Adaptive Fast Boundary Element Methods in Industrial Applications

Söllerhaus, October 2nd, 2004.

Efficient Update of Hierarchical Matrices

joint work with L. Grasedyck, W. Hackbusch and S. Le Borne

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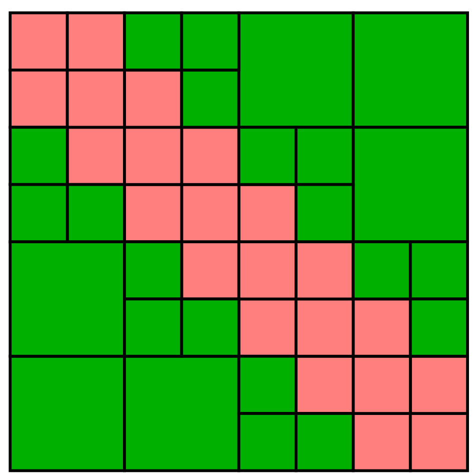
- Concept of hierarchical (or $\mathcal{H}$-) matrices
- Motivation for update of $\mathcal{H}$-matrices
- Update algorithm
- Numerical results

Properties of $\mathcal{H}$-Matrices

- $\mathcal{H}$-matrix is an approximation of full matrix that e.g. arises from discretisation of integral operator.
- $\mathcal{H}$-matrices have a block structure - each block is either rank k (`Rk`) or dense (`full`) matrix.
- With $\mathcal{H}$-matrices is possible to perform matrix operations (MVM,MM,Inv) with almost linear complexity.



Some construction remarks

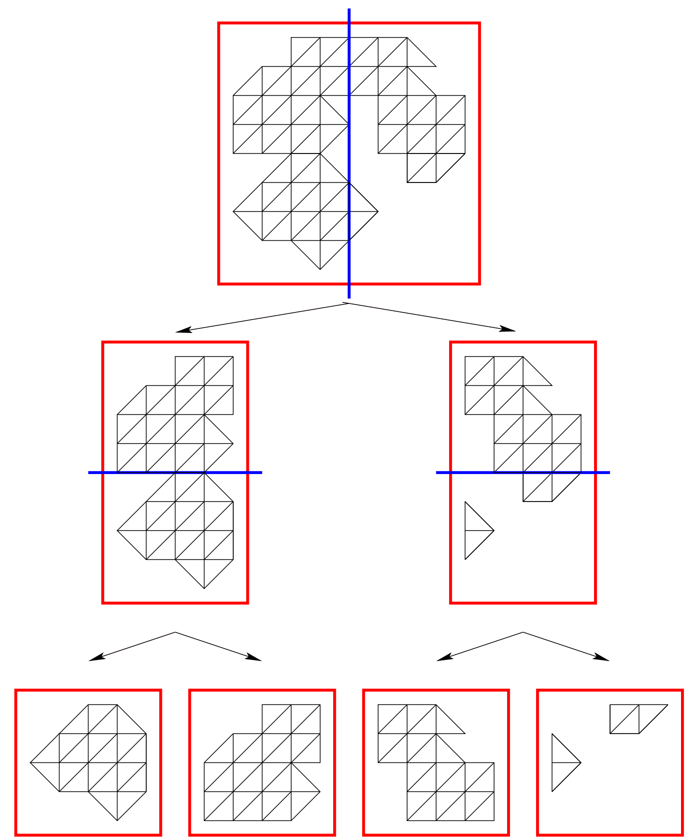
- $\mathcal{H}$-matrices are based on the given block cluster tree $T_{\mathcal{I}\times\mathcal{I}}$.
- The block cluster tree $T_{\mathcal{I}\times\mathcal{I}}$ is constructed using the cluster tree $T_{\mathcal{I}}$ (and an admissibility condition).
- The cluster tree $T_{\mathcal{I}}$ is determined and based on a partitioned grid τ and an index set $\mathcal{I}$.

In general: $\#$Basis functions $= |\mathcal{I}|$.
Example: Piece-wise constant ansatz leads to the $|\tau| = |\mathcal{I}|$.

Geometrically regular clustering

Compute a box, that contains the whole domain to whom grid τ belongs.

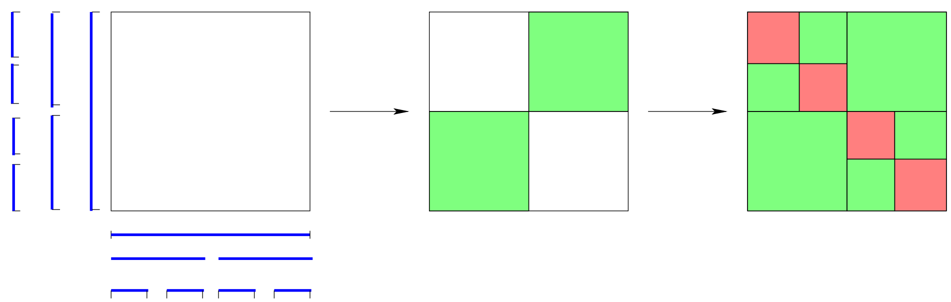
1. Determine the maximal extent.
2. Split box in that direction.
3. Repeat the process as long as it is necessary.



Remark: This clustering routine is independent of the grid.

