Fast algorithms and numerical methods for the solution of Boundary Element Methods

Session 5: Hierarchical matrices

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Outline

1. Main concepts introduced during last session: low-rank approximations
2. Hierarchical matrices
3. $\mathcal{H}$-matrices based Solvers

How to reduce the costs of the BEM?

- Boundary integral equation to solve (EFIE)

$$\int_{\Gamma} G(\boldsymbol{x}-\boldsymbol{y})p(\boldsymbol{y})dS_{\boldsymbol{y}} = -u^{inc}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

- Helmholtz fundamental solution: $G(\boldsymbol{x}-\boldsymbol{y}) = \dfrac{\exp(ik|\boldsymbol{x}-\boldsymbol{y}|)}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}$

BEM discretization $\Rightarrow$ fully-populated system $\mathbb{A}\boldsymbol{p} = \boldsymbol{b}$

- Assembly of the matrix system and matrix-vector product: $O(N^2)$

How can we reduce the costs?

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How can we reduce the costs?

- Not possible to speed-up the solution of the initial system
- But it is possible for an approximate system

- BEM system is not low-rank (because invertible)
- But it can be approximated by a data-sparse system with low-rank blocks: reduction of storage and solution time

Low-rank approximation for the BEM matrix?

$\mathbb{A} \in \mathbb{R}^{N\times N}$ of rank r is called low-rank if $2rN \ll N^2$

- $\mathbb{A} = \mathbb{U}\mathbb{V}^T$ with $\mathbb{U} \in \mathbb{R}^{N\times r}$ and $\mathbb{V} \in \mathbb{R}^{N\times r}$
- Then the storage is reduced from N^2 to $2rN$

We know how to derive the low-rank approximation in a fast way

- Truncated SVD: best low-rank approximation $O(rN^3)$ operations

$$\mathbb{A}_r = \sum_{i=1}^{r} \mathbb{U}_i \boldsymbol{\Sigma}_{ii} \mathbb{V}_i^*.$$

- We use the Adaptative Cross Approximation

$$\mathbb{A} = \mathbb{B}_k + \mathbb{R}_k, \quad \mathbb{R}_k = \mathbb{A} - \sum_{\ell=1}^{k} \mathbf{u}_\ell \mathbf{v}_\ell^T$$

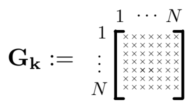
The existence of a data-sparse approximation is related to $\mathbb{G}$.

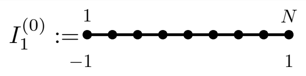
Behavior of the BEM system matrix

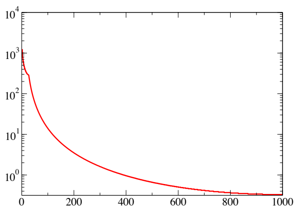
Model problem: Kernel function $(\mathbb{G})_{ij} = G(\boldsymbol{x}_i, \boldsymbol{y}_j)$

$$\mathbb{G}_k = \sum_{i=1}^{k} \mathbf{U}_i \mathbf{\Sigma}_{ii} \mathbf{V}_i^*, \quad \varepsilon_k = \frac{||\mathbb{G} - \mathbb{G}_k||_F}{||\mathbb{G}||_F}, \quad ||\mathbb{G} - \mathbb{G}_k||_F^2 = \sum_{i=k+1}^{N} \sigma_i^2$$

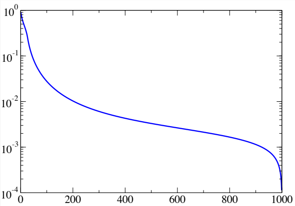
Truncated SVD of the kernel function ($N = 1000$, $[-1:1]$, $k = 10\pi$)







Decay of the sing. values

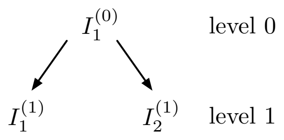


Error decay

As expected, BEM matrix is not low-rank (numerical observation)

