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

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Overview

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Model problem

Darcy's equation for groundwater flow leads to

$$\begin{aligned} -\operatorname{div} K(x) \operatorname{grad} u(x) &= f(x) && \text{for all } x \in \Omega, \\ u(x) &= 0 && \text{for all } x \in \partial\Omega. \end{aligned}$$

with discontinuous, possibly anisotropic, permeabilities $K > 0$.

Discretization by finite element scheme leads to linear system

$$Ax = b \qquad \text{with } A \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}},\ b \in \mathbb{R}^{\mathcal{I}}.$$

Usually it is ill-conditioned, i.e., not suitable for Krylov solvers.

Goal: Find preconditioner $C \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}}$ to reduce condition number of A, then solve

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

Ideal preconditioner

Inverse matrix $C := A^{-1}$ would reduce the condition number to one.

Problem: Computing A^{-1} directly

- takes too long and
- requires too much storage.

Approach: Find an approximation of A^{-1}.

Even better: Find an approximation of an LR or Cholesky factorization, evaluate preconditioner by forward and backward substitution.

Properties of the inverse

Positivity: Even for simple examples, we have $(A^{-1})_{ij} > 0$ for all $i, j \in \mathcal{I}$.
$\rightarrow$ Cannot use sparse representation. Not even as an approximation.

Diffusion: For infinite time, the solution y of the vector-valued ODE

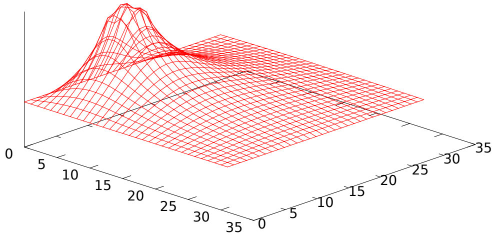
$$y'(t) = b - Ay(t) \qquad \text{for all } t \in \mathbb{R}$$

converges to x, i.e., $\lim_{t\to\infty} y(t) = x = A^{-1}b$.
In the continuous setting: limit of a diffusion process.

Smoothness: Diffusion processes tend to smoothe the solution, at least in the absence of driving forces.

Example: Locally smooth solution

Model problem: $K = 1$, b locally supported.



Observation: Solution increasingly smooth outside of the support of b.

Generalized regularity result

Observation: Let $t, s \subseteq \mathcal{I}$ be subsets of indices that are “geometrically far away” from each other. Then we have

$$\mathrm{supp}(b) \subseteq s \quad \Rightarrow \quad x|_t = (A^{-1}b)|_t \text{ smooth}$$

Idea: Smooth functions can be approximated by polynomials, i.e., in a low-dimensional space $\mathcal{V}$.

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Generalization: This property also holds (with a different space $\mathcal{V}$) for non-smooth and anisotropic coefficient functions K.

Hackbusch/Bebendorf (2003), B. (2010), Faustmann/Melenk/Praetorius (2013)

Low-rank matrices

Generalized regularity: If $t, s \subseteq \mathcal{I}$ are "far away" from each other, we can find a subspace $\mathcal{V} \subseteq \mathbb{R}^t$ of low dimension k such that

$$\operatorname{supp}(b) \subseteq s \quad \Rightarrow \quad x|_t \approx \widetilde{x} \in \mathcal{V}.$$

Projection: Choose orthogonal $V \in \mathbb{R}^{t \times k}$ with $\operatorname{range}(V) = \mathcal{V}$, then VV^* is the orthogonal projection into $\mathcal{V}$ and we have

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Result: $A^{-1}|_{t\times s} \approx V(V^* A^{-1}|_{t\times s})$, rank-$k$ approximation.

Overview

Factorization

Farfield of a set $t \subseteq \mathcal{I}$ given by

$$\mathrm{far}(t) := \{j \in \mathcal{I} \ : \ \mathrm{dist}(j, t) \geq \mathrm{diam}(t)\}.$$

Generalized regularity: For $t, s \subseteq \mathcal{I}$ we find orthogonal V_t, W_s such that

$$A^{-1}|_{t \times \mathrm{far}(t)} \approx V_t V_t^* A^{-1}|_{t \times \mathrm{far}(t)}, \qquad A^{-1}|_{\mathrm{far}(s) \times s} \approx A^{-1}|_{\mathrm{far}(s) \times s} W_s W_s^*.$$

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$$A^{-1}|_{t \times s} \approx V_t V_t^* A^{-1}|_{t \times s} W_s W_s^* = V_t S_{ts} W_s^*, \qquad S_{ts} \in \mathbb{R}^{k \times k}.$$

Nested bases

Generalized regularity: Consider $t' \subseteq t \subseteq \mathcal{I}$.
Let orthogonal matrices $V_{t'}$, V_t be given as before. We have