Given: cluster tree $T_{\mathcal{I}}$ with root $\mathcal{I} = \{1, \ldots, n\}$

Seeking: block cluster tree $T_{\mathcal{I}\times\mathcal{I}}$

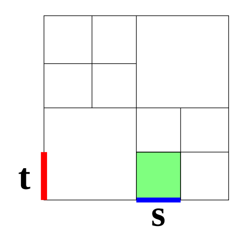


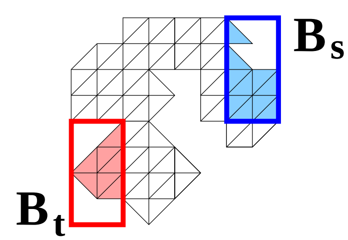
Start: $\mathcal{I} \times \mathcal{I}$. Iterate: subdivide inadmissible blocks:

$$\mathrm{sons}(t \times s) := \mathrm{sons}(t) \times \mathrm{sons}(s).$$

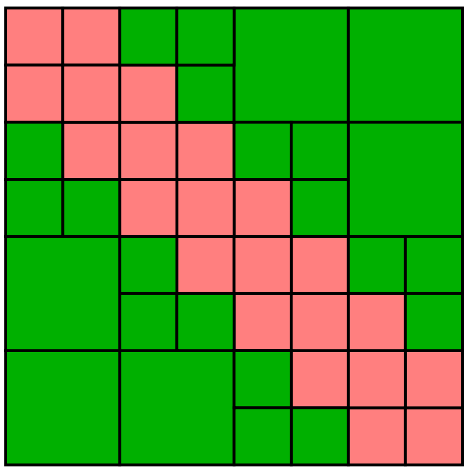
Admissibility condition:

$\min(\mathrm{diam}(B_t), \mathrm{diam}(B_s)) \leq \eta \, \mathrm{dist}(B_t, B_s)$

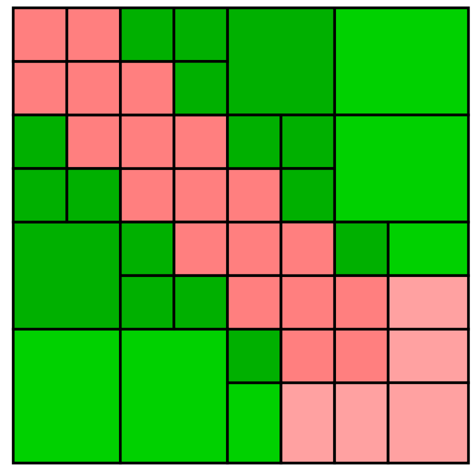




The grid τ **locally refined**
Cluster tree $T_{\mathcal{I}}$, based on $\mathcal{I}$.
Matrix $G \in \mathcal{H}(T_{\mathcal{I}\times\mathcal{I}}, k)$.



Grid τ' is obtained.
Cluster tree $T_{\mathcal{I}'}$, based on $\mathcal{I}'$.
Matrix $G' \in \mathcal{H}(T_{\mathcal{I}'\times\mathcal{I}'}, k)$.



Question: Can G be **used** in the construction of the G', an $\mathcal{H}$-matrix that corresponds to the refined grid τ'?

Idea: **Recycle** the $\mathcal{H}$-matrix instead of constructing new one = **Update** of $\mathcal{H}$-matrix.

$\mathcal{H}$-Matrix Update Algorithm

Let $G \in \mathcal{H}(T_{\mathcal{I}\times\mathcal{I}}, k)$ be an $\mathcal{H}$-matrix. Update of G can be done in three steps:

- Update of cluster tree $T_{\mathcal{I}}$ (removing old and adding new indices in tree).
- Update of block cluster tree $T_{\mathcal{I}\times\mathcal{I}}$ using already changed cluster tree $T_{\mathcal{I}}$.
- Update of `Rk` and `full` matrix blocks from G.

- τ' is the grid obtained after local refinement of the grid τ.
- $\mathcal{I}'$ is an index set that corresponds to the grid τ'.
- For $\mathcal{I}'$ there holds:

$$\mathcal{I}' = (\mathcal{I} \setminus \mathcal{I}_{out}) \quad \dot{\cup} \quad \mathcal{I}_{in}$$

- $\mathcal{I}_{out} \subset \mathcal{I}$ is the set of indices that have to be removed from $\mathcal{I}$.
- $(\mathcal{I} \setminus \mathcal{I}_{out})$ is the set of indices that correspond to the unchanged basis functions.
- $\mathcal{I}_{in}$ is the set of indices, that correspond to the new basis functions.

Update of the cluster tree

The cluster tree $T_{\mathcal{I}'}$ that corresponds to the refined grid τ' can be represented as

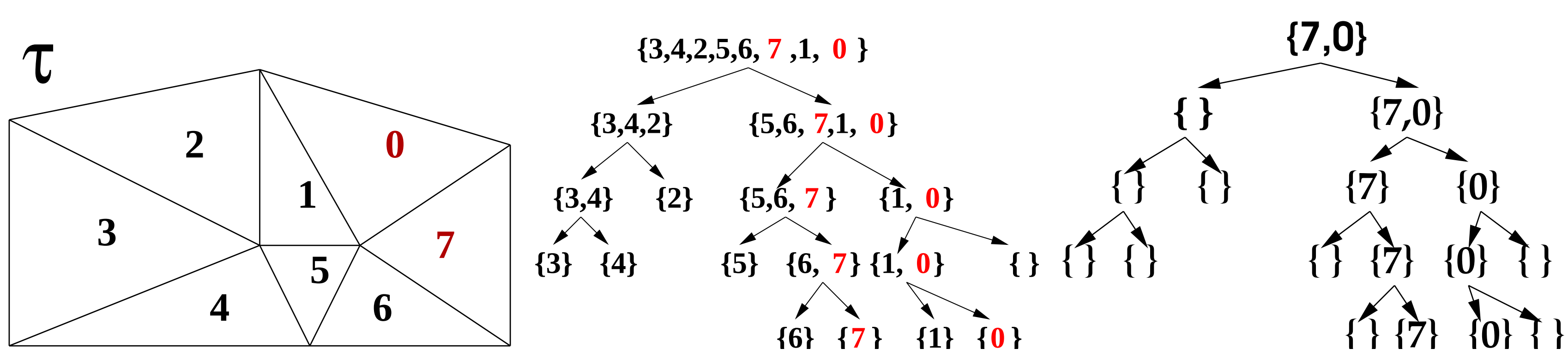
$$T_{\mathcal{I}'} = (T_{\mathcal{I}} \setminus T_{\mathcal{I}_{out}}) \quad \cup \quad T_{\mathcal{I}_{in}}$$

