An Introduction to
Fast Multipole Boundary Element Methods

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Workshop Fast BEM & BETI
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Examples and Applications
Outline

Model Problem and Boundary Element Method

Motivation of Low Rank Approximation

Clustering and Admissibility Condition

Fast Multipole Method

Numerical Examples
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Numerical Examples
Indirect BEM Approach

Laplace Dirichlet boundary value problem

\[-\Delta u(x) = 0 \quad \text{for} \; x \in \Omega \subset \mathbb{R}^3\]

\[u(x) = g(x) \quad \text{for} \; x \in \Gamma = \partial\Omega\]
Indirect BEM Approach

Laplace Dirichlet boundary value problem

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\[u(x) = g(x) \quad \text{for } x \in \Gamma = \partial \Omega\]

Single layer potential ansatz:

\[u(\tilde{x}) := \frac{1}{4\pi} \int_{\Gamma} \frac{1}{|x - y|} w(y) ds_y \quad \text{for } \tilde{x} \in \Omega\]

is a solution of the Laplace equation.
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Determine density function \( w \) from the boundary integral equation

\[(Vw)(x) = \frac{1}{4\pi} \int_{\Gamma} \frac{1}{|x - y|} w(y)ds_y = g(x) \quad \text{for } x \in \Gamma\]
Discrete Problem

Variational formulation: Find $w \in H^{-1/2}(\Gamma)$

$$\int_{\Gamma} (Vw)(x)v(x)ds_x = \int_{\Gamma} g(x)v(x)ds_x \quad \forall v \in H^{-1/2}(\Gamma)$$
Discrete Problem

Variational formulation: Find \( w \in H^{-1/2}(\Gamma) \)

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\int_{\Gamma} (Vw)(x)v(x) \, ds_x = \int_{\Gamma} g(x)v(x) \, ds_x \quad \forall v \in H^{-1/2}(\Gamma)
\]

Triangulation of the surface \( \rightarrow \) discrete approximation:

\[
w_h(x) = \sum_{k=1}^{N} w_k \psi_k(x) \in S_h^0(\Gamma) \subset H^{-1/2}(\Gamma)
\]
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Galerkin variational formulation:

\[
w_h \in S_0^0(\Gamma) : \quad \int_{\Gamma} (Vw_h)(x)v_h(x)ds_x = \int_{\Gamma} g(x)v_h(x)ds_x \quad \forall v_h \in S_0^0(\Gamma)
\]
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Triangulation of the surface $\rightarrow$ discrete approximation:

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$$

equivalent system of linear equations: $V_h w = g$

where

$$
V_h[\ell, k] = \int_{\Gamma} (V \psi_k)(x)\psi_\ell(x)ds_x \quad g_\ell = \int_{\Gamma} g(x)\psi_\ell(x)ds_x
$$
Data-sparse Boundary Element Methods

Matrix times vector multiplication $\mathbf{v} = V_h \mathbf{w}$ for $\ell = 1, \ldots, N$:

$$
v_{\ell} = \sum_{k=1}^{N} V_h[\ell, k] w_k = \frac{1}{4\pi} \sum_{k=1}^{N} w_k \int_{\tau_{\ell}} \int_{\tau_{k}} \frac{1}{|x - y|} \, ds_x \, ds_y \quad \rightarrow O(N^2)
$$
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Fast / Data-sparse boundary element methods:

- Fast Multipole Method [Rokhlin 1985; Greengard, Rokhlin 1987]
- Panel Clustering [Hackbusch, Nowak 1989]
- Wavelets [Dahmen, Prössdorf, Schneider 1993]
- Adaptive Cross Approximation [Bebendorf, Rjasanow 2003]
- $\mathcal{H}$ matrices [Hackbusch 1999]
- $\mathcal{H}^2$ matrices [Hackbusch, Khoromskij, Sauter 1999]
### Comparison: Standard BEM and Fast BEM

- **quadratic vs almost linear complexity**
- **Standard BEM**: limited to 20000/30000 boundary elements
- **memory requirements** for 458752 elements: 1643 GB vs 3.4 GB
- **computational time** for 458752 elements: 875 h vs 20 min
- **uniform FE mesh**: 37.75 millions tetrahedrons, 458752 boundary elements
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Numerical Examples
Low Rank Approximation, Singular Value Decomposition

