$\mathcal{H}^2$-matrix preconditioners

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Christian-Albrechts-Universität zu Kiel

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Overview

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1. $\mathcal{H}^2$-matrices
2. Algebraic operations
3. Current projects

Model problem

Darcy's equation for groundwater flow leads to

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\begin{aligned}
-\operatorname{div} K(x) \operatorname{grad} u(x) &= f(x) && \text{for all } x \in D, \\
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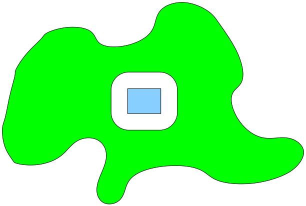
Goal: Find preconditioner $C \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}}$ reducing condition of A, then solve

$$CAx = Cb \qquad \text{or} \qquad C^{1/2}AC^{1/2}\widehat{x} = C^{1/2}b.$$

Approach: Approximate optimal preconditioner $C := A^{-1}$.

Generalized regularity result



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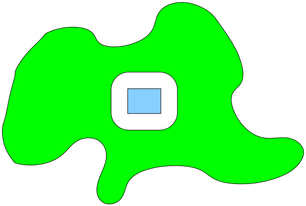

Generalized regularity result: For right-hand sides b with $\mathrm{supp}(b) \subseteq F_t$, the solution $x = A^{-1}b = Cb$ satisfies

$$x|_t \approx V_t V_t^* x|_t$$

with a low-rank isometric matrix $V_t^{t \times k}$ depending only on t.

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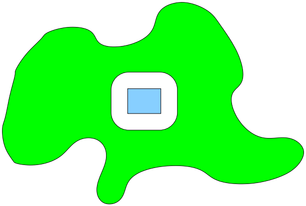

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Low-rank representation: $C|_{t\times s} \approx V_t V_t^* C|_{t\times s}$ for all $s \subseteq F_t$, i.e., for all $s \subseteq \mathcal{I}$ with $\mathrm{dist}(t,s) \geq \mathrm{diam}(t)$.

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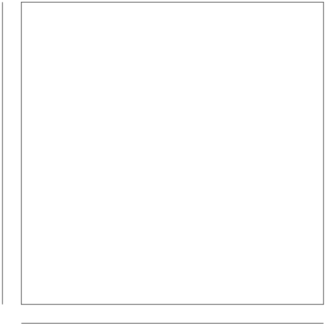
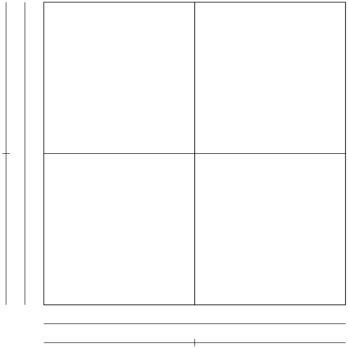
Result: We can restrict to nested bases, i.e.,

$$V_t \approx \begin{pmatrix} V_{t_1} E_{t_1} \\ V_{t_2} E_{t_2} \end{pmatrix} \qquad \text{with transfer matrices } E_{t_1}, E_{t_2} \in \mathbb{R}^{k\times k}.$$



Split matrix into admissible submatrices.

$\mathcal{H}^2$-matrix



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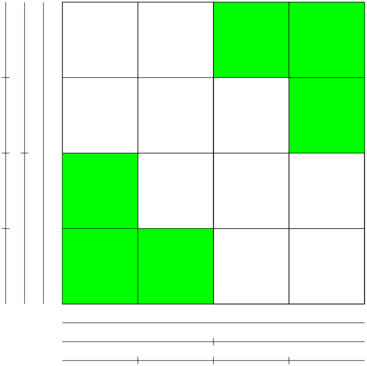

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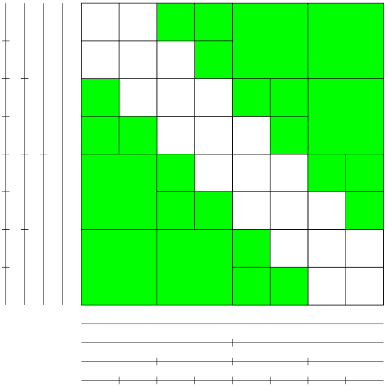