where $T_{\mathcal{I}_{out}}, T_{\mathcal{I}_{in}}$ are the cluster trees that correspond to the index sets $\mathcal{I}_{out}$ and $\mathcal{I}_{in}$.

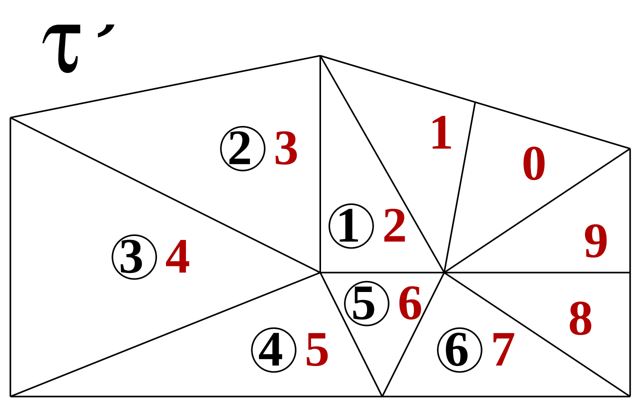
Problem: How to construct those cluster trees?

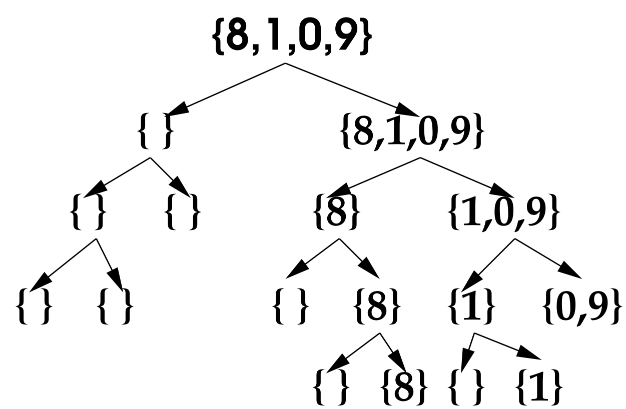
The algorithm that describes the construction (not clustering) of the tree $T_{\mathcal{I}'}$ has the following steps:

1a.**Construct** the cluster tree $T_{\mathcal{I}_{out}}$ as **index reproduction** of the given cluster tree $T_{\mathcal{I}}$.

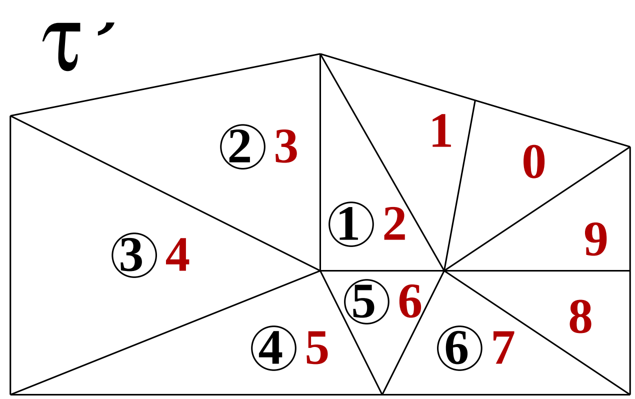


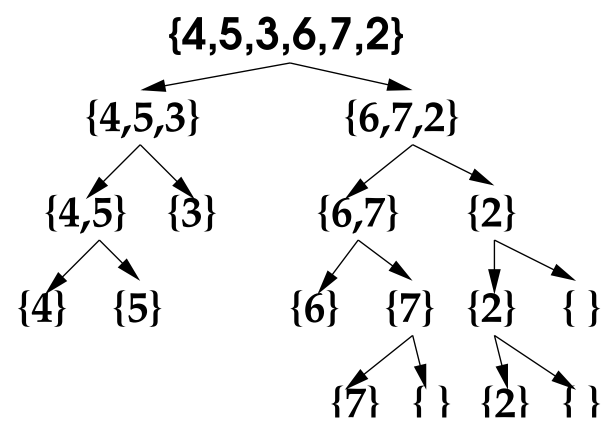
1b.**Construct** the cluster tree $T_{\mathcal{I}_{in}}$ as **bounding box reproduction** of the given cluster tree $T_{\mathcal{I}}$.