Matrix block

\[ A \in \mathbb{R}^{m \times n} \quad \text{with} \quad \mu = \text{rank} A \leq \min\{m, n\} \]

Low rank approximation

\[ A_k = \sum_{i=1}^{k} u_i v_i^\top \quad u_i \in \mathbb{R}^m, \quad v_i \in \mathbb{R}^n \]

The singular value decomposition

\[ A = U \Sigma V^\top = \sum_{i=1}^{\mu} \sigma_i(A) u_i v_i^\top \]

can be defined by means of the eigenvalue decomposition of the symmetric matrix \( A^\top A \).
1. Example [Rjasanow, Steinbach 2007]

Low rank approximation by SVD of $A$ where

$$A[k, \ell] = K(x_k, y_\ell), \ k, \ell = 1, \ldots, N$$

and a uniform discretization of the domain $[0, 1] \times [0, 1]$ by nodes

$$(x_k, y_\ell) = ((k - 1)h, (\ell - 1)h), \ h = \frac{1}{N - 1}$$

for $k, \ell = 1, \ldots, N$. 
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for $k, \ell = 1, \ldots, N$.

Function

$$ K(x, y) = \frac{1}{\alpha + x + y}, $$

with an artificial “singularity” for a small parameter $\alpha > 0$. 
Singular Values of $A$

$N = 32$

$N = 1024$

- Logarithmic plot for $\alpha = 10^{-4}$
- Most singular values are almost zero.
- A few singular values are sufficient for a good approximation $A_k$ by SVD.
Largest 32 Singular Values of $A$

$N = 32, 64, 128$

$N = 256, 512, 1024$

- Number of significant singular values increases only slightly with increasing dimension $N$. 
Relative Accuracy of Low Rank Approximation $A_k$

$N = 32, 64, 128$

$N = 256, 512, 1024$

- relative accuracy over $k = 1, \ldots, 32$

$$\varepsilon(k) = \frac{\|A - A_k\|_F}{\|A\|_F}$$

- Number of singular values determines the quality of the approximation.
- The results just slightly depend on $\alpha$, they even improve for smaller $\alpha$. 

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2. Example: Function with Stronger Singularity

\[ K(x, y) = \frac{1}{\alpha + (x - y)^2} \]

with artificial “singularity” along the diagonal \( \{(x, x)\} \).

- Rank \( k(10^{-6}) \) for accuracy \( 10^{-6} \) of \( A_k \) as function of \( \alpha \) for \( N = 256 \)
- horizontal axis: \(-\log_2(\alpha)\) with \( \alpha \in [2^0, 2^{-8}] \)
- left: strong dependency of the rank on \( \alpha \) for \([0, 1] \times [0, 1] \)
- right: For \([0, 0.5] \times [0.5, 1]\) (separation of \( x \) and \( y \)) well behaved.
2. Example: Singular Values of $A$ for Several $\alpha$

complete square $[0, 1] \times [0, 1]$

quarter $[0, 0.5] \times [0.5, 1]$

▷ lower curve: $\alpha = 10^{-1}$; upper curve: $\alpha = 10^{-8}$; $N = 256$

▷ Total matrix (with singularity) cannot be approximated by low rank but the subblock (“without” singularity).
2. Example: Hierarchical Low Rank Approximation

- $N = 256$, $\alpha = 2^{-9}$, numbers = rank $k(10^{-6})$
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- main idea: Subdivide matrix $A$. First step: 4 blocks for subdomains 
  
  $[0, 0.5] \times [0, 0.5]$, $[0, 0.5] \times [0.5, 1]$, $[0.5, 1] \times [0, 0.5]$, $[0.5, 1] \times [0.5, 1]$

- Off diagonal blocks can be approximated efficiently.
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- Diagonal blocks: same structure as $A$ but half the size $\rightarrow$ Subdivisioning.
- Block which require a large rank are subdivided.
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  \]