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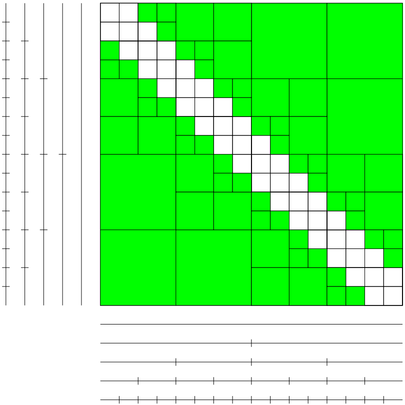

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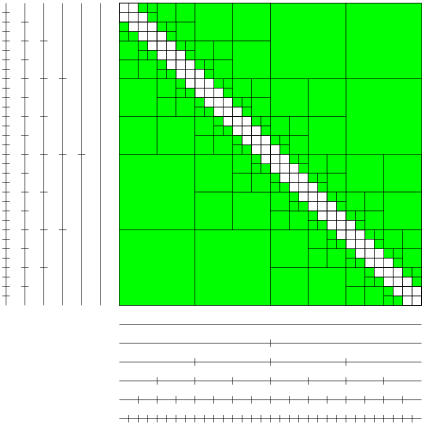

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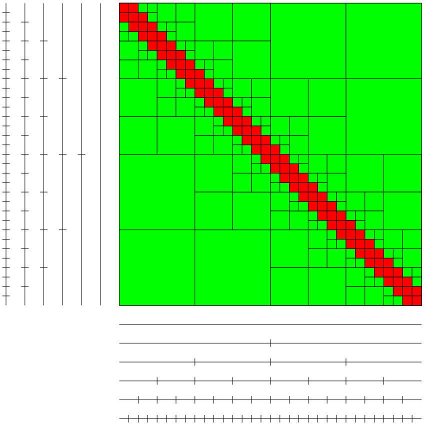

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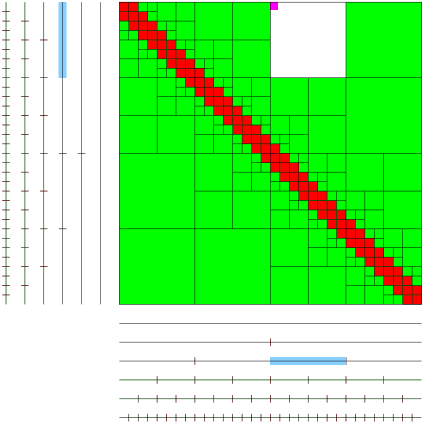

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Use factorized representation

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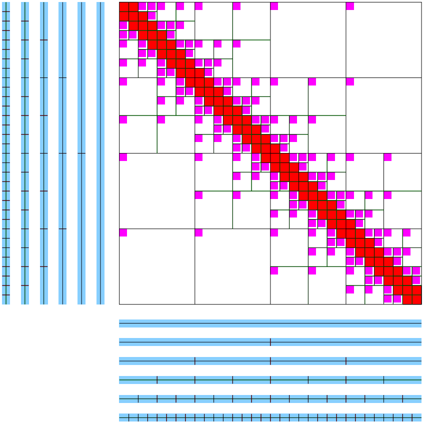

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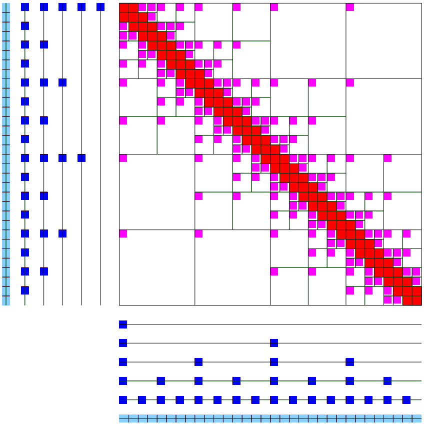