Finding submatrices that are low-rank

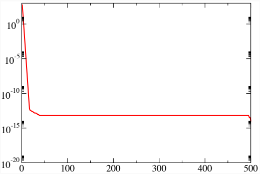
Partitioning of the unknowns



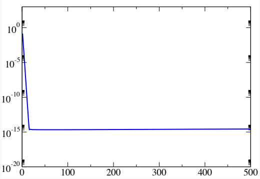
$$\mathbf{G_k} := \begin{array}{c} \\ I_1^{(1)} \\ I_2^{(1)} \end{array} \begin{array}{c} \begin{array}{cc} I_1^{(1)} & I_2^{(1)} \end{array} \\ \left[\begin{array}{c:c} & \\ \hdashline & \end{array}\right] \end{array}$$

Numerical constatation: behavior of singular values $(\mathbb{G})_{ij} = G(\boldsymbol{x}_i, \boldsymbol{y}_j)$

Off-diagonal block: $\mathbf{x}_i \in [-1, 0], \mathbf{y}_j \in [0, 1]; I_1^{(1)} \times I_2^{(1)}$



Decay of the sing. values

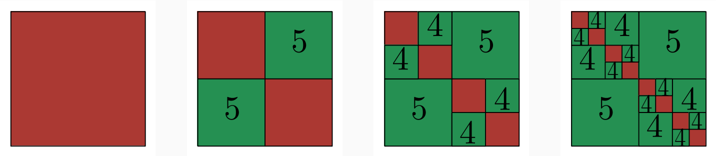


Error decay

For complex geometries, unknowns are reordered: cluster tree to avoid to do the permutations at each level

Low-rank approximation of the blocks

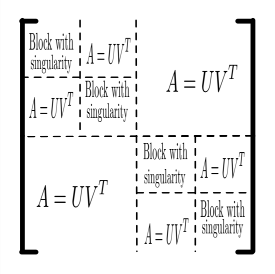
Numerical constatation: Rank of the blocks



Entire matrix *1 level* *2 levels* *3 levels*

Partitioning of the matrix: block cluster tree

- Diagonal blocks contain all singularities: as $||\boldsymbol{x} - \boldsymbol{y}||$ tends to 0
- Off-diagonal blocks: separated target and source points



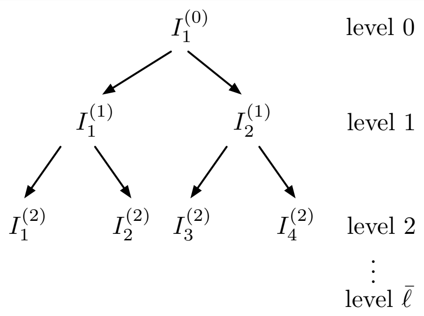
Compression rate: $\tau = 1 - \frac{2r}{N}$

- storage: from N^2 to $2rN$
- increases with level

Outline

Basic concepts of Hierarchical matrices

- Classical block partitioning: fixed partitioning of $I = \{1, \ldots, N\}$ into disjoints subsets $P = \{I_j : 1 \le j \le k\}$ with $I = \cup_{j=1}^{k} I_j$
- We need coarse partitionings and fine partitionings: $\mathcal{H}$-tree



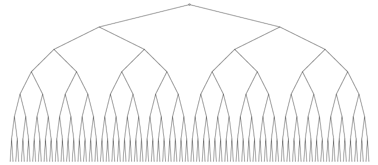
- Cluster: set of indices corresponding to points that are "close" in some sense
- Leaf: node without son
- Binary tree: max of 2 sons per cell
- Root cell encloses all the points
- Recursive subdivision until stopping criteria (min # of points) is achieved

W. Hackbusch. *A sparse arithmetic based on $\mathcal{H}-$matrices. Part I: Introduction to $\mathcal{H}-$matrices.* Computing, 1999.

