Master in High Performance Computing

Numerical Solution of PDEs using the Finite Element Method

The devil is in the details: boundary conditions and constraints

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Poisson problem revisited

Homogeneous Dirichlet case, constant coefficient equal to 1:

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

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

$$V := H^1_0(\Omega) := \{v \,|\, v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\partial\Omega} v = 0\}$$

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

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

Poisson problem revisited

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

$$-\Delta u = f \qquad \text{in } \Omega$$
$$u = g \qquad \text{on } \partial\Omega$$

$$V_0 := H^1_0(\Omega) := \{v \mid v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\partial\Omega} v = 0\}$$

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

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

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

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ICTP The Abdus Salam International Centre for Theoretical Physics

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Poisson problem revisited

Mixed boundary conditions, non-constant coefficients

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

$$V_{0,\Gamma_D} := H^1_0(\Omega) := \{ v \,|\, v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\Gamma_D} v = 0 \}$$

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

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

Trial spaces VS test spaces

$$V_{0,\Gamma_D} := H^1_0(\Omega) := \{v \,|\, v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\Gamma_D} v = 0\}$$

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

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

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

Trial spaces VS test spaces

$$V_{0,\Gamma_D} := H^1_0(\Omega) := \{v \,|\, v \in L^2(\Omega), \nabla v \in L^2(\Omega), \gamma_{\Gamma_D} v = 0\}$$

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

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

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 $H^1_{0,\Gamma_D}(\Omega)$ < n_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

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

- 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 $$\tilde{A} \mapsto \begin{pmatrix} A_{OO} & 0 \\ 0 & \alpha I_{CC} \end{pmatrix} \qquad u \mapsto \begin{pmatrix} u_O \\ u_D \end{pmatrix} \qquad \tilde{F} \mapsto \begin{pmatrix} \tilde{F}_O - A_{OC} g_D \\ \alpha g_D \end{pmatrix}$$

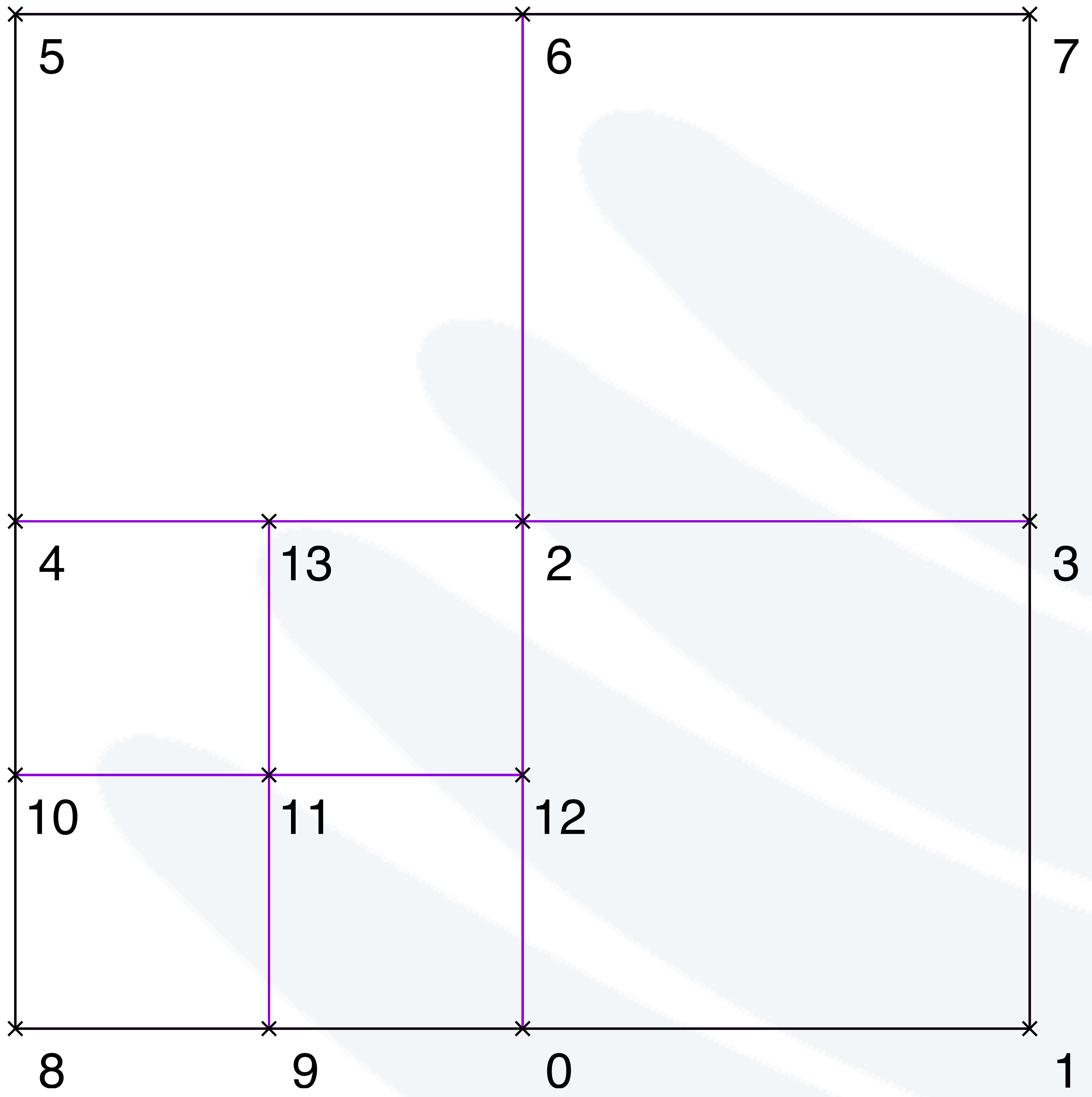
Special case of AffineConstraints

- General case: constrained dofs are a subset of all dofs $\mathcal{N}_C \subset \mathcal{N}$
- AffineConstraints: $x_i = \sum_{j \in \mathcal{N} \setminus \mathcal{N}_C} C_{ij} x_j + b_i \qquad \forall i \in \mathcal{N}_C$
- 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