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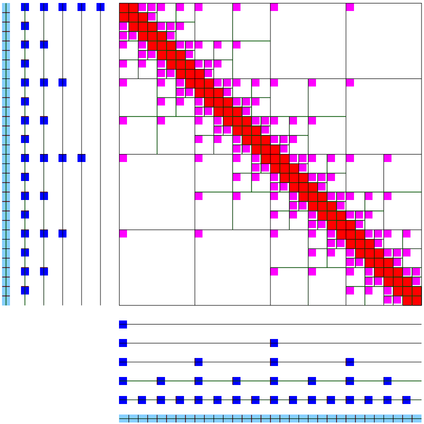

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Result: $\mathcal{O}(nk)$ units of storage, $\mathcal{O}(nk)$ operations for $x \leftarrow x + Cy$.

Overview

Goal

We know that $C = A^{-1}$ can be approximated by an $\mathcal{H}^2$-matrix.

We want to compute this approximation efficiently.

Approach:

- Express C in terms of submatrices.
- Take advantage of low-rank factorizations to reduce work.

Block inverse

Block LR factorization yields

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I & \\ A_{21}A_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix}.$$

Denoting the Schur complement by $S := A_{22} - A_{21}A_{11}^{-1}A_{12}$, we find

$$C = A^{-1} = \begin{pmatrix} A_{11}^{-1} & -A_{11}^{-1}A_{12}S^{-1} \\ & S^{-1} \end{pmatrix} \begin{pmatrix} I & \\ -A_{21}A_{11}^{-1} & I \end{pmatrix}.$$

Result: Inverse represented by products and inverses of submatrices.
Inverses of submatrices can be handled by simple recursion.
$\rightarrow$ We need an efficient matrix multiplication algorithm.

Approximation of S^{-1}: 🖹 Faustmann/Melenk/Praetorius (2013)

Matrix multiplication

Goal: Compute $A \leftarrow A + BC$.

Recursion applied if B and C are not admissible and subdivided.

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \leftarrow \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} + \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}.$$

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Low-rank case: B or C is admissible, therefore given in factorized form.

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$$A + BC = A + V_t(S_{ts} W_s^* C) = A + V_t Z^*.$$

Compute $Z = C^* W_s S_{ts}^*$ and perform low-rank update.

Low-rank update

Goal: Update $A \leftarrow A + XY^*$ with $\mathcal{H}^2$-matrix A and $X, Y \in \mathbb{R}^{\mathcal{I} \times k}$.

Observation: $A + XY^*$ is already an $\mathcal{H}^2$-matrix,
for admissible blocks $t \times s$ we have

$$(A + XY^*)|_{t \times s} = V_t S_{ts} W_s^* + X|_{t \times k} Y|_{s \times k}^* \\ = \underbrace{\begin{pmatrix} V_t & X|_{t \times k} \end{pmatrix}}_{=: \widetilde{V}_t} \underbrace{\begin{pmatrix} S_{ts} & \\ & I \end{pmatrix}}_{=: \widetilde{S}_{ts}} \underbrace{\begin{pmatrix} W_s & Y|_{s \times k} \end{pmatrix}^*}_{=: \widetilde{W}_s^*}.$$

Problem: The rank of $A + XY^*$ increases.

Recompression

Goal: Reduce the rank of $\widetilde{V}_t$ while keeping the resulting error within acceptable bounds.

Tool: Singular value decomposition

$$\widetilde{V}_t = \sum_{\nu=1}^{2k} q_\nu \sigma_\nu p_\nu^*,$$

with singular values $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{2k} \geq 0$ and orthonormal bases $\{q_1, \ldots, q_{2k}\}$ and $\{p_1, \ldots, p_{2k}\}$.

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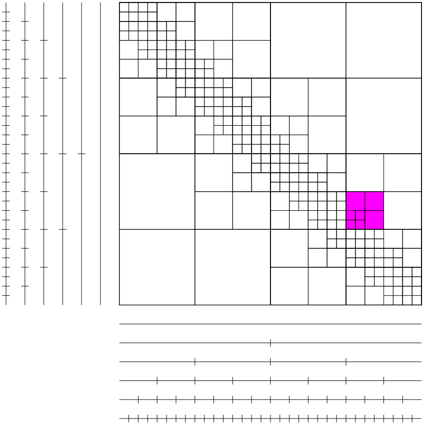
Weight matrices $\widetilde{B}_t$ used to implement error control.