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▶ Off diagonal blocks can be approximated efficiently.
▶ Diagonal blocks: same structure as $A$ but half the size $\rightarrow$ Subdivisioning.
▶ Block which require a large rank are subdivided.
▶ Memory requirements are decreased: $146N$, $94N$, $74N$ and $72N$.
▶ The rank of the separated blocks grows logarithmically ($7 - 8 - 9$).
Essential Ingredients of Hierarchical Approximation

for dense matrices with singularity along the “diagonal”:

- construction of the clusters for the variables $x$ and $y$
- determine admissible blocks (separation of $x$ and $y$)
- partitioning of the matrix
- efficient low rank approximation of the admissible blocks.
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Possible ways to construct a low rank approximation:

- SVD (not efficient)
- adaptive cross approximation
- expansion of the kernel (Taylor, spherical harmonics, ...)
- interpolation of the kernel (Chebychev polynomials (+SVD))
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Clustering of elements: subdivide box into similar boxes (alt.: bisection)
Simple admissibility condition: direct neighbors are not admissible.
Geometric Clustering and Matrix Partitioning in 1D

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Geometric Clustering and Matrix Partitioning in 2D
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\[ \Omega_1 \quad \Omega_2 \quad \Omega_3 \quad \Omega_4 \]

nearfield

\[ l_1^1 \quad l_2^1 \quad l_3^1 \quad l_4^1 \]
Geometric Clustering and Matrix Partitioning in 2D

\[ \Omega_1^2 \quad \Omega_2^2 \quad \Omega_3^2 \quad \Omega_4^2 \quad \Omega_5^2 \quad \Omega_6^2 \quad \Omega_7^2 \quad \Omega_8^2 \quad \Omega_9^2 \quad \Omega_{10}^2 \quad \Omega_{11}^2 \quad \Omega_{12}^2 \quad \Omega_{13}^2 \quad \Omega_{14}^2 \quad \Omega_{15}^2 \quad \Omega_{16}^2 \]

- farfield
- nearfield

\[ I_1^2 \quad I_2^2 \quad I_3^2 \quad I_4^2 \quad \ldots \quad I_{16}^2 \]
Partitioning of a BEM Matrix

Sphere, 3D, $N = 5120$
Admissibility Condition and Complexity

Definition

A pair of cluster \((\omega_i^\lambda, \omega_j^\lambda)\) is admissible, if

\[
\max\{\text{diam } \omega_i^\lambda, \text{diam } \omega_j^\lambda\} \leq \eta \text{ dist}(\omega_i^\lambda, \omega_j^\lambda)
\]

for a fixed parameter \(\eta < 1\).
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\]

for a fixed parameter \(\eta < 1\).

Memory requirements for \(\mathcal{H}\) matrix:

\[
O\left(\frac{1}{\eta^{d-1}}\right) k(L + 1) 2N
\]

where

- rank \(k\) approximation of admissible blocks \((k \sim \log N)\)
- \(L + 1\) level in the cluster tree \((1 + L \sim \log N)\)
- \(N\) boundary elements
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Kernel Approximation

Matrix times vector product $v = V_h w$ for $\ell = 1, \ldots, N$:

$$v_\ell = \sum_{k=1}^{N} V_h[\ell, k] w_k = \frac{1}{4\pi} \sum_{k=1}^{N} w_k \int_{\tau_\ell} \int_{\tau_k} \frac{1}{|x - y|} ds_y ds_x \quad \rightarrow O(N^2)$$
Kernel Approximation

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\[
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\]

If \(|\mathbf{x} - \mathbf{y}|^{-1} = f(\mathbf{x})g(\mathbf{y})\) hold, we would get:

\[
v_\ell = \frac{1}{4\pi} \int_{\tau_\ell} f(\mathbf{x}) \, ds_\mathbf{x} \sum_{k=1}^{N} \mathbf{w}_k \int_{\tau_k} g(\mathbf{y}) \, ds_\mathbf{y} \quad \rightarrow \mathcal{O}(N)
\]

