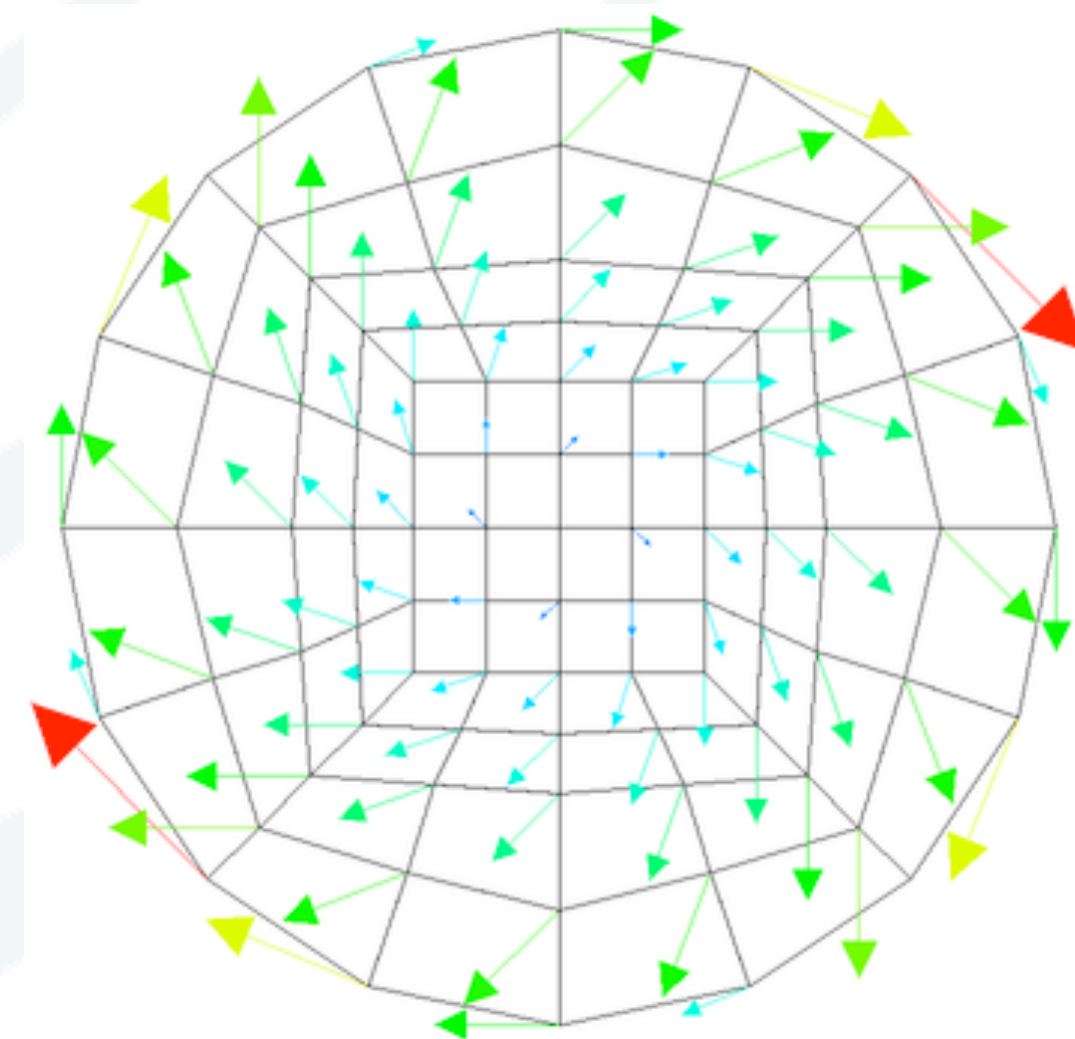
6.667e-01 -1.667e-01 -1.667e-01 -3.333e-01
-1.667e-01 1.333e+00 -3.333e-01 -3.333e-01 0.000e+00
-1.667e-01 -3.333e-01 1.333e+00 -3.333e-01 0.000e+00 0.000e+00
-3.333e-01 -3.333e-01 -3.333e-01 2.667e+00 0.000e+00 0.000e+00
0.000e+00 0.000e+00 0.000e+00 1.333e+00 0.000e+00
0.000e+00 0.000e+00 0.000e+00 0.000e+00 1.333e+00

```




Applying constraints: the AffineConstraints class

- This class is used for
 - Hanging nodes
 - Dirichlet and periodic constraints
 - Other constraints
- Linear constraints of the the form $u_C = Cu_O + b$





Applying constraints: the AffineConstraints class

- System setup
- Hanging node constraints created using
`DoFTools::make_hanging_node_constraints()`
- Will also use for boundary values from now on:
`VectorTools::interpolate_boundary_values(..., constraints);`
- Need different SparsityPattern creator
`DoFTools::make_sparsity_pattern (... , constraints, ...)`
 - Can remove constraints from linear system
`DoFTools::make_sparsity_pattern (... , constraints,
/ *keep_constrained_dofs = * / false)`
- Sort, rearrange, optimise constraints
`constraints.close()`



Applying constraints: the AffineConstraints class

- Assembly
- Assemble local matrix and vector as normal
- Eliminate while transferring to global matrix:
`constraints.distribute_local_to_global (`
 `cell_matrix, cell_rhs,`
 `local_dof_indices,`
 `system_matrix, system_rhs);`
- Solve and then set all constraint values correctly:
`ConstraintMatrix::distribute(...)`