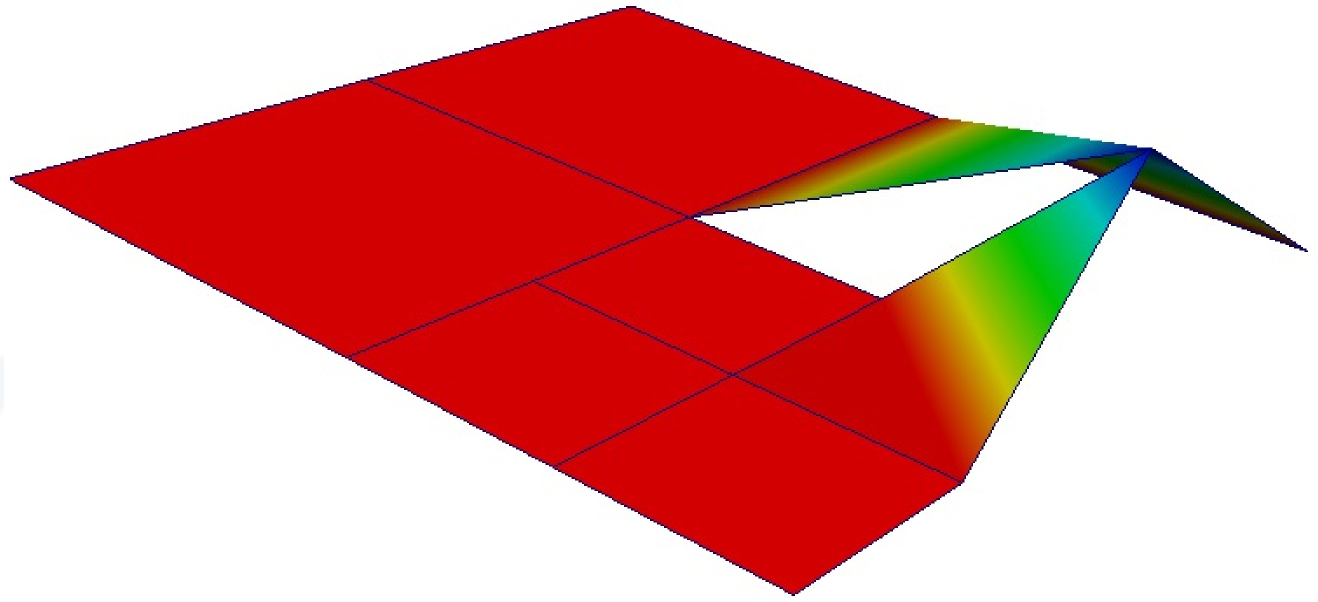


Discontinuous FE space!