Result: Low-rank update in $\mathcal{O}(nk^2)$ operations.

Local update

Goal: Update submatrix $A|_{t \times s} \leftarrow A|_{t \times s} + XY^*$.



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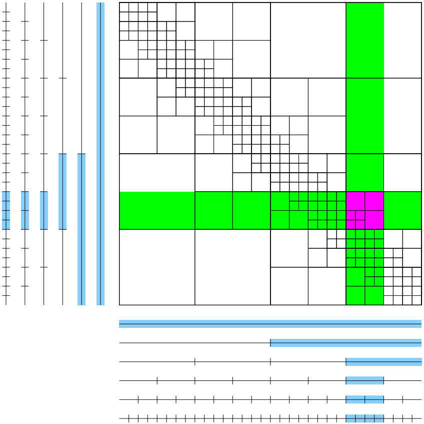
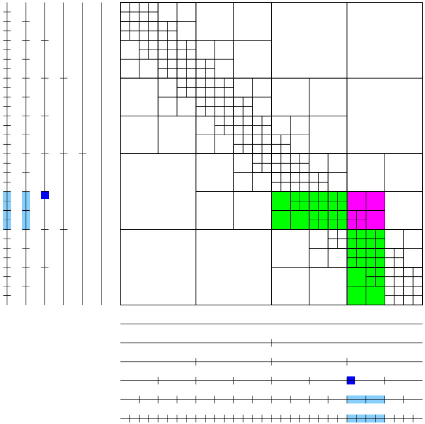


Challenge: Changing the cluster bases V_t, W_s influences other blocks.

Local update

Goal: Update submatrix $A|_{t\times s} \leftarrow A|_{t\times s} + XY^*$.

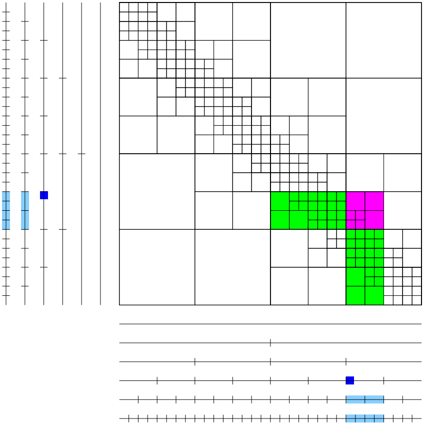


Challenge: Changing the cluster bases V_t, W_s influences other blocks.

Solution: We only change the transfer matrices E_t and F_s.

Local update

Goal: Update submatrix $A|_{t\times s} \leftarrow A|_{t\times s} + XY^*$.



Challenge: Changing the cluster bases V_t, W_s influences other blocks.

Solution: We only change the transfer matrices E_t and F_s.

Result: Local update takes $\mathcal{O}(k^2(\#t + \#s))$ operations.

Summary

Matrix inversion and matrix multiplication can be expressed by

- matrix-vector multiplication of k vectors by submatrix $X|_{t\times s}$,
- low-rank updates $X|_{t\times s} \leftarrow X|_{t\times s} + YZ^*$,

and simple recursion.

Both elementary operations take $\mathcal{O}(k^2(\#t + \#s))$ operations, leading to a total complexity of $\mathcal{O}(nk^2 \log n)$.

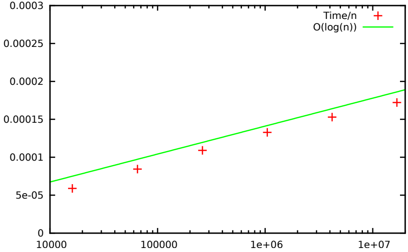
Other algebraic operations can be treated similarly, e.g.,

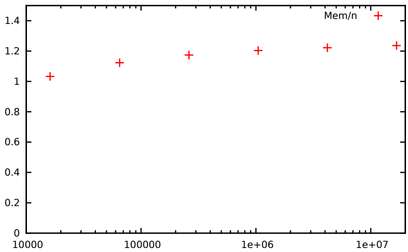
- LR factorization,
- LDL^* and Cholesky factorization,
- matrix exponential.