Approximation of the kernel by expansion für \(|\mathbf{x}| < |\mathbf{y}|\)

\[
\frac{1}{|\mathbf{x} - \mathbf{y}|} \approx \sum_{n=0}^{p} \sum_{m=-n}^{n} |\mathbf{x}|^{n} Y_{n}^{-m}(\hat{\mathbf{x}}) Y_{n}^{m}(\hat{\mathbf{y}}) \frac{Y_{n}^{m}(\hat{\mathbf{y}})}{|\mathbf{y}|^{n+1}}
\]

with spherical harmonics für \(m \geq 0\) and \(\hat{\mathbf{x}} = \mathbf{x}/|\mathbf{x}|\):

\[
Y_{n}^{\pm m}(\hat{\mathbf{x}}) = \sqrt{\frac{(n-m)!}{(n+m)!}} (-1)^{m} \frac{d^{m}}{d\hat{x}^{m}} P_{n}(\hat{x}_{3})(\hat{x}_{1} \pm i\hat{x}_{2})^{m}.
\]
Fast Multipole Method

Inserting expansion into matrix entry where $|x| < |y|$

$$\int_{\tau_\ell} \int_{\tau_k} \frac{1}{|x - y|} ds_y ds_x \approx \int_{\tau_\ell} \int_{\tau_k} \left( \sum_{n=0}^{p} \sum_{m=-n}^{n} |x|^n Y_{n}^{-m}(\hat{x}) \frac{Y_{n}^{m}(\hat{y})}{|y|^{n+1}} \right) ds_y ds_x$$
Fast Multipole Method

Inserting expansion into matrix entry where $|x| < |y|

\[
\int_{\tau_\ell} \int_{\tau_k} \frac{1}{|x - y|} \, ds_y \, ds_x \approx \int_{\tau_\ell} \int_{\tau_k} \left( \sum_{n=0}^{p} \sum_{m=-n}^{n} |x|^n Y_n^{-m}(\hat{x}) \frac{Y_m^m(\hat{y})}{|y|^{n+1}} \right) \, ds_y \, ds_x
\]

\[
= \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} \left( |x|^n Y_n^{-m}(\hat{x}) \right) \, ds_x \int_{\tau_k} \frac{Y_m^m(\hat{y})}{|y|^{n+1}} \, ds_y
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\int_{\tau_{k}} \int_{\tau_{k}} \frac{1}{|x - y|} \, ds_{y} \, ds_{x} \approx \int_{\tau_{k}} \int_{\tau_{k}} \left( \sum_{n=0}^{p} \sum_{m=-n}^{n} |x|^{n} Y_{n}^{-m}(\hat{x}) \frac{Y_{n}^{m}(\hat{y})}{|y|^{n+1}} \right) \, ds_{y} \, ds_{x}
\]

\[
= \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_{k}} (|x|^{n} Y_{n}^{-m}(\hat{x})) \, ds_{x} \int_{\tau_{k}} \frac{Y_{n}^{m}(\hat{y})}{|y|^{n+1}} \, ds_{y}
\]

Splitting in near- and farfield and interchanging the summation order:

\[
\nu_{\ell} = \sum_{k \in \text{NF}(\ell)} V_{h}[\ell, k] w_{k} + \sum_{k \in \text{FF}(\ell)} V_{h}[\ell, k] w_{k}
\]
Fast Multipole Method

Inserting expansion into matrix entry where $|x| < |y|

$$\int_{\tau_\ell} \int_{\tau_k} \frac{1}{|x-y|} \, ds_y \, ds_x \approx \int_{\tau_\ell} \int_{\tau_k} \left( \sum_{n=0}^{p} \sum_{m=-n}^{n} |x|^n Y_n^{-m}(\hat{x}) \frac{Y_n^m(\hat{y})}{|y|^{n+1}} \right) \, ds_y \, ds_x = \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} (|x|^n Y_n^{-m}(\hat{x})) \, ds_x \int_{\tau_k} \frac{Y_n^m(\hat{y})}{|y|^{n+1}} \, ds_y$$