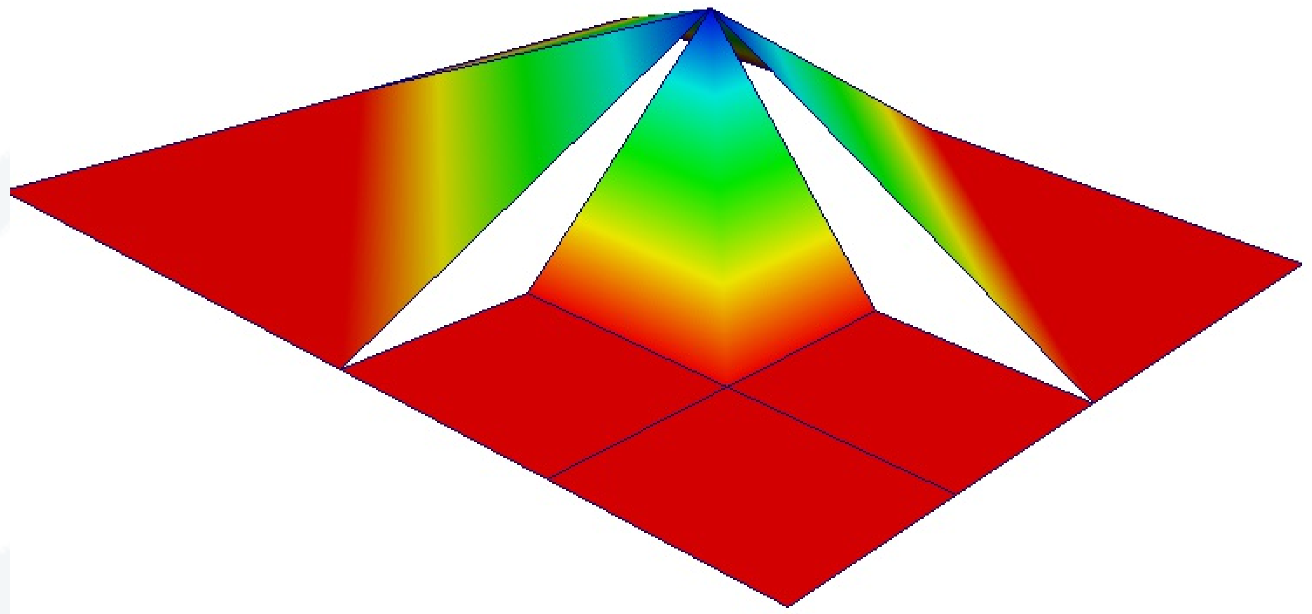
Not a subspace of H^1

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

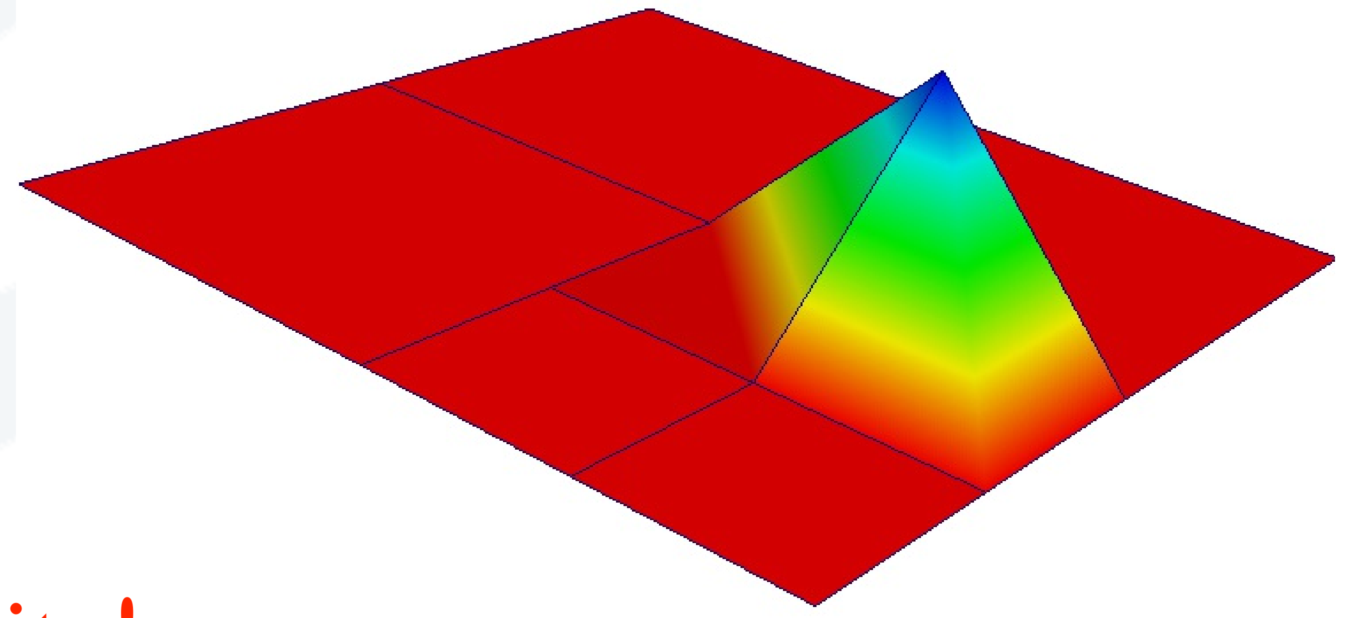
$N_0(\mathbf{x})$:



$N_2(\mathbf{x})$:



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

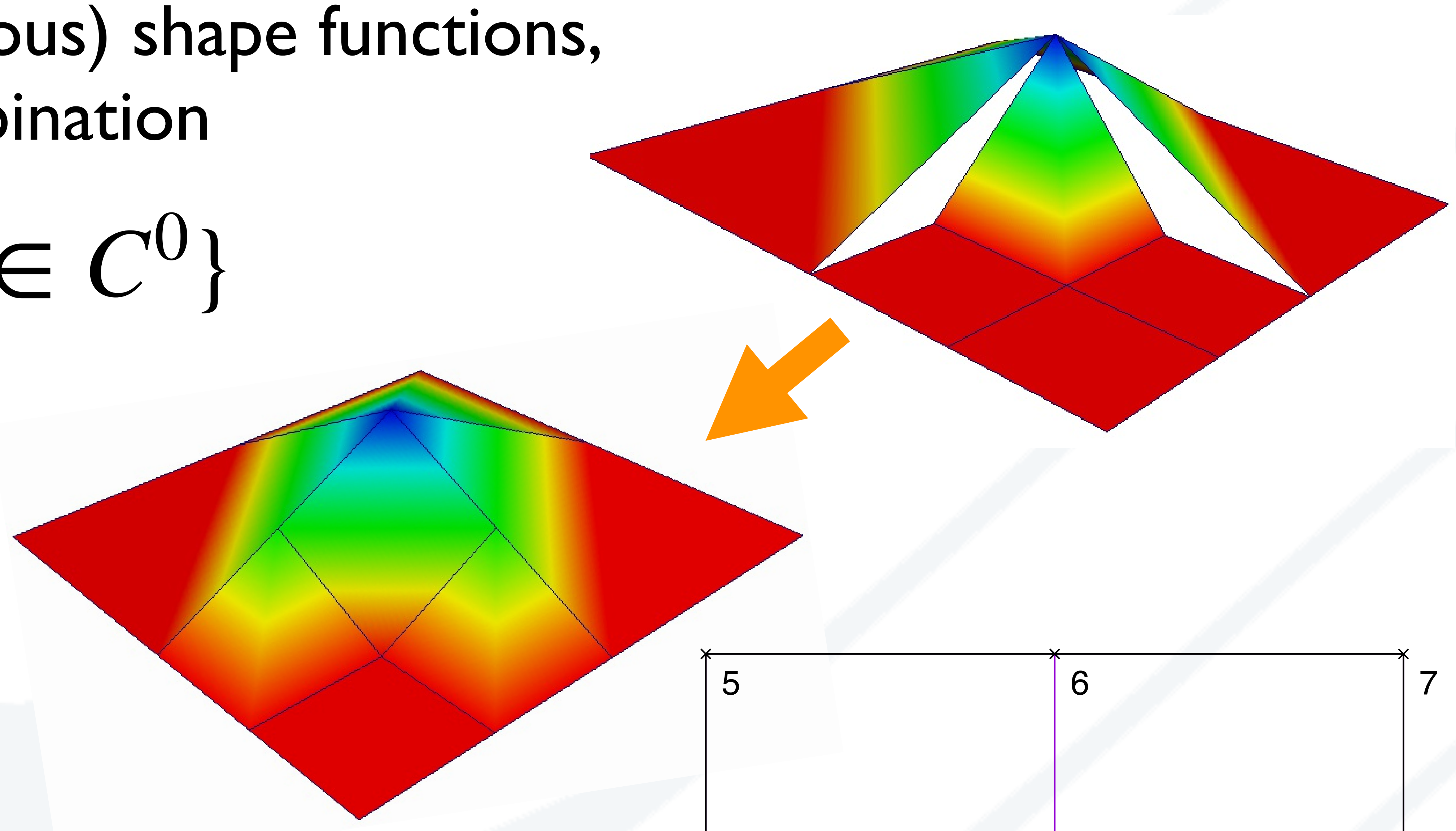


Solution: introduce constraints to require continuity!

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.

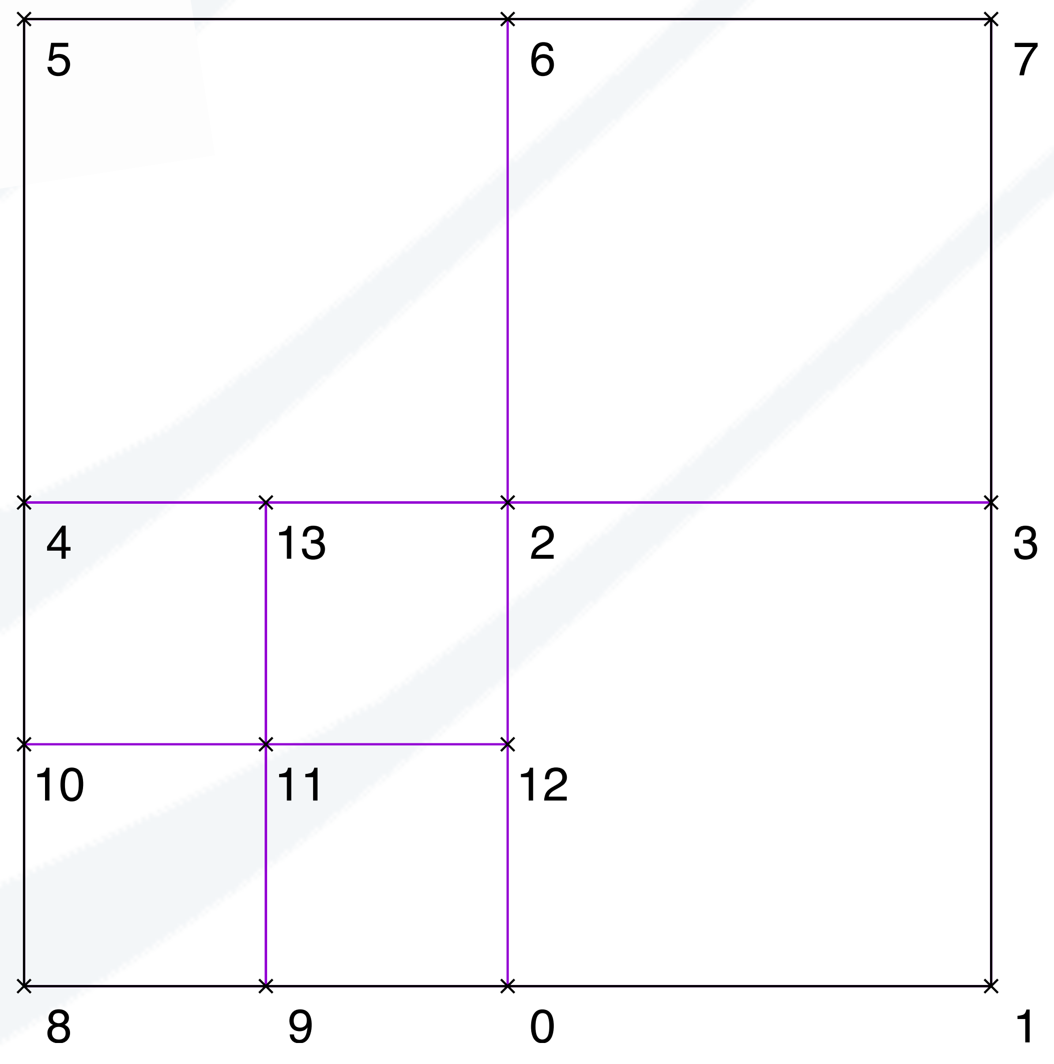
We can make the function continuous by making it continuous at vertices 12 and 13:

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

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

define a subset of all DoFs to be constrained

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



The general form:

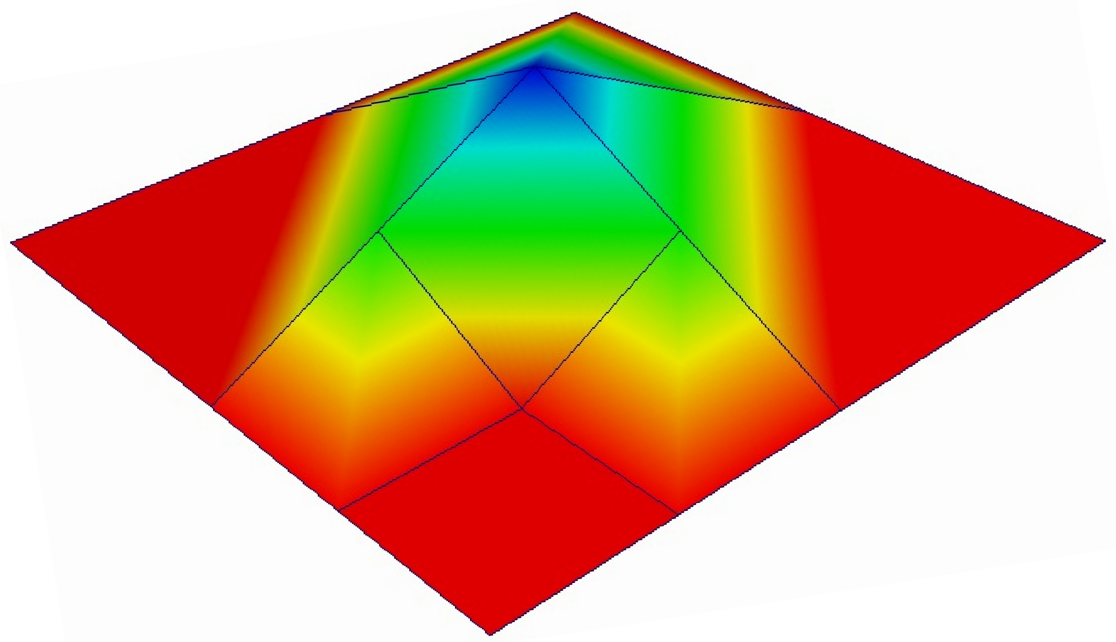
$$u_i = \sum_{j\in\mathcal{N}} c_{ij}\, u_j + b_i \quad \forall i \in \mathcal{N}_C$$

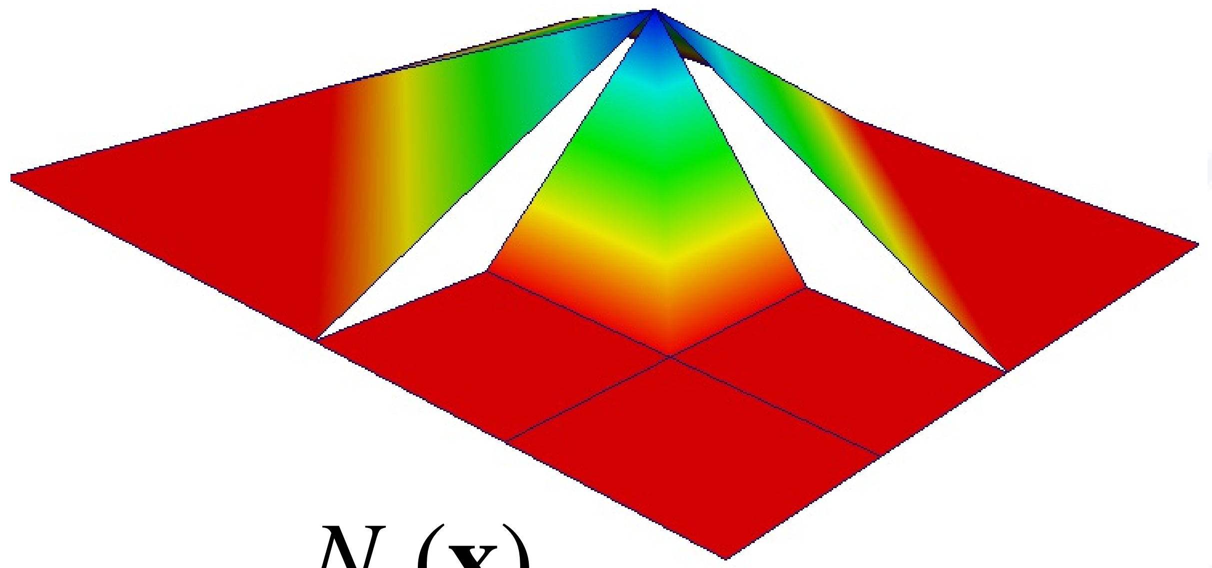
similar constraints arise from boundary conditions (normal/ tangential component) or hp-adaptive FE

Condensed shape functions

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

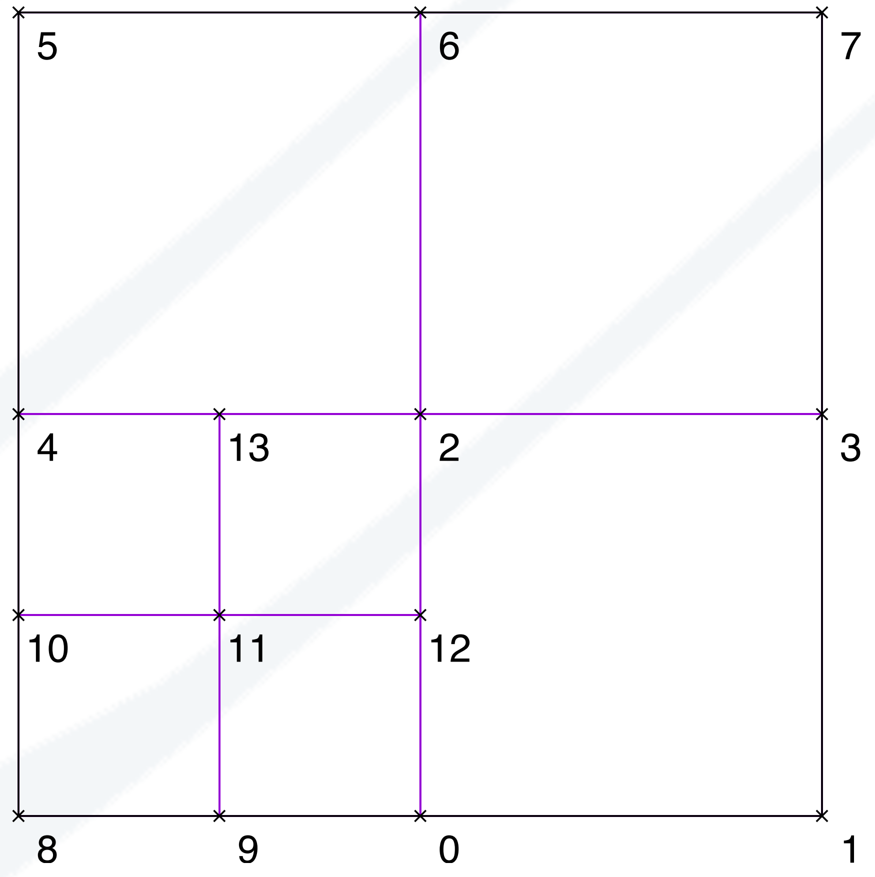
$$\widetilde{N}_2 := N_2 + \frac{1}{2}N_{13} + \frac{1}{2}N_{12}$$