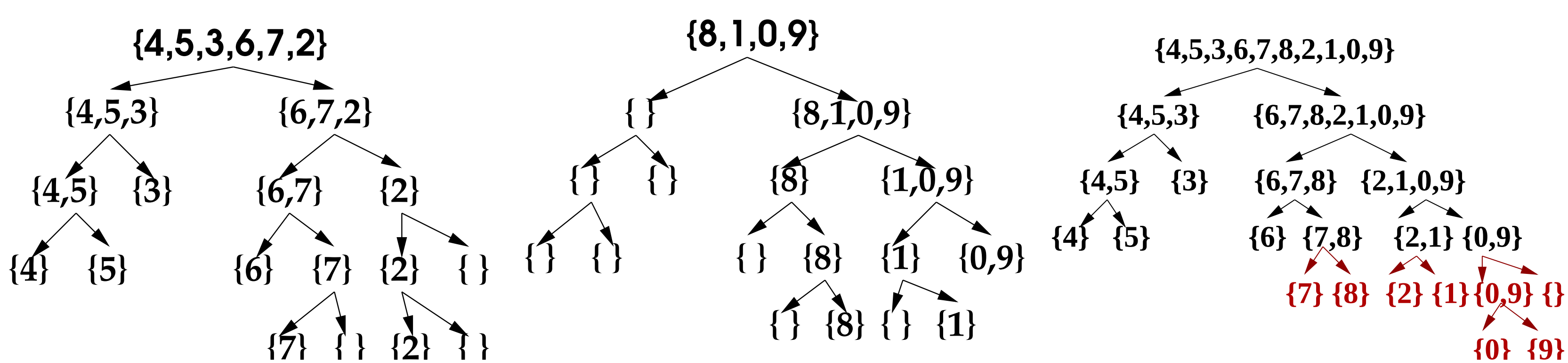
2. **Restrict** the cluster tree $T_{\mathcal{I}}$. The result is the cluster tree $(T_{\mathcal{I}} \setminus T_{\mathcal{I}_{out}})$.





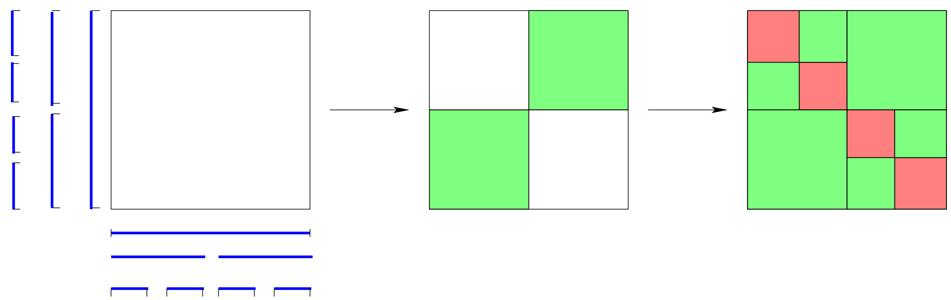
3. Do a **fusion** (union) of the trees $T_{\mathcal{I}} \setminus T_{\mathcal{I}_{out}}$ and $T_{\mathcal{I}_{in}}$. We obtain the preliminary tree $T'_{\mathcal{I}'}$, that might have some leaves whose size is greater than given n_{min}.

3a. **Subdivide** only those leaves whose size are larger than n_{min}. The final result is the tree $T_{\mathcal{I}'}$.



Given: cluster tree $T_{\mathcal{I}}$ with root $\mathcal{I} = \{1, \ldots, n\}$

Seeking: block cluster tree $T_{\mathcal{I}\times\mathcal{I}}$



Start: $\mathcal{I} \times \mathcal{I}$. Iterate: subdivide inadmissible blocks:

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Admissibility condition:
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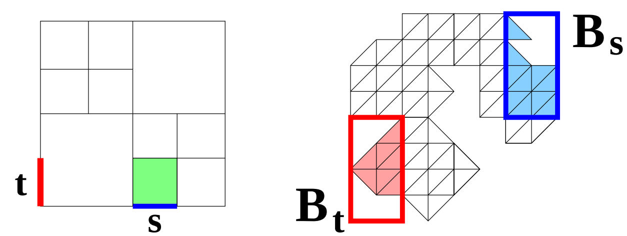
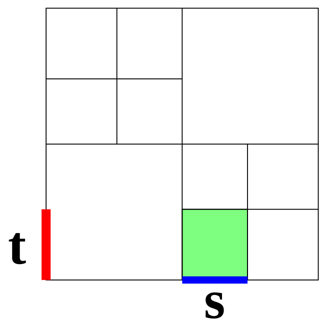


Update: Since the cluster trees $T_{\mathcal{I}}$ and $T_{\mathcal{I}'}$ have the same bounding boxes, there is one-one correspondence between block cluster trees $T_{\mathcal{I}\times\mathcal{I}}$ and $T_{\mathcal{I}'\times\mathcal{I}'}$.

Update of the $\mathcal{H}$-matrix $G \in \mathcal{H}(T_{\mathcal{I}\times\mathcal{I}}, k)$,$G' \in \mathcal{H}(T_{\mathcal{I}'\times\mathcal{I}'}, k)$

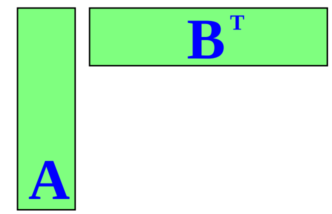
The algorithm for constructing the matrix G' (based on the block cluster tree $T_{\mathcal{I}'\times\mathcal{I}'}$) using the $\mathcal{H}$-matrix G is:

- if the leaf of the block cluster tree remained unchanged then **copy** the corresponding block matrix (`Rk` or `full` block).
- if the leaf of the block cluster tree contains all new indices than construct **new** matrix block.
- if the leaf of the block cluster tree contains some new indices **update** the corresponding block.