B./Reimer (2014)

Experiment: FEM Cholesky decomposition

Goal: Approximate Cholesky decomposition of a FEM stiffness matrix.



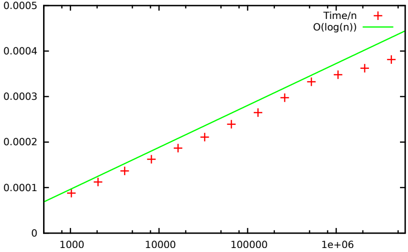


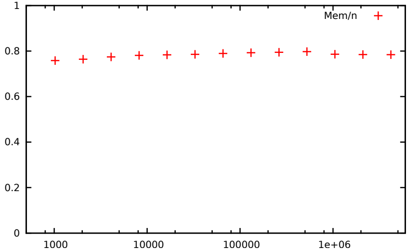
Results:

- Accuracy $\|I - \widetilde{L}^{-*}\widetilde{L}^{-1}A\|_2 \approx 0.1$.
- Factorization in $\sim n \log n$ operations.
- Storage requirements $\sim n$.

Experiment: BEM 2D Cholesky decomposition

Goal: Approximate Cholesky decomposition of a BEM stiffness matrix.



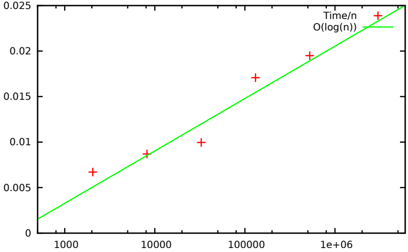


Results:

- Accuracy $\|I - \widetilde{L}^{-*}\widetilde{L}^{-1}A\|_2 \approx 0.2$.
- Factorization in $\sim n \log n$ operations.
- Storage requirements $\sim n$.

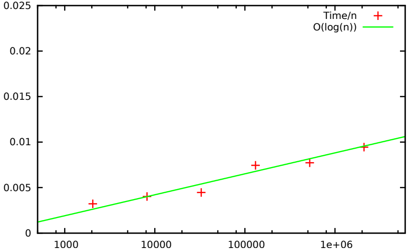
Experiment: BEM 3D Cholesky decomposition

Goal: Approximate Cholesky decomposition of a BEM stiffness matrix.



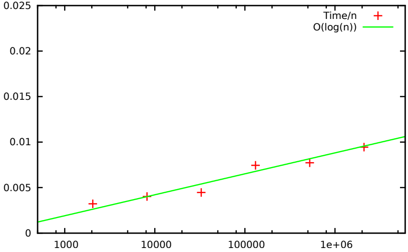
Experiment: BEM 3D Cholesky decomposition

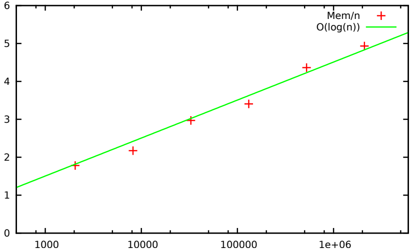
Goal: Approximate Cholesky decomposition of a BEM stiffness matrix.



Experiment: BEM 3D Cholesky decomposition

Goal: Approximate Cholesky decomposition of a BEM stiffness matrix.





Results:

- Less than 12 cg steps.
- Factorization in $\sim n \log n$ operations.
- Storage requirements $\sim n \log n$.

Overview

Stochastic PDE

Consider a domain $D \subseteq \mathbb{R}^d$ and a probability space $(\Omega, \mathcal{M}, P)$.