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$$v_\ell = \sum_{k \in \text{NF}(\ell)} V_h[\ell, k] \, w_k + \sum_{k \in \text{FF}(\ell)} V_h[\ell, k] \, w_k \approx \sum_{k \in \text{NF}(\ell)} V_h[\ell, k] \, w_k + \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} (|x|^n Y_n^{-m}(\hat{x})) \, ds_x \sum_{k \in \text{FF}(\ell)} \frac{w_k}{4\pi} \int_{\tau_k} \frac{Y_n^m(\hat{y})}{|y|^{n+1}} \, ds_y$$

$$= L_n^m(\ell)$$
Fast Multipole Method

Inserting expansion into matrix entry where $|x| < |y|$

$$\int_{\tau_\ell} \int_{\tau_k} \frac{1}{|x - y|} ds_y ds_x \approx \int_{\tau_\ell} \int_{\tau_k} \left( \sum_{n=0}^{p} \sum_{m=-n}^{n} |x|^n Y_n^{-m}(\hat{x}) \frac{Y_m^m(\hat{y})}{|y|^{n+1}} \right) ds_y ds_x$$

$$= \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} (|x|^n Y_n^{-m}(\hat{x})) ds_x \int_{\tau_k} \frac{Y_m^m(\hat{y})}{|y|^{n+1}} ds_y$$

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$$v_\ell = \sum_{k \in \text{NF}(\ell)} V_h[\ell, k] w_k + \sum_{k \in \text{FF}(\ell)} V_h[\ell, k] w_k$$

$$\approx \sum_{k \in \text{NF}(\ell)} V_h[\ell, k] w_k + \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} (|x|^n Y_n^{-m}(\hat{x})) ds_x \sum_{k \in \text{FF}(\ell)} \frac{w_k}{4\pi} \int_{\tau_k} \frac{Y_m^m(\hat{y})}{|y|^{n+1}} ds_y$$

$$= L_n^m(\ell)$$

But: coefficients $L_n^m(\ell)$ depend on $\ell \rightarrow$ fast computation???
Matrix Representation

\[
\sum_{k \in NF(\ell)} V_h[\ell, k] w_k + \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} |x|^n Y^{-m}_n(\hat{x}) ds_x \sum_{k \in FF(\ell)} \frac{w_k}{4\pi} \int_{\tau_k} \frac{Y^m_n(\hat{y})}{|y|^{n+1}} ds_y \]

\[
= L^m_n(\ell)
\]
Idea of the Algorithm of FMM

matrix times vector product

\[ \tilde{v}_\ell = \sum_{k \in \text{NF}(\ell)} V_h[\ell, k] w_k + \sum_{n=0}^{p} \sum_{m=-n}^{n} \left| x \right|^n Y_{n}^{-m}(\hat{x}) ds_x \sum_{k \in \text{FF}(\ell)} w_k \frac{\int_{\tau_k} Y_{n}^{m}(\hat{y}) \left| y \right|^{n+1} ds_y}{4\pi} = L_{n}^{m}(\ell) \]
Idea of the Algorithm of FMM

Matrix times vector product

\[
\tilde{v}_\ell = \sum_{k \in \text{NF}(\ell)} V_h[\ell, k] w_k + \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} |x^n Y_{n}^{-m}(\hat{x})| \, ds_x \sum_{k \in \text{FF}(\ell)} \frac{w_k}{4\pi} \int_{\tau_k} \frac{Y_{n}^{m}(\hat{y})}{|y|^{n+1}} \, ds_y
\]

Fast computation by means of hierarchical structure and kernel expansion:

\[
= L^m_n(\ell)
\]

→ almost linear complexity
Expansions of FMM

\[ \frac{1}{|x - y_\ell|} \approx \Phi_\ell(x) = \sum_{n=0}^{p} \sum_{m=-n}^{n} \overline{S}_n^m(x)R_n^m(y_\ell) \]

\( \triangleright \) multipole expansion for \( \ell \in I_i^\lambda \)

\[ \Phi_\ell(x) = \sum_{n=0}^{p} \sum_{m=-n}^{n} \overline{S}_n^m(x - C_i^\lambda)M_n^m(C_i^\lambda, \ell) \]  \( \triangleright \) Compute multipole coefficients of a cluster

\[ \tilde{M}_n^m(C_i^L, I_i^L) = \sum_{\ell \in I_i^L} q_\ell M_n^m(C_i^L, \ell) \]  \( \triangleright \) local expansion

\[ \Psi_\ell(x) = \sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m(C_j^\lambda, \ell)R_n^m(x - C_j^\lambda) \]

where

\[ L_n^m(C_j^\lambda, \ell) = \overline{S}_n^m(y_\ell - C_j^\lambda) \]
FMM Operations