$$G_{ij} = \int_\Gamma \int_\Gamma \phi_i(x) g(x,y) \phi_j(y) \, \mathrm{d}\Gamma_x \mathrm{d}\Gamma_y$$

$$G|_{t\times s} \approx AB^T, A \in \mathbb{R}^{\#t\times k}, B \in \mathbb{R}^{\#s\times k}.$$



Interpolation:

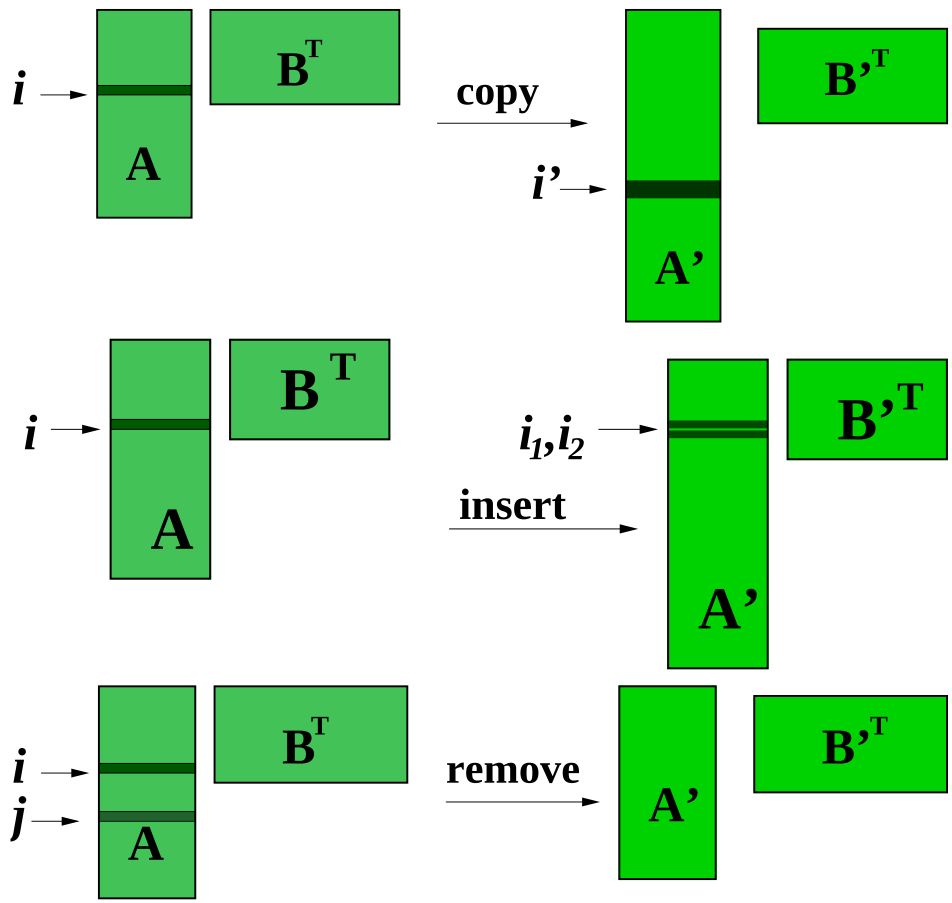
$$g(x,y) \approx \sum_{\nu=1}^{m^3} L_\nu(x) g(x_\nu, y)$$

$$A_{i\nu} = \int_\Gamma \phi_i(x) L_\nu(x) \, \mathrm{d}\Gamma_x, \quad B_{j\nu} = \int_\Gamma \phi_j(y) g(x_\nu, y) \, \mathrm{d}\Gamma_y$$

$$G'|_{t'\times s'} = A'B'^T \in \mathbb{R}^{\#t'\times\#s'}$$

$$A'_{i\nu} = \begin{cases} A_{i\nu} & i \in t \\ \int_\Gamma \phi_i(x) L_\nu(x) \, \mathrm{d}\Gamma_x & i \in t' \setminus t \end{cases}$$

$$B'_{j\nu} = \begin{cases} B_{j\nu} & j \in s \\ \int_\Gamma \phi_j(y) g(x_\nu, y) \, \mathrm{d}\Gamma_y & j \in s' \setminus s \end{cases}$$