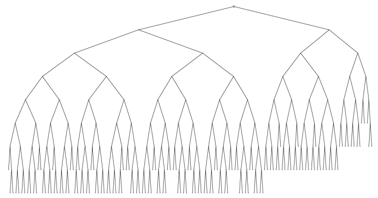
Comparison of two cluster trees

Two algorithms: to balance the tree based on

- $\#$ of points: constant in each cell t (Median bisection)
- geometry: cell is subdivided according to the geometry (Geometric bisection)



Median

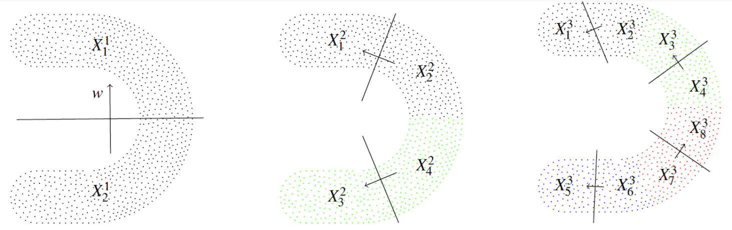


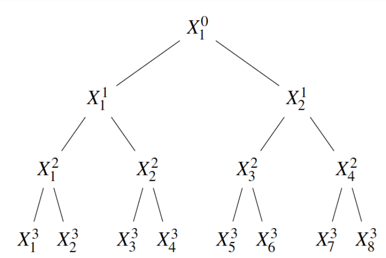
Geometric

B. Lizé. *Résolution directe rapide pour les éléments finis de frontière en électromagnétisme et acoustique: $\mathcal{H}$-Matrices. Parallélisme et Applications industrielles.* Thèse, Paris 13, 2014.

Balanced tree: principal direction based bisection

Method to balance the number of degrees of freedom



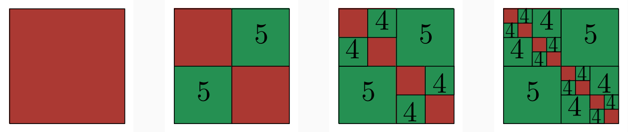


- Center of mass of the cluster X
- Covariance matrix of the cluster
  $$\mathbf{C} = \sum_{k=1}^{N} (x_k - X)(x_k - X)^T$$
- Eigenvalues $\&$ Eigenvectors of $\mathbf{C}$
- Separation plane: through X and orthogonal to largest eigenvalue

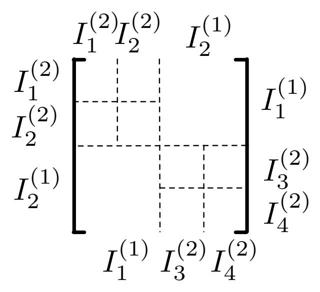
Messner. *Fast Boundary Element Methods in Acoustics*, PhD Dissertation, 2011.

Basic concepts of Hierarchical matrices (matrix case)

Traditional block partitioning of a matrix: $P_2 = P \times P$
We need finer blocks close to the diagonal and coarser far away



General block partitioning of $I \times I$: allows subsets of $I \times I$
$\mathcal{H}-$partitionings: hierarchical structure similar to vector case



Overview of the algorithm

$$\boxed{\int_\Gamma G(\boldsymbol{x} - \boldsymbol{y}) p(\boldsymbol{y}) dS_{\boldsymbol{y}} = -u^{inc}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma}$$

1. Renumbering of the unknowns (according to the geometry): each index $i \in I$ in the cluster tree carry a position $\mathbf{x}_i \in \mathbb{R}^3$
2. Subdivision of the BEM matrix: Block Cluster tree
3. Admissibility condition to determine which blocks are low-rank
   - $\Rightarrow$ Defines the stopping criteria in the construction of the block cluster tree (as soon as we have a low rank matrix, we do not need to subdivide the block)
   - $\Rightarrow$ Algorithms to generate automatically the block cluster tree

B. Lizé. *Résolution directe rapide pour les éléments finis de frontière en électromagnétisme et acoustique: $\mathcal{H}$-Matrices. Parallélisme et Applications industrielles*, Thèse, Paris 13, Juin 2014.