- **M2M**

\[
\tilde{M}_n^m(C_j^\lambda, I_j^\lambda) = \sum_{\omega_i^{\lambda+1} \in \text{sons}(\omega_j^\lambda)} \sum_{s=0}^{n} \sum_{t=-s}^{s} R_s^t(C_j^\lambda C_i^{\lambda+1}) \tilde{M}_{n-s}^{m-t}(C_i^{\lambda+1}, I_i^{\lambda+1})
\] (4)

- **M2L** for \((\omega_i^\lambda, \omega_j^\lambda)\) admissible

\[
\tilde{L}_n^m(C_i^\lambda, I_i^\lambda)) = \sum_{s=0}^{\infty} \sum_{t=-s}^{s} (-1)^n S_{n+s}^{m+t}(C_j^\lambda C_i^\lambda) \tilde{M}_s^t(C_j^\lambda, I_j^\lambda)
\] (5)

- **L2L**

\[
\tilde{L}_n^m(C_j^{\lambda+1}, \text{FF}(\omega_i^\lambda)) = \sum_{s=n}^{p} \sum_{t=-s}^{s} R_{s-n}^t(C_i^\lambda C_j^{\lambda+1}) \tilde{L}_s^t(C_i^\lambda, \text{FF}(\omega_i^\lambda))
\] (6)

\[
v_\ell \approx \sum_{k \in \text{NF}(\ell)} V_{h}[\ell, k] w_k + \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} (|x|^n Y_{-m}^n(\hat{x})) \, ds_x \sum_{\tilde{k} \in \text{FF}(\ell)} \frac{W_k}{4\pi} \int_{\tau_k} \frac{Y_{n}^{m}(\hat{y})}{|y|^{n+1}} \, ds_y
\]

\[= L_n^m(\ell)\]
Demo of the FMM Algorithm

Ramani Duraiswami: http://www.umiacs.umd.edu/~ramani/fmm/
Fast Boundary Element Methods

Analysis of FMM: [GO, Steinbach, Wendland 2006]

- preserves essential properties of the boundary integral operators
- control of the error of FMM
- almost linear complexity ($O(N \log^{d-1} N)$)
- can be extended to volume potentials [GO, Steinbach, Urthaler 2010]
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Preconditioning:
- operator of opposite order [Steinbach, Wendland 1998; GO, Steinbach 2003]
- artificial multi-level preconditioner [Steinbach 2003]
- algebraic multigrid method for FMM [GO 2008]
Outline

Model Problem and Boundary Element Method

Motivation of Low Rank Approximation

Clustering and Admissibility Condition

Fast Multipole Method

Numerical Examples
Industrial Application: Controllable Reactor

with ABB, EU project CASOPT

Reactor coil

Control coils
Linear Elastostatics

- Fast multipole BEM extendable to linear elastostatics
  \[\text{GO, Steinbach, Wendland 2005; GO, Steinbach, Urthaler 2010}\]
Linear Elastostatics

- Fast multipole BEM extendable to linear elastostatics
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Linear Elasticity: Newton Potentials

- Mixed boundary conditions, $\Omega = (0, 1)^3$
- Indirect computation of $N_1 f$
- $u(x) = (x_1^3, x_2^3, x_3^3)^T$

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Linear Elastostatics: Newton Potentials

- mixed boundary conditions, $\Omega = (0, 1)^3$
- indirect computation of $N_1 f$
- $u(x) = (x_1^3, x_2^3, x_3^3)^\top$

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Vibration Analysis of Ships

[Wilken, GO, Cabos, Steinbach 2009; Brunner, GO, Junge, Steinbach, Gaul 2010; GO, Steinbach 2011]

- fluid structure interaction
- FEM BEM coupling
- ship in sea (with A. von Graefe, GL)
Some References

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The fast multipole method for the symmetric boundary integral formulation.

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Applications of a fast multipole Galerkin boundary element method in linear elastostatics.

L. Greengard and V. Rokhlin
A fast algorithm for particle simulations.