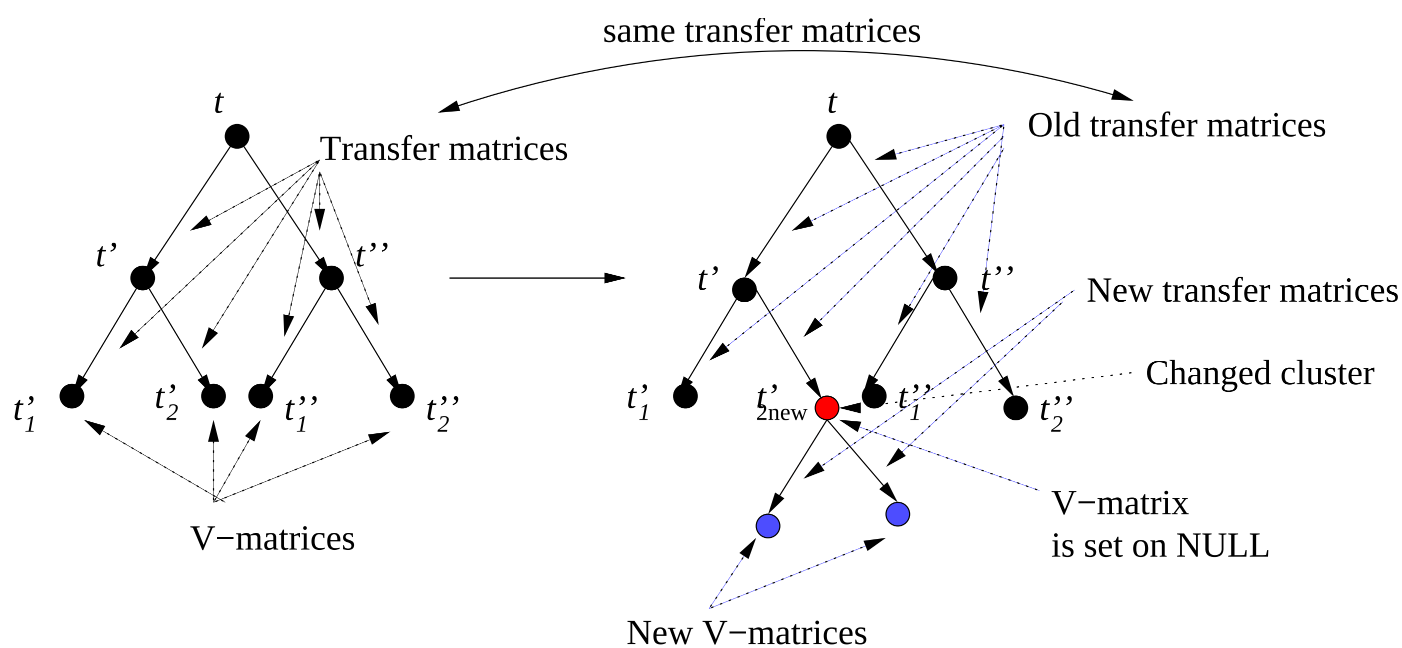

i
A
B'T
copy
i'
A'
B''T
i
A
BT
i1,i2
insert
A'
B'T
i
j
A
BT
remove
A'
B'T

$$
\begin{aligned}
\tilde{g}^{t,s}(x,y) &:= (\mathcal{J}_m^t \otimes \mathcal{J}_m^s)[g](x,y) = \sum_{\nu\in K}\sum_{\mu\in K} g(x_\nu^t, x_\mu^s)\mathcal{L}_\nu^t(x)\mathcal{L}_\mu^s(y). \\
\tilde{G}_{ij} &:= \int_\Omega \varphi_i(x) \int_\Omega \tilde{g}^{t,s}(x,y)\varphi_j(y)\,\mathrm{d}y\,\mathrm{d}x \\
&= \sum_{\nu\in K}\sum_{\mu\in K} g(x_\nu^t, x_\mu^s) \underbrace{\left(\int_\Omega \varphi_i(x)\mathcal{L}_\nu^t(x)\,\mathrm{d}x\right)}_{=V_{i\nu}^t} \underbrace{\left(\int_\Omega \varphi_j(y)\mathcal{L}_\mu^s(y)\,\mathrm{d}y\right)}_{=V_{j\mu}^s} \\
&= V^t S^{t,s} V^{s\top} \\
S_{\nu\mu}^{t,s} &:= g(x_\nu^t, x_\mu^s). \\
T_{\nu',\nu}^{t',t} &:= \mathcal{L}_\nu^t(x_{\nu'}^{t'}), \quad V^t = \begin{pmatrix} V^{t_1}\cdot T^{t_1,t} \\ V^{t_2}\cdot T^{t_2,t} \end{pmatrix}.
\end{aligned}
$$

- Matrix S depends **only** on bounding box.
- Matrices V^t depend only on the cluster but they will be computed only for the leaves.
- Transfer matrices $T^{t,t'}$ depend also only on bounding boxes.

Update of $\mathcal{H}^2$-Matrices

- $T^{t,t'}$ and S matrices need not to be updated, since bounding boxes do not change.
- V matrices are updated in the same way as Rk matrices are updated.



$$\mathcal{G}[u](x) = f(x), \quad f := \mathcal{V}\partial_n u, \quad x \in \Gamma := \partial\Omega, \Omega := [-1,1]^3$$

- $\mathcal{G}$ is the double layer potential operator
  $\mathcal{G}[u](x) = \frac{1}{2}u(x) + \frac{1}{4\pi}\int_\Gamma \frac{\langle n(y), x-y\rangle u(y)}{\|x-y\|^3} d\Gamma_y$
- $\mathcal{V}$ is the single layer potential operator
  $\mathcal{V}[u](x) := \frac{1}{4\pi}\int_\Gamma \frac{\partial_n u(y)}{\|x-y\|} d\Gamma_y$.
- $u(x) = \frac{1}{\|x-y_0\|}$, $y_0 = (1.0, 1.0, 1.001)$.
- Machine: `SUN ULTRASPARC III` with 900 MHz CPU clock rate and 150 MHz memory clock rate.