What do we need next?

$$\boxed{\int_\Gamma G(\boldsymbol{x}-\boldsymbol{y})p(\boldsymbol{y})dS_{\boldsymbol{y}} = -u^{inc}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma}$$

Important tools:

$\surd$ Renumbering of the unknowns (according to the geometry): each index $i \in I$ in the cluster tree carry a position $\mathbf{x}_i \in \mathbb{R}^3$

(2) Subdivision of the BEM matrix: Block Cluster tree

(3) Admissibility condition to determine which blocks are low-rank

- Points on the mesh are partitioned the with a $\mathcal{H}-$tree over I
- We need to find submatrices of $\mathbb{A}$ which will be low-rank $\rightarrow$ Block Cluster tree

What do we need next?

$$\boxed{\int_\Gamma G(\boldsymbol{x}-\boldsymbol{y})p(\boldsymbol{y})dS_{\boldsymbol{y}} = -u^{inc}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma}$$

$\surd$ Renumbering of the unknowns (according to the geometry): each index $i \in I$ in the cluster tree carry a position $\mathbf{x}_i \in \mathbb{R}^3$

$\surd$ Subdivision of the BEM matrix: Block Cluster tree

(3) Admissibility condition to determine which blocks are low-rank

We need a simple tool to determine the low-rank submatrices:

- The blocks should be as large as possible to obtain a compression rate as large as possible

$$\tau = 1 - \frac{2k}{N} \text{ (storage is reduced from } N^2 \text{ to } 2kN)$$

- Computing explicitly the rank of the submatrices is too expensive

Determine *a priori* if the submatrix has a low-rank approximation?

- The condition depends on the nature of the matrix
- The condition depends on the kernel used

Theory for Asymptotically smooth kernels

Ex: $f(\mathbf{x}, \mathbf{y}) = (4\pi||\mathbf{x} - \mathbf{y}||)^{-1}$ is asymptotically smooth

Taylor series to build theoretically a low rank approximation with r[1] terms

$$s^r(\mathbf{x}, \mathbf{y}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^3, |\boldsymbol{\alpha}| \leq m} (\mathbf{x} - \mathbf{x}_0)^{\boldsymbol{\alpha}} \frac{1}{\boldsymbol{\alpha}!} \partial_x^{\boldsymbol{\alpha}} s(\mathbf{x}_0, \mathbf{y}) + \underbrace{R_s^r}_{\text{remainder}} \qquad \mathbf{x} \in X, \quad \mathbf{y} \in Y$$

How does the Taylor series converge($\mathbf{x} \in X$ and $\mathbf{y} \in Y$)?

$s(.,.)$ is asymptotically smooth if $\exists c_1, c_2$ and $\sigma \in \mathbb{N}$ (singularity degree) such that $\forall z \in \{x_j, y_j\}$ and $n \in \mathbb{N}$, $\forall \mathbf{x} \neq \mathbf{y}$

$$|\partial_{\mathbf{z}}^n s(\mathbf{x}, \mathbf{y})| \leq n! c_1 (c_2 ||\mathbf{x} - \mathbf{y}||)^{-n-\sigma}$$

$$|R_s^r(\mathbf{x}, \mathbf{y})| \leq C' \sum_{\ell=m}^{\infty} \left(\frac{||\mathbf{x} - \mathbf{x}_0||}{c_2 ||\mathbf{x}_0 - \mathbf{y}||} \right)^{\ell}$$

Convergence of R_s^r for all $\mathbf{y} \in Y$ such that $\gamma_x := \frac{\max_{\mathbf{x} \in X} ||\mathbf{x} - \mathbf{x}_0||}{c_2 ||\mathbf{x}_0 - \mathbf{y}||} < 1$

[1] $r := \#\{\boldsymbol{\alpha} \in \mathbb{N}_0^3 : |\boldsymbol{\alpha}| \leq m\}$

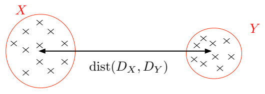
Taylor expansion converges exponentially with convergence rate γ_x since

$$|R_s^r(\mathbf{x},\mathbf{y})| \leq \quad C' \frac{\gamma_x^m}{1-\gamma_x} \xrightarrow[m\to\infty]{} 0$$