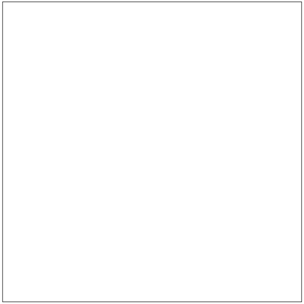
$$A^{-1}|_{t\times \mathrm{far}(t)} \approx V_t V_t^* A^{-1}|_{t\times \mathrm{far}(t)},$$
$$A^{-1}|_{t'\times \mathrm{far}(t')} \approx V_{t'} V_{t'}^* A^{-1}|_{t\times \mathrm{far}(t')}.$$

Restrict to t' and use $\mathrm{far}(t) \subseteq \mathrm{far}(t')$ to get

$$A^{-1}|_{t'\times \mathrm{far}(t)} \approx V_t|_{t'\times k} V_t^* A^{-1}|_{t\times \mathrm{far}(t)},$$
$$A^{-1}|_{t'\times \mathrm{far}(t)} \approx V_{t'} V_{t'}^* A^{-1}|_{t'\times \mathrm{far}(t)}.$$

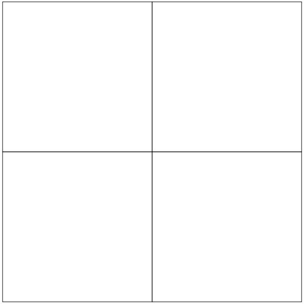
Result: Assume $V_t|_{t'\times k} = V_{t'} E_{t',t}$ with transfer matrix $E_{t',t} \in \mathbb{R}^{k\times k}$.

Block structure



Start with entire matrix.

Block structure



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Split into submatrices,

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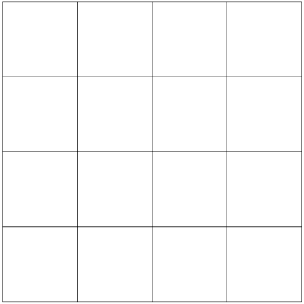

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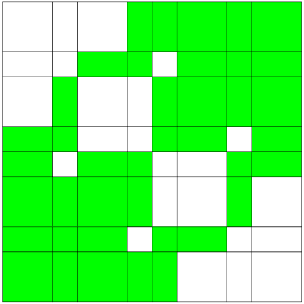

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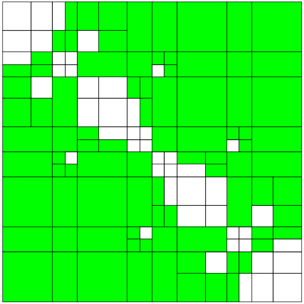

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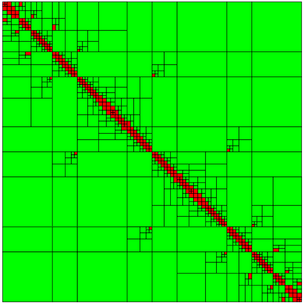

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Split into submatrices,
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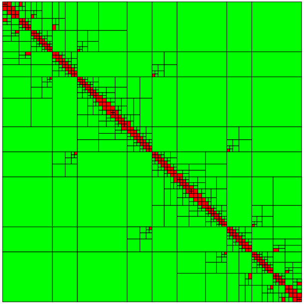
until remaining matrices small enough.

Block structure



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Result:

- Hierarchy of clusters $t \subseteq \mathcal{I}$.
- Hierarchy of blocks $t \times s \subseteq \mathcal{I} \times \mathcal{I}$.

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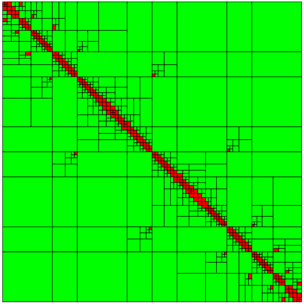

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Matrix representation:

- Farfield blocks in factorized form $A^{-1}|_{t \times s} \approx V_t S_{ts} W_s^*$.
- Nearfield blocks are small, stored in standard form.
- Cluster bases V_t and W_s in nested form.

$\rightarrow \mathcal{H}^2$-matrix representation, $\mathcal{O}(nk)$ units of storage instead of n^2.

Overview

Goal

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

We want to compute this approximation efficiently.

Approach:

- Express A^{-1} 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

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

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.

Matrix multiplication

Goal: Update $A \leftarrow A + BC$ with $A \in \mathbb{R}^{t \times r}$, $B \in \mathbb{R}^{t \times s}$ and $C \in \mathbb{R}^{s \times r}$.

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.

$$A + BC = A + V_t \; S_{ts} W_s^* C$$

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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 $A \in \mathcal{H}^2(V, W)$ 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

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

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 $\mathcal{O}(k^2(\#t + \#s))$ 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 $\mathcal{O}(nk^2 \log n)$.