Model problem: Poisson's equation with stochastic loading.

$$-\Delta u(x, \omega) = f(x, \omega) \qquad \text{for all } x \in D,\ \omega \in \Omega.$$

Goal: Compute two-point correlation

$$C_u(x, y) := \int_\Omega u(x, \omega) u(y, \omega)\, dP(\omega) \qquad \text{for all } x, y \in D.$$

Approach: C_u is solution of $2d$-dimensional PDE

$$\Delta_x \Delta_y C_u(x, y) = C_f(x, y) \qquad \text{for all } x, y \in D.$$

Schwab/Todor (2003)

Matrix equation

Goal: Approximate solution of

$$\Delta_x \Delta_y C_u(x,y) = C_f(x,y) \qquad \text{for all } x,y \in D.$$

Approach: Galerkin discretization with tensor basis functions $\varphi_{ij} = \varphi_i \otimes \varphi_j$ leads to

$$AXA^* = B,$$

where A is the standard Poisson stiffness matrix.

Regularity: X can be approximated by an $\mathcal{H}^2$-matrix.

Pentenrieder/Schwab (2011)

Solver: Approximate $A^{-1}BA^{-*}$ by $\mathcal{H}^2$-matrix, e.g., by using $A \approx LR$.

For $\mathcal{H}$-matrices: Dölz/Harbrecht/Schwab (2014)

Darcy's equation

Goal: Simulate groundwater flow based on Darcy's law.

$$
\begin{aligned}
K(x)^{-1} f(x) + \nabla p(x) &= 0 && \text{for all } x \in \Omega,\\
-\nabla \cdot f(x) &= 0 && \text{for all } x \in \Omega,\\
\langle f(x), n(x) \rangle &= g(x) && \text{for all } x \in \partial\Omega.
\end{aligned}
$$

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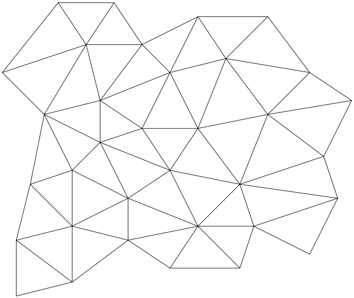
Discretization by mixed FEM:



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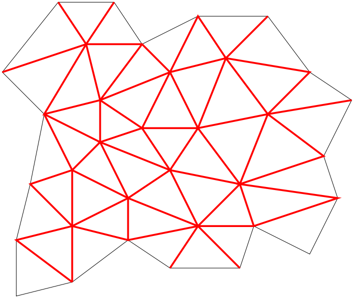
Discretization by mixed FEM:

- flux by Raviart-Thomas elements,



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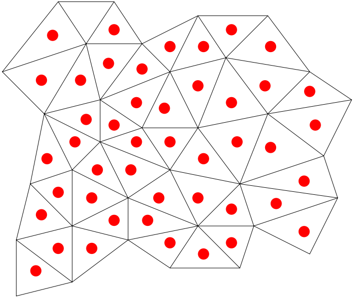
Discretization by mixed FEM:

- flux by Raviart-Thomas elements,
- pressure by piecewise constants,



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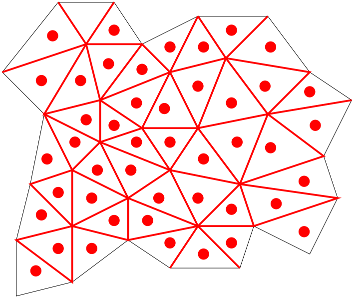
Discretization by mixed FEM:

- flux by Raviart-Thomas elements,
- pressure by piecewise constants,
- total index set $\mathcal{I} = \mathcal{I}_f \cup \mathcal{I}_p$.



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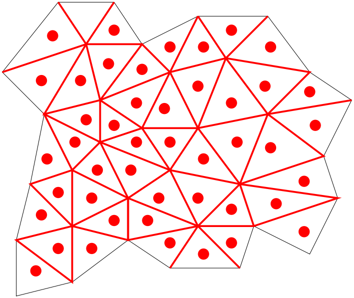
- total index set $\mathcal{I} = \mathcal{I}_f \cup \mathcal{I}_p$.