Derivation of a sufficient condition independent of $\mathbf{x}_0$, be observing that

$$\max_{\mathbf{x}\in X} ||\mathbf{x}-\mathbf{x}_0|| \leq \mathrm{diam}\, X \quad \text{and} \quad \mathrm{dist}(\mathbf{x}_0, Y) \geq \mathrm{dist}(X,Y)$$

X and Y are said to be η-*admissible* ($\eta > 0$) if



$$\min\Big(\mathrm{diam}\, X, \mathrm{diam}\, Y\Big) < \eta \times \mathrm{dist}(X,Y)$$

How do we choose η?

$$\max_{\mathbf{x}\in X} ||\mathbf{x}-\mathbf{x}_0|| \leq \mathrm{diam}\, X \leq \eta\, \mathrm{dist}(X,Y) \leq \eta\, \mathrm{dist}(\mathbf{x}_0, Y) \quad \rightarrow \quad \gamma_x \leq \frac{\eta}{c_2}$$

Exponential convergence if X and Y are η-*admissible* and if $\eta < c_2$

Efficiency of $\mathcal{H}$-matrix repres. for asymptotically smooth kernels

Hackbusch. Hierarchical Matrices: algorithms and analysis, Springer, 2015.

What can we expect for the Helmholtz kernel?

$G(\mathbf{x},\mathbf{y}) = \exp(ik||\mathbf{x}-\mathbf{y}||)f(\mathbf{x},\mathbf{y})$ with $f(\mathbf{x},\mathbf{y})$ asymptotically smooth

$\exists c_1, c_2$ and $\sigma \in \mathbb{N}$ such that $\forall z \in \{x_j, y_j\}$ and $n \in \mathbb{N}$

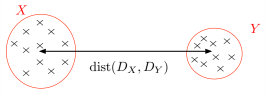
$$|\partial_{\mathbf{z}}^n G(\mathbf{x},\mathbf{y})| \leq n! c_1 (1 + k||\mathbf{x}-\mathbf{y}||)^n (c_2||\mathbf{x}-\mathbf{y}||)^{-n-\sigma}$$

Taylor series to build theoretically a low rank approximation with r terms

$$|R_\kappa^r(\mathbf{x},\mathbf{y})| \leq C' \sum_{\ell=m}^{\infty} \left((1 + k||\mathbf{x}_0-\mathbf{y}||)\frac{||\mathbf{x}-\mathbf{x}_0||}{c_2||\mathbf{x}_0-\mathbf{y}||}\right)^\ell.$$

R_s^r converges $\forall \mathbf{y} \in Y$ such that $\gamma_{\kappa,x} := (1 + k||\mathbf{x}_0-\mathbf{y}||)\frac{\max_{\mathbf{x}\in X}||\mathbf{x}-\mathbf{x}_0||}{c_2||\mathbf{x}_0-\mathbf{y}||} < 1$

The exponential convergence is now conditioned by the η_k-admissibility (criterion to determine *a priori* low-rank blocks)



$$\min\Big(\operatorname{diam} X, \operatorname{diam} Y\Big) < \eta(k) \times \operatorname{dist}(X, Y)$$

Are $\mathcal{H}$-matrix repres. of the 3 BEM matrix efficient?

Low-frequency regime: η_k-admissibility similar to η-admissibility

method as efficient as for asymptotically smooth kernels

Higher frequencies: admissibility condition depends linearly on ω

more involved methods to handle this case (directional approaches, ...)

We keep η fixed netherveless (standard $\mathcal{H}$-matrices easier to implement)

$$\mathbb{A}_{\sigma\times\tau} \text{ is a priori low-rank} \quad \text{if } \min\Big(\text{diam}(\sigma), \text{diam}(\tau)\Big) < \eta \times \text{dist}(\sigma, \tau)$$

Study of Taylor expansion $\rightarrow$ memory savings will not be optimal.
What can we expect? Frequency range where it can be a useful tool?