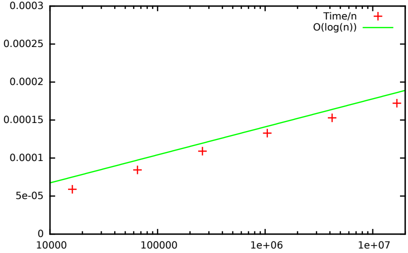
Other algebraic operations can be treated similarly, e.g.,

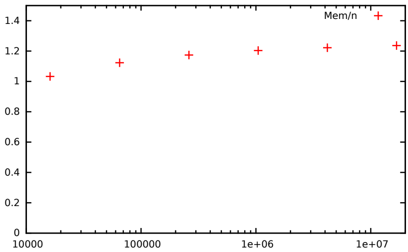
- LR factorization,
- LDL^* and Cholesky factorization,
- matrix exponential.

Grasedyck/Hackbusch (2003), 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 $\sim n$.

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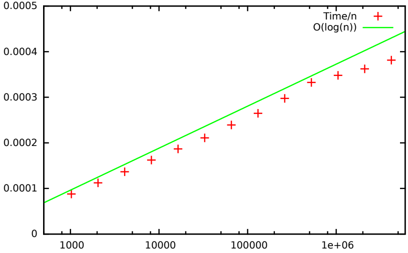

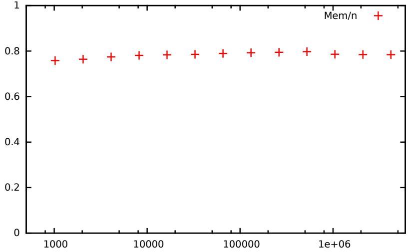

Results:

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

Overview

Eigenvalue problems

Goal: Compute *m*-th eigenvalue of a symmetric matrix *A*.

Approach: Slicing the spectrum.

1. Start with an interval $[\alpha, \beta]$ containing the eigenvalue.
2. Check how many eigenvalues are less than $\gamma := (\alpha + \beta)/2$.
3. Repeat for $[\alpha, \gamma]$ or $[\gamma, \beta]$.

Parlett (1980)

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Higher efficiency: Replace exact factorization by $\mathcal{H}^2$-approximation computed in $\mathcal{O}(n \log n)$ operations.

Parlett (1980), Benner/B./Mach/Reimer (2014)

Experiment: FEM eigenvalues

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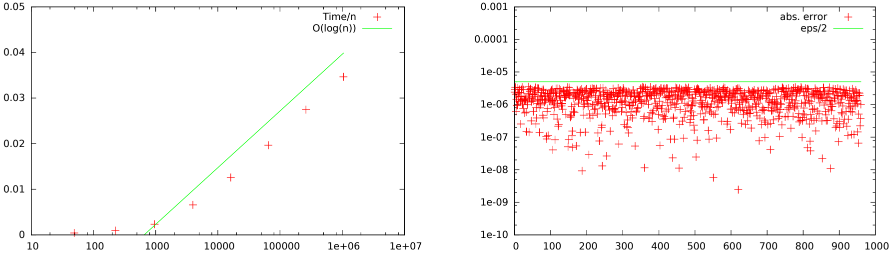

Results:

- One slice takes $\sim n \log n$ operations.
- Prescribed accuracy guaranteed for all eigenvalues.

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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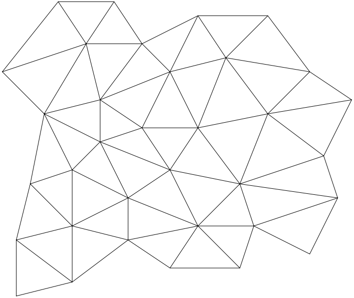
Discretization by mixed FEM:



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,\\
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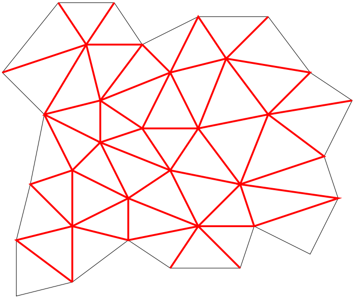
Discretization by mixed FEM:

- flux by Raviart-Thomas elements,



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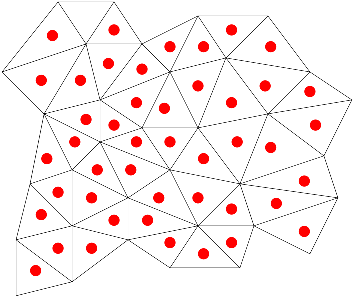
$$

Discretization by mixed FEM:

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



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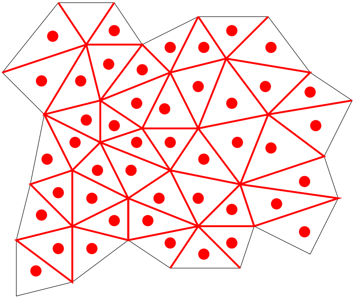
Discretization by mixed FEM:

- 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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Discretization by mixed FEM:

- flux by Raviart-Thomas elements,
- pressure by piecewise constants,
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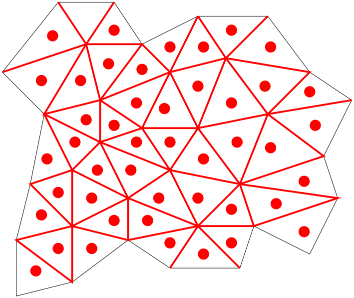
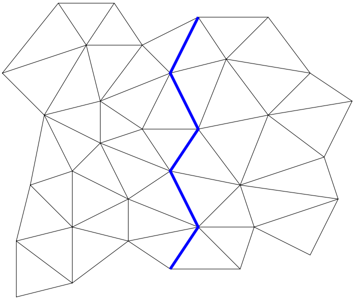
$$
\begin{pmatrix} M & B^* \\ B & \end{pmatrix} \begin{pmatrix} f \\ p \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix}
$$



Domain decomposition clustering

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

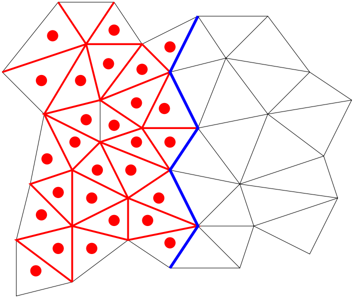
$$\begin{pmatrix} & & \\ & & \\ & & M_{33} \end{pmatrix}$$



Domain decomposition clustering

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

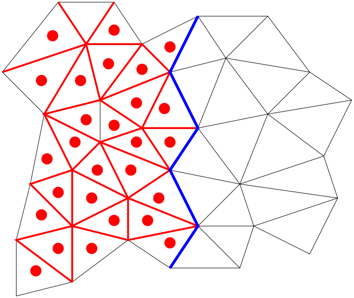
$$\begin{pmatrix} M_{11} & B_{11}^* & & \\ B_{11} & & & \\ & & & \\ & & & M_{33} \end{pmatrix}$$



Domain decomposition clustering

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

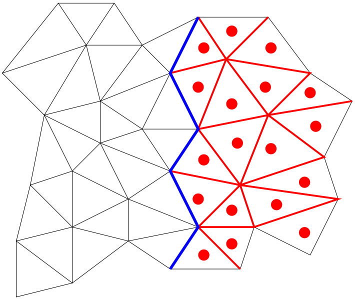
$$\begin{pmatrix} M_{11} & B_{11}^* & & M_{13} \\ B_{11} & & & B_{13} \\ & & & \\ M_{31} & B_{13}^* & & M_{33} \end{pmatrix}$$



Domain decomposition clustering

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

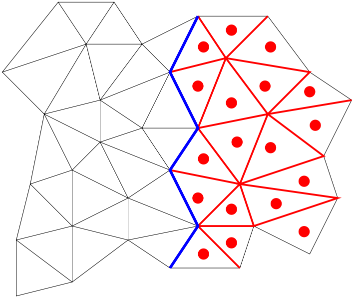
$$\begin{pmatrix} M_{11} & B_{11}^* & & & M_{13} \\ B_{11} & & & & B_{13} \\ & & M_{22} & B_{22}^* & \\ & & B_{22} & & \\ M_{31} & B_{13}^* & & & M_{33} \end{pmatrix}$$



Domain decomposition clustering

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

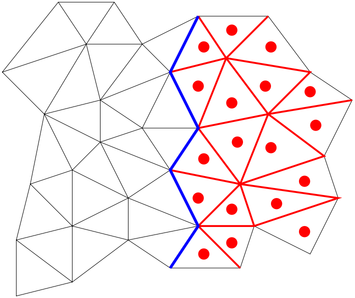
$$\begin{pmatrix} M_{11} & B_{11}^* & & & M_{13} \\ B_{11} & & & & B_{13} \\ & & M_{22} & B_{22}^* & \color{red}{M_{23}} \\ & & B_{22} & & \color{red}{B_{23}} \\ M_{31} & B_{13}^* & \color{red}{M_{32}} & \color{red}{B_{23}^*} & M_{33} \end{pmatrix}$$



Domain decomposition clustering

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

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



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.

Applications to preconditioners, symmetric eigenvalue problems and saddle-point problems.

Software package H2Lib scheduled for release in October, 2014.