Time (in seconds) for the update of the (double-layer potential operator) $\mathcal{H}$-matrix compared to reassembly starting with n_1 degrees of freedom.

n_1 =12288	n_2 =12422	n_2 =13002	n_2 =15806
new	2.1%	10.9%	44.5%
adaptive (G')	1.02	5.76	23.16
reassembly (G'')	29.5	31.67	40.82
savings(costs)	97%(3%)	82%(18%)	44%(56%)
$\frac{\|G''-G'\|_2}{\|G''\|_2}$	6.04×10^{-16}	6×10^{-16}	5.29×10^{-16}

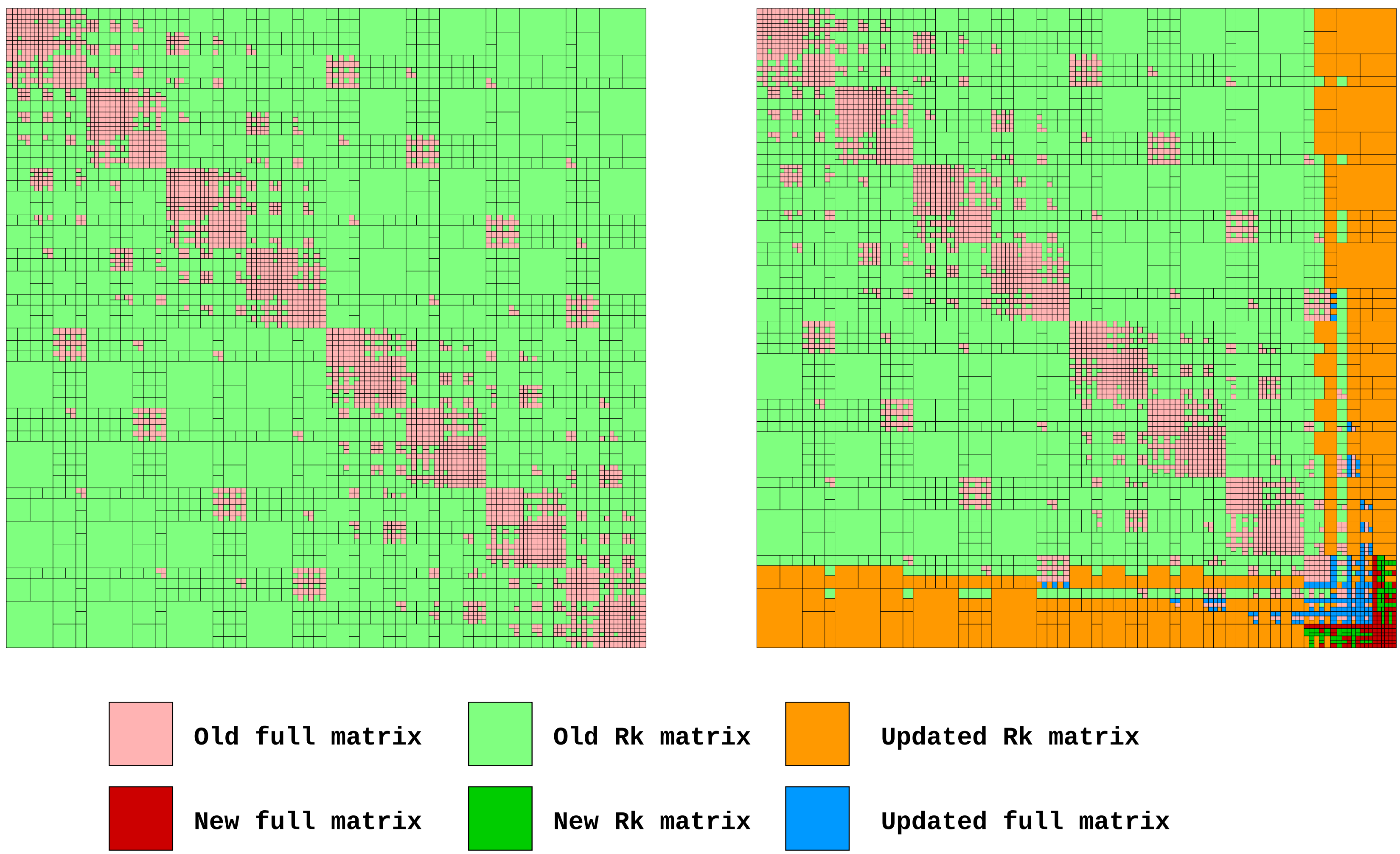
$n_1 = 49152$	n_2 =49682	n_2 =51880	n_2 =62544
new	2.1%	10.5%	42.8%
adaptive (G')	6.05	31.8	121.78
reassembly (G'')	169	209.6	252.7
savings(costs)	97%(3%)	85%(15%)	52%(48%)
$\frac{\|G''-G'\|_2}{\|G''\|_2}$	7.05×10^{-16}	7.05×10^{-16}	6.44×10^{-16}

$n_1 = 196608$	n_2 =198686	n_2 =207190	n_2 = 248290
new	2.1%	10.2%	42%
adaptive (G')	42.91	147.65	543.55
reassembly (G'')	791	875.8	1068.48
savings(costs)	95%(5%)	83%(17%)	51%(49%)
$\frac{\|G''-G'\|_2}{\|G''\|_2}$	7.90×10^{-16}	7.80×10^{-16}	4.3×10^{-16}

Time (in seconds) for the update of the $\mathcal{H}^2$-matrix compared to reassembly starting with $n_1 = 49152(196608)$ degrees of freedom.

n_1 =49152	n_2 =49676	n_2 =51734	n_2 =62462
new	2.1%	10%	42.6%
adaptive	2.3	9.5	50.1
reassembly	67.6	71	86.8
savings(costs)	97%(3%)	87%(13%)	42%(58%)

n_1 = 196608	n_2 =198672	n_2 =206754	n_2 =247984
new	2.1%	9.8 %	41.4%
adaptive	14.1	55.3	291.4
reassembly	455.6	471.2	547.2
savings (costs)	97%(3%)	88%(12%)	47%(53%)


Old full matrix
Old Rk matrix
Updated Rk matrix
New full matrix
New Rk matrix
Updated full matrix

Outlook

- $\mathcal{H}$- and $\mathcal{H}^2$-matrices can be efficiently updated.
- If `Rk` matrices are computed using ACA (Adaptive Cross Approximation), updated of $\mathcal{H}$-matrices can be as well efficiently performed.