$N_2(\mathbf{x})$

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



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

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

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

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

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

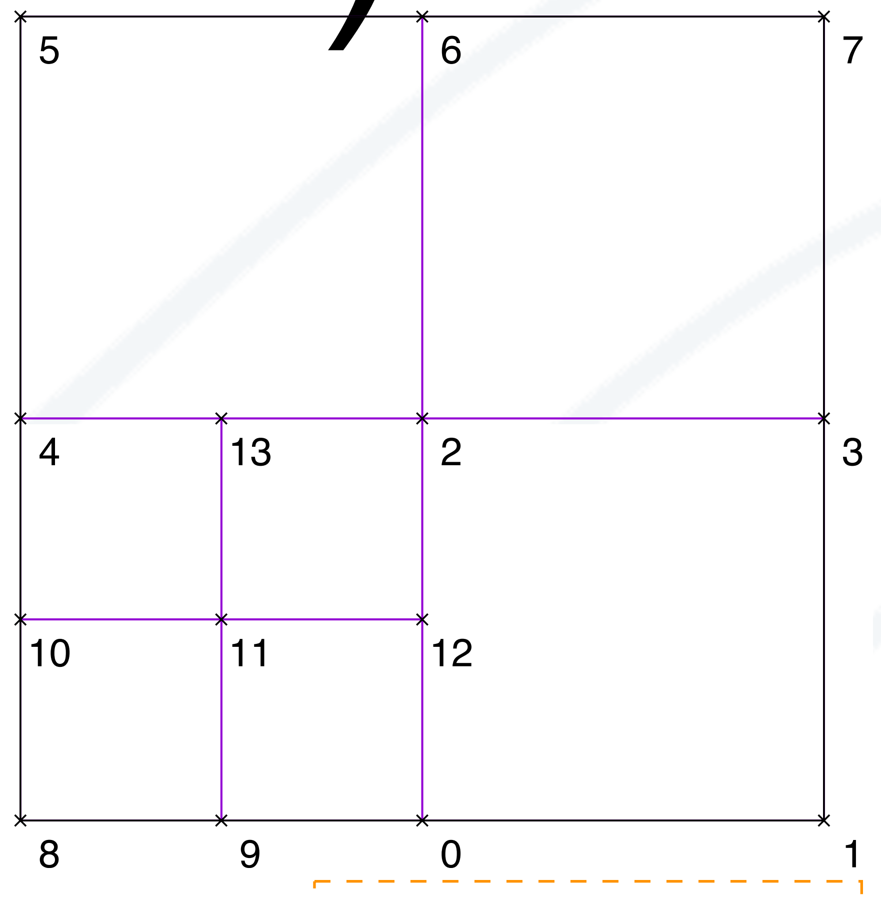
Step 3: Solve $\mathbf{K} \cdot \mathbf{u} = \mathbf{F}$