Estimated memory requirements

Storage estimate (N: # DOFs)

$$N_{st} \leq C \max(r^{\max}, N_{\text{leaf}}) N \log N$$

$N_{\text{leaf}} (= 100)$: parameter to stop the DOF clustering

$r^{\max}$: maximum numerical rank observed among all the η-admissible blocks

Estimated maximum rank: Study of the Taylor expansion $\rightarrow$ rank depends on ω

If circular frequency ω is fixed, rank should stay constant while N increases

$$\boxed{N_{st} = O(N \log N)}$$

If density of points is fixed, maximum rank expected to grow linearly with the frequency until the high-frequency regime is achieved

- $h = O(\lambda_S) = O(\omega^{-1})$ + BEM mesh $\rightarrow h = O(N^{-2})$
- The maximum numerical rank is thus expected $O(N^{1/2})$

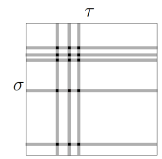
$$\boxed{N_{st} \leq O(N^{3/2} \log N)}$$

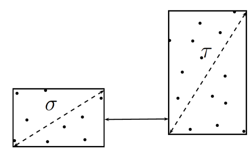
Admissibility criteria: in practice

- Helmholtz kernel is not similar to $1/r$ kernels
- But in practice we use the same condition even though it can be suboptimal for high frequencies

$$f(\sigma,\tau) = \begin{cases} 1 & \text{if } \max\Big(\text{diam}(\sigma), \text{diam}(\tau)\Big) < \eta . d(\sigma,\tau) \\ 0 & \text{otherwise} \end{cases}$$

- Diameter of a group too expensive: diameter of enclosing cell
- Distance: distance between closest faces of enclosing cells





Condition computed in $O(1)$ operations

Hierarchical algorithm: summary

Use of a hierarchical algorithm

Leaves of the block cluster tree

- if blocks are not admissible: store in a component-wise fashion
- otherwise admissibility condition guarantees low-rank sub-block: compute the low-rank approximation

Non leaf blocks

- if blocks are not admissible: the block is subdivided
- otherwise admissibility condition guarantees low-rank sub-block: compute the low-rank approximation

Iterations until admissible block or the stopping criteria

3 kinds of blocks: $\mathcal{H}$-matrices; full- and low-rank blocks

S. Börm, L. Grasedyck and W. Hackbusch. *Hierarchical matrices*, 2003.

Outline

How to use $\mathcal{H}-$matrices to derive an iterative solver

Only operation needed for the iterative solver: matrix-vector product

$$\mathbf{y} = \mathbb{A}\mathbf{x} := \text{MVM}(\mathbb{A}, \tau \times \sigma, \mathbf{x}, \mathbf{y})$$

MVM$(\mathbb{A}, \tau \times \sigma, \mathbf{x}, \mathbf{y})$

if $\tau \times \sigma$ not a leaf cell **then**
  for all $\tau' \times \sigma' \in S(\tau \times \sigma)$ **do**
    Matrix-vector product: MVM$(\mathbb{A}, \tau' \times \sigma', \mathbf{x}, \mathbf{y})$
  end for
else
  $\mathbf{y}_{|\tau} := \mathbf{y}_{|\tau} + \mathbb{A}_{\tau \times \sigma} \mathbf{x}_{|\sigma}$
end if

How to use $\mathcal{H}-$matrices to derive an iterative solver

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    Matrix-vector product: MVM$(\mathbb{A}, \tau' \times \sigma', \mathbf{x}, \mathbf{y})$
  end for
else
  $\mathbf{y}_{|\tau} := \mathbf{y}_{|\tau} + \mathbb{A}_{\tau \times \sigma}\mathbf{x}_{|\sigma}$
end if

Matrix-vector product for the leaf cells

- If it is a full-block: standard matrix-vector product
- If it is an admissible block: $\mathbb{A}_{\tau \times \sigma} = \mathbb{U}\mathbb{V}^T$
  1. $\mathbf{w} \leftarrow \mathbb{V}^T \mathbf{x}_{|\sigma}$
  2. $\mathbf{y}_{|\tau} \leftarrow \mathbb{U}\mathbf{w}$