Current work

- Implementation of local error estimators.
- Update of $\mathcal{H}$-matrices if `Rk` matrices are computed using HCA (Hybrid Cross Approximation).

`www.hmatrix.org`

Adaptive Cross Approximation (ACA)

Aim Construct an approximation of the form $\sum_{\nu=1}^{k} a_\nu b_\nu^T$ to a matrix $M \in \mathbb{R}^{n\times m}$ up to a relative error $\|M - \sum_{\nu=1}^{k} a_\nu b_\nu^T\|_2 \approx \epsilon \|M\|_2$. **Algorithm**

Input: A function that returns the matrix entry M_{ij} for an index pair (i, j).

Step $\nu = 1 \ldots k$:

1. Determine (and **save**) a pivot index (i^*, j^*).
2. Compute the entries of the two vectors $a_\nu \in \mathbb{R}^n, b_\nu \in \mathbb{R}^m$ by

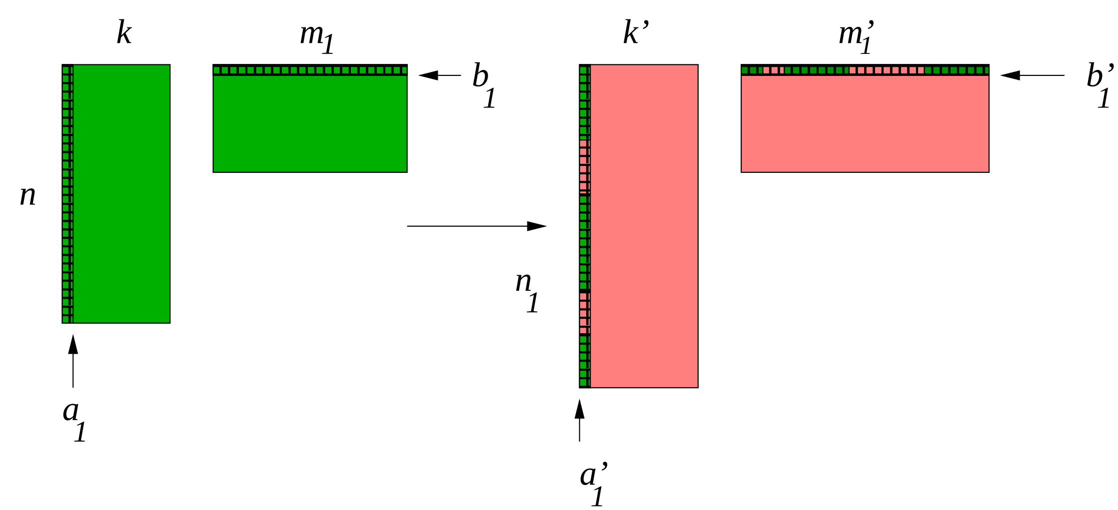
$$(a_\nu)_i := M_{ij^*} - \sum_{\nu=1}^{\mu-1} (a_\nu)_i (b_\nu)_{j^*}, (b_\nu)_j := \frac{1}{\delta}\Big(M_{i^*j} - \sum_{\nu=1}^{\mu-1} (a_\nu)_{i^*} (b_\nu)_j\Big).$$

Stop if $\|a_\nu\|_2 \|b_\nu\|_2 \le \epsilon \|a_1\|_2 \|b_1\|_2$.

Output: The factorisation $AB^T \approx M$.

Since the pivot elements are saved in the update of Rk matrix (computed by ACA) we distinguish three cases:

- All pivot pairs can be reused.
- First $t, t < k$ pivot pairs can be used, rest has to be computed as in the original algorithm.
- There is no pivot pair that can be used again, there is no update possible, i.e. Rk matrix is completely new.



Time (in seconds) for the update of the SLP $\mathcal{H}$-matrix compared to reassembly starting with $n_1 = 12288$ ($n_1 = 49152$) degrees of freedom

n_1 =12288 new	n_2 =12422 2.2%	n_2 =13014 11.2%	n_2 = 15790 44.4%
adaptive G_{ad}	1.5	8.6	32.4
reassembly G_{or}	33.7	35.5	44.1
savings (costs)	94%(6%)	76%(24%)	26%(74%)
$\|G_{ad} - G_{exact}\|_2$	9.5×10^{-7}	8.33×10^{-7}	1.54×10^{-6}
$\|G_{or} - G_{exact}\|_2$	9.22×10^{-7}	8.26×10^{-5}	6.70×10^{-7}

Numerical test for ACA

n_1 =49152	n_2 = 49682	n_2 =51870	n_2 =62494
new	2.1%	10.5%	42.7%
adaptive G_{ad}	10	43.2	146
reassembly G_{or}	167.2	177.1	213.7
savings(costs)	94%(6%)	76%(24%)	32%(68%)
$\|G_{ad} - G_{exact}\|_2$	3.37×10^{-7}	4.85×10^{-7}	4.21×10^{-7}
$\|G_{or} - G_{exact}\|_2$	3.36×10^{-7}	1.75×10^{-7}	1.93×10^{-7}