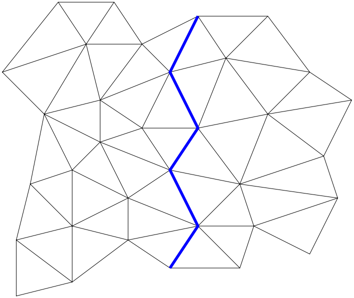
$$\begin{pmatrix} M & B^* \\ B & \end{pmatrix} \begin{pmatrix} f \\ p \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix}$$



Domain decomposition clustering

Goal: Construct cluster tree ensuring that sub-problems are well-posed Darcy systems.

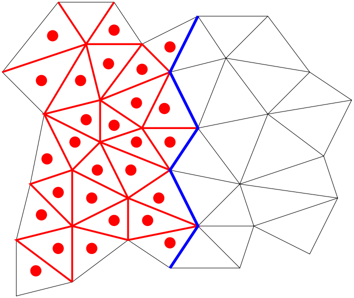
$$\begin{pmatrix} & & \\ & & \\ & & M_{33} \end{pmatrix}$$



Domain decomposition clustering

Goal: Construct cluster tree ensuring that sub-problems are well-posed Darcy systems.

$$\begin{pmatrix} M_{11} & B_{11}^* & & \\ B_{11} & & & \\ & & & \\ & & & M_{33} \end{pmatrix}$$



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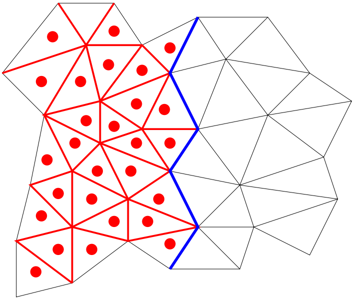
$$\begin{pmatrix} M_{11} & B_{11}^* & & M_{13} \\ B_{11} & & & B_{13} \\ & & & \\ M_{31} & B_{13}^* & & M_{33} \end{pmatrix}$$



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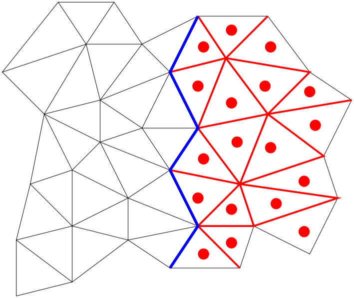

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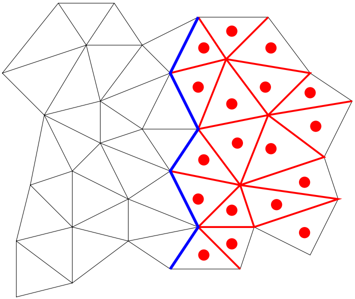
$$\begin{pmatrix} M_{11} & B_{11}^* & & & M_{13} \\ B_{11} & & & & B_{13} \\ & & M_{22} & B_{22}^* & \color{red}{M_{23}} \\ & & B_{22} & & \color{red}{B_{23}} \\ M_{31} & B_{13}^* & \color{red}{M_{32}} & \color{red}{B_{23}^*} & M_{33} \end{pmatrix}$$



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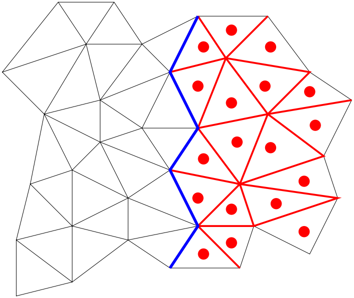

Clustering strategy: Split cluster t into separator cluster $t_0 \subseteq \mathcal{I}_f \cap t$ and domain clusters $t_1, t_2 \subseteq t$ following domain decomposition approach.

Grasedyck/Kriemann/LeBorne (2009)

Conclusion

$\mathcal{H}^2$-matrices take advantage of low-rank structure to approximate inverses and LR or Cholesky factors in $\mathcal{O}(nk)$ units of storage.

Local low-rank updates allow us to construct approximations in $\mathcal{O}(nk^2 \log n)$ operations.

Current projects: stochastic PDEs, matrix equations, saddle-point problems, parallelization.

Software package H2Lib scheduled for release in October, 2014.