Easy Implementation of an iterative solver for $\mathcal{H}-$matrices

How to use $\mathcal{H}-$matrices to derive a direct solver

$$\begin{pmatrix} \mathbb{L}_{11} & 0 \\ \mathbb{L}_{21} & \mathbb{L}_{22} \end{pmatrix} \begin{pmatrix} \mathbb{U}_{11} & \mathbb{U}_{12} \\ 0 & \mathbb{U}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix}$$

- Forward step: solve $\mathbb{L}Y = B$

$$\begin{cases} \mathbb{L}_{11}\mathbf{y}_1 & = & \mathbf{b}_1 \\ \mathbb{L}_{22}\mathbf{y}_2 & = & \mathbf{b}_2 - \mathbb{L}_{21}\mathbf{y}_1 \end{cases}$$

- Backward step: solve $Y = \mathbb{U}X$

$$\begin{cases} \mathbf{x}_2 & = & \mathbb{U}_{22}^{-1}\mathbf{y}_2 \\ \mathbf{x}_1 & = & \mathbb{U}_{11}^{-1}\mathbf{y}_1 - \mathbb{U}_{11}^{-1}\mathbb{U}_{12}\mathbf{x}_2 \end{cases}$$

How to use $\mathcal{H}-$matrices to derive a direct solver

$$\begin{pmatrix} \mathbb{L}_{11} & 0 \\ \mathbb{L}_{21} & \mathbb{L}_{22} \end{pmatrix} \begin{pmatrix} \mathbb{U}_{11} & \mathbb{U}_{12} \\ 0 & \mathbb{U}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix}$$

- Forward step: solve $\mathbb{L}Y = B$

$$\begin{cases} \mathbb{L}_{11}\mathbf{y}_1 = \mathbf{b}_1 \\ \mathbb{L}_{22}\mathbf{y}_2 = \mathbf{b}_2 - \mathbb{L}_{21}\mathbf{y}_1 \end{cases}$$

- Backward step: solve $Y = \mathbb{U}X$

$$\begin{cases} \mathbf{x}_2 = \mathbb{U}_{22}^{-1}\mathbf{y}_2 \\ \mathbf{x}_1 = \mathbb{U}_{11}^{-1}\mathbf{y}_1 - \mathbb{U}_{11}^{-1}\mathbb{U}_{12}\mathbf{x}_2 \end{cases}$$

LU-solver for 2x2 Block System

$$\begin{pmatrix} \mathbb{A}_{\tau_1\tau_1} & \mathbb{A}_{\tau_1\tau_2} \\ \mathbb{A}_{\tau_2\tau_1} & \mathbb{A}_{\tau_2\tau_2} \end{pmatrix} = \begin{pmatrix} \mathbb{L}_{\tau_1\tau_1} & \mathbf{0} \\ \mathbb{L}_{\tau_2\tau_1} & \mathbb{L}_{\tau_2\tau_2} \end{pmatrix} \begin{pmatrix} \mathbb{U}_{\tau_1\tau_1} & \mathbb{U}_{\tau_1\tau_2} \\ \mathbf{0} & \mathbb{U}_{\tau_2\tau_2} \end{pmatrix}$$

1. LU decomposition to compute: $\mathbb{L}_{\tau_1\tau_1}$ and $\mathbb{U}_{\tau_1\tau_1}$
2. Compute $\mathbb{U}_{\tau_1\tau_2}$ from $\mathbb{A}_{\tau_1\tau_2} = \mathbb{L}_{\tau_1\tau_1}\mathbb{U}_{\tau_1\tau_2}$
3. Compute $\mathbb{L}_{\tau_2\tau_1}$ from $\mathbb{A}_{\tau_2\tau_1} = \mathbb{L}_{\tau_2\tau_1}\mathbb{U}_{\tau_1\tau_1}$
4. LU decomposition to compute: $\mathbb{A}_{\tau_2\tau_2} - \mathbb{L}_{\tau_2\tau_1}\mathbb{U}_{\tau_1\tau_2} = \mathbb{L}_{\tau_2\tau_2}\mathbb{U}_{\tau_2\tau_2}$

New definitions of algebraic operations for $\mathcal{H}-$matrices

Bebendorf. *Hierarchical LU decomposition-based preconditioners for BEM.* Computing, 2005.