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            -3.333e-01 -1.667e-01
-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             0.000e+00  0.000e+00 -3.333e-01 -1.667e-01 -1.667e-01
-3.333e-01 -1.667e-01 -3.333e-01  1.333e+00                       -3.333e-01 -1.667e-01
 0.000e+00            -1.667e-01             1.333e+00 -1.667e-01 -3.333e-01                                  -1.667e-01 -3.333e-01            -1.667e-01
                      -3.333e-01            -1.667e-01  6.667e-01 -1.667e-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
                                                                                         6.667e-01 -1.667e-01 -1.667e-01 -3.333e-01
-1.667e-01             0.000e+00                                                        -1.667e-01  1.333e+00 -3.333e-01 -3.333e-01 -3.333e-01
                       0.000e+00            -1.667e-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                                  -3.333e-01 -3.333e-01 -3.333e-01  2.667e+00 -3.333e-01 -3.333e-01
-1.667e-01            -1.667e-01                                                                   -3.333e-01            -3.333e-01  1.333e+00 -3.333e-01
                      -1.667e-01            -1.667e-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                                             -3.333e-01            -5.000e-01  0.000e+00
-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            -1.667e-01 -1.667e-01 -6.667e-01  0.000e+00  0.000e+00
-3.333e-01 -1.667e-01 -3.333e-01  1.333e+00                       -3.333e-01 -1.667e-01
-8.333e-02            -8.333e-02             1.500e+00 -1.667e-01 -3.333e-01                                  -3.333e-01 -5.000e-01             0.000e+00
                      -3.333e-01            -1.667e-01  6.667e-01 -1.667e-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
                                                                                         6.667e-01 -1.667e-01 -1.667e-01 -3.333e-01
-3.333e-01            -1.667e-01                                                        -1.667e-01  1.333e+00 -3.333e-01 -3.333e-01  0.000e+00
                      -1.667e-01            -3.333e-01                                  -1.667e-01 -3.333e-01  1.333e+00 -3.333e-01             0.000e+00
-5.000e-01            -6.667e-01            -5.000e-01                                  -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             0.000e+00  1.333e+00  0.000e+00
                       0.000e+00             0.000e+00                                                         0.000e+00  0.000e+00  0.000e+00  1.333e+00
```

Approach 2:

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

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

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

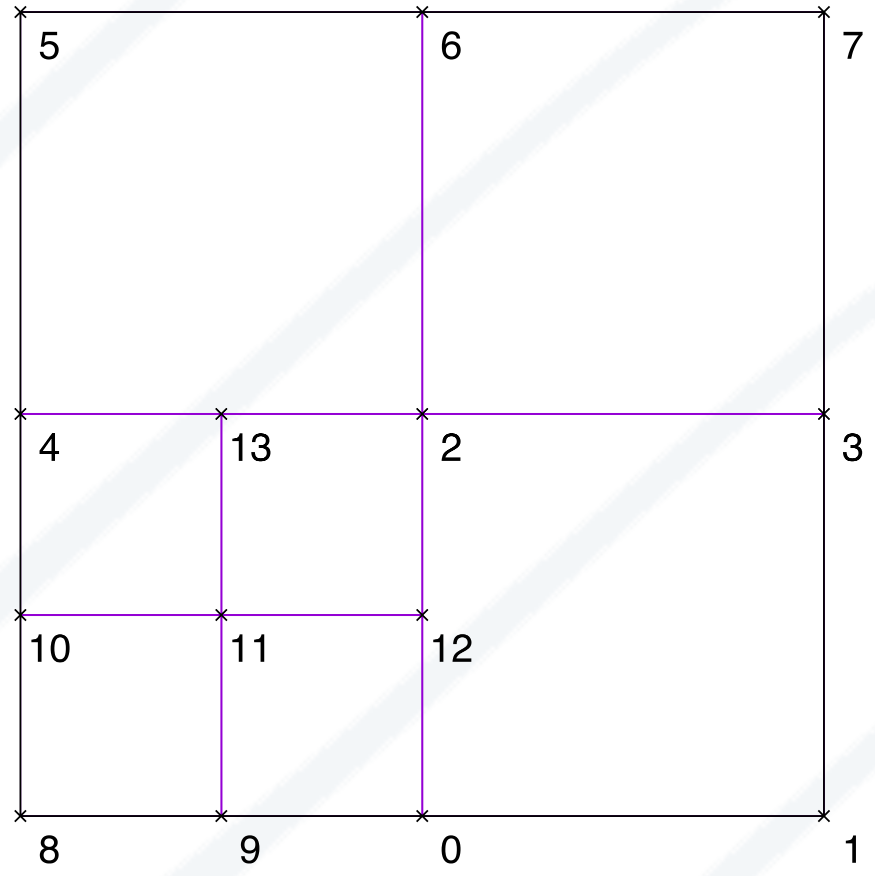
Step 2: Apply constraints during assembly operation (local-to-global) $\mathbf{K}_K, \mathbf{F}_K$

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

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

Approach 2 (example):

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




```
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================= matrix ==================
 1.500e+00 -1.667e-01 -8.333e-02 -3.333e-01 -8.333e-02                                             -3.333e-01            -5.000e-01  0.000e+00
-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            -1.667e-01 -1.667e-01 -6.667e-01  0.000e+00  0.000e+00
-3.333e-01 -1.667e-01 -3.333e-01  1.333e+00                       -3.333e-01 -1.667e-01
-8.333e-02            -8.333e-02             1.500e+00 -1.667e-01 -3.333e-01                                  -3.333e-01 -5.000e-01             0.000e+00
                      -3.333e-01            -1.667e-01  6.667e-01 -1.667e-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
                                                                                         6.667e-01 -1.667e-01 -1.667e-01 -3.333e-01
-3.333e-01            -1.667e-01                                                        -1.667e-01  1.333e+00 -3.333e-01 -3.333e-01  0.000e+00
                      -1.667e-01            -3.333e-01                                  -1.667e-01 -3.333e-01  1.333e+00 -3.333e-01             0.000e+00
-5.000e-01            -6.667e-01            -5.000e-01                                  -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             0.000e+00  1.333e+00  0.000e+00
                       0.000e+00             0.000e+00                                                        0.000e+00  0.000e+00  0.000e+00  1.333e+00
```
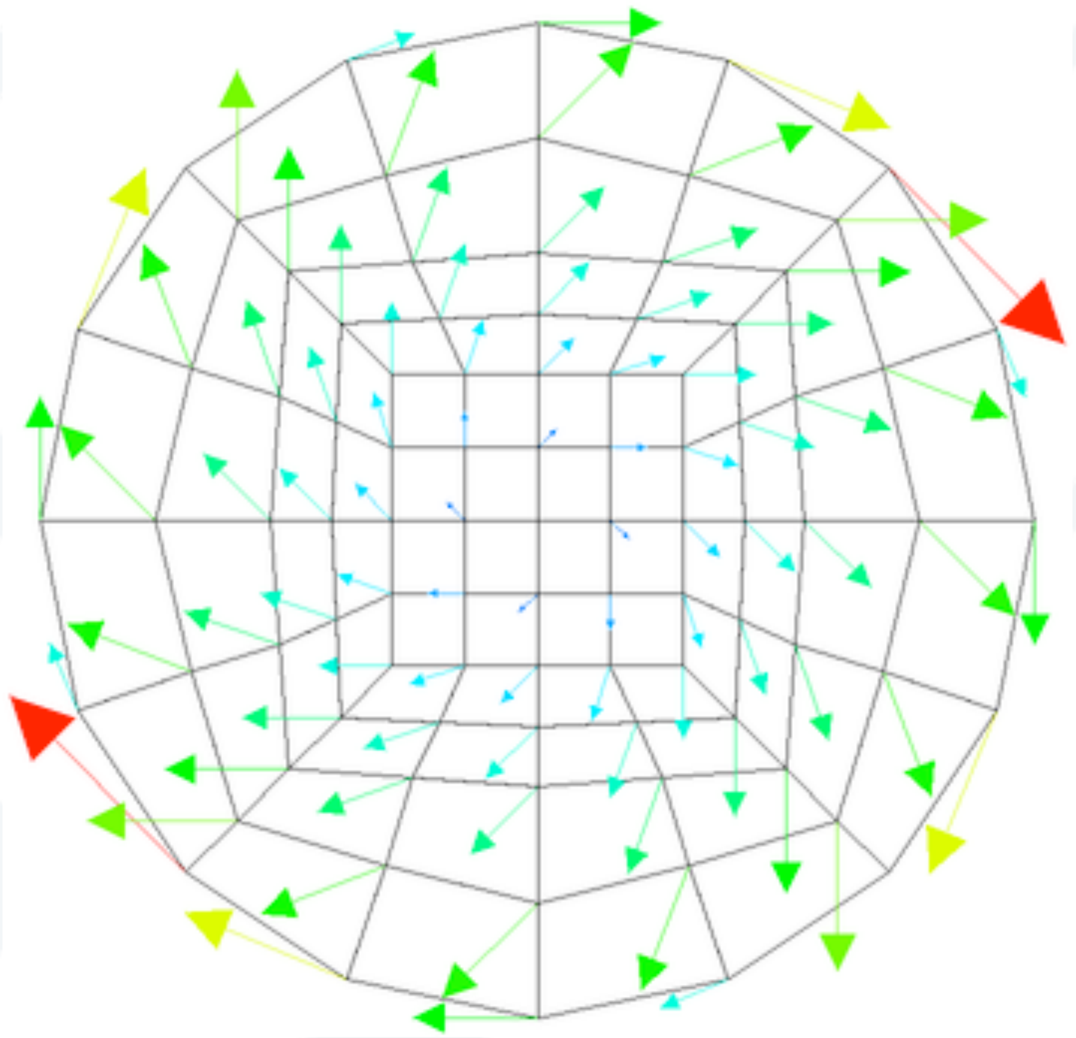

Applying constraints: the AffineConstraints class

- 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

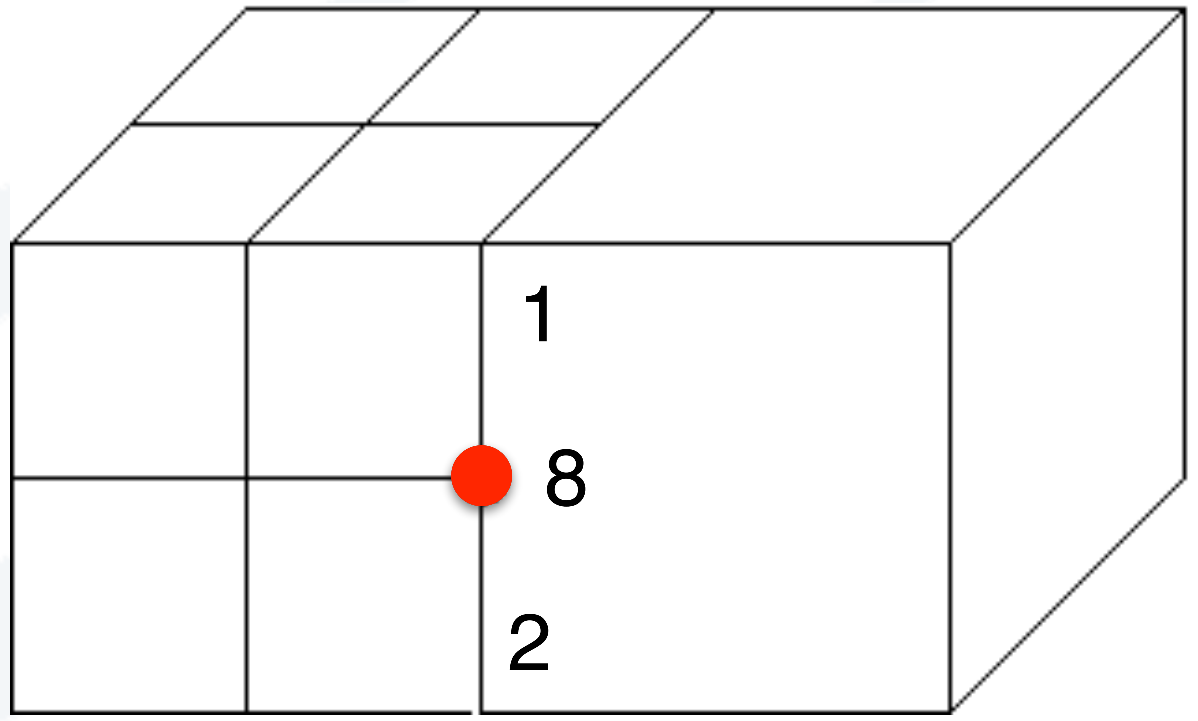
- Assembly
  - Assemble local matrix and vector as normal
  - Eliminate while transferring to global matrix:
```
constraints.distribute_local_to_global (
   cell_matrix, cell_rhs,
   local_dof_indices,
   system_matrix, system_rhs);
```
  - Solve and then set all constraint values correctly:
```
ConstraintMatrix::distribute(...)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

Applying constraints: Conflicts

- When writing into a AffineConstraints, existing constraints are not overwritten.

- Can merge constraints together:
```
constraints.merge (other_constraints,
MergeConflictBehavior::left_object_wins);
```

- Which is right? $u_8 = \bar{u}$ or
$$u_8 = \frac{1}{2}\left[u_1 + u_2\right]$$



- Careful on loops: $u_1 = u_2\ ;\ u_2 = u_3\ ;\ u_3 = u_1$