Fast multipole accelerated boundary element method for solution of 3D scattering problems

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- BEM strategy for large problems
- Peculiarities of the FMM used
- fGMRES and FMM based preconditioning
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Introduction

- Several publications on BEM/FMM
- Wideband FMM is a problem:
  - Low frequencies
  - High frequencies
- As problem is solved iteratively, efficient BIE formulation and preconditioning are important
- Different sources of errors should be consistently balanced
- BEM should be modified to fit memory/speed requirements
- Parallelization is relatively easy
\[ \nabla^2 \phi + k^2 \phi = 0 \]

<table>
<thead>
<tr>
<th>f, kHz</th>
<th>k, m^{-1}</th>
<th>D, m</th>
<th>kD</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>400</td>
<td>10^{-5}</td>
<td>0.004</td>
</tr>
<tr>
<td>50</td>
<td>200</td>
<td>30</td>
<td>600</td>
</tr>
<tr>
<td>4</td>
<td>70</td>
<td>0.3</td>
<td>20</td>
</tr>
<tr>
<td>2</td>
<td>40</td>
<td>5</td>
<td>200</td>
</tr>
<tr>
<td>1</td>
<td>20</td>
<td>50</td>
<td>1000</td>
</tr>
</tbody>
</table>
The number of mesh vertices/panels, $N$, increases proportionally to $(kD)^2$ so the minimal memory/speed complexity $O((kD)^2)$.

The FMM error and complexity depends on the truncation numbers, $p$, which depend on $kD$.

Efficiency of translations is critical. If $p^2$ is the size of representation and translation is performed with complexity $O(p^n)$, then the complexity of the FMM for simple shapes is $O((kD)^n)$.

If $n \geq 4$ the direct method for matrix-vector product is comparable or faster than the FMM.

Use of diagonal forms of translation operators provides translation exponent $n=2$, while some problems appear at low $kD$.

To compute a problem with $kD = 500$ and several elements per wavelength one needs mesh size with 1 million vertices (2 million elements).

Small $kD$ cases may require also large meshes if the geometry of the problem is complex.
Formulation

\[ \nabla^2 \phi + k^2 \phi = 0, \quad \mathbf{x} \in \mathcal{V} \subset \mathbb{R}^3, \quad k \in \mathbb{R}, \]

For external problems:

\[ \lim_{|\mathbf{x}| \to \infty} \left( |\mathbf{x}| \left( \frac{\partial \phi}{\partial |\mathbf{x}|} - i k \phi \right) \right) = 0. \]

Boundary conditions:

\[ \alpha(\mathbf{x}) \phi(\mathbf{x}) + \beta(\mathbf{x}) q(\mathbf{x}) = \gamma(\mathbf{x}), \quad \mathbf{x} \in S, \]

where \( q(\mathbf{x}) = \frac{\partial \phi}{\partial n}(\mathbf{x}) = \mathbf{n}(\mathbf{x}) \cdot \nabla \phi(\mathbf{x}). \)
Boundary Integral Equation

Green’s Identity

\[ \pm \phi(y) = L[q] - M[\phi], \quad y \notin S, \]

\[ L[q] = \int_S q(x)G(x, y)dS(x), \quad M[\phi] = \int_S \phi(x)\frac{\partial G(x, y)}{\partial n(x)}dS(x), \]

\[ G(x, y) = \frac{e^{ikr}}{4\pi r}, \quad r = |x - y|, \]

\[ \pm \frac{1}{2} \phi(y) = L[q] - M[\phi], \quad y \in S. \]
Boundary Integral Equation
(Burton-Miller / Combined / Direct)

Maue Identity

$$\pm \frac{1}{2} q(y) = L'[q] - M'[\phi], \quad y \in S,$$

$$L'[q] = \int_S q(x) \frac{\partial G(x,y)}{\partial n(y)} dS(x), \quad M'[\phi] = \frac{\partial}{\partial n(y)} \int_S \phi(x) \frac{\partial G(x,y)}{\partial n(x)} dS(x),$$

Combined Equation

$$\pm \frac{1}{2} [\phi(y) + \lambda q(y)] = (L + \lambda L')[q] - (M + \lambda M')[\phi],$$

$$A[\psi] = c.$$
Basic notes concerning the use of the FMM in the BEM

- Precomputations (singular elements, etc.) should be performed in \( O(N) \) or \( O(N \log N) \) computational and memory complexity.
- “On the fly” computation of integrals should be computationally cheap as much as possible.
- Since the FMM is \( O(N) \) or \( O(N \log N) \) algorithm it is preferable to increase the size of the mesh and use low order integrals than use rough meshes and high order integration.
- Increase of the mesh size is also preferable in terms of overall accuracy increase, since a larger mesh provides better shape approximation.
Computational domain (3D cube) is partitioned by octree.

**Upward pass** (get S-expansions for all boxes (skip empty))
(S-expansion means singular, or multipole, or far field expansion)

1. Get S-exp for Max Level
2. Get S-exp for other levels (use S|S-translations)
FMM

**Downward pass** (get R-expansions for all boxes (skip empty))
(R-expansion means regular, or local, or near field expansion)

1. Get R-exp from S-exp’s of the boxes in the neighborhood (use S|R-translations)
2. Get R-exp from parent (use R|R-translations)
**FMM**

**Final evaluation** (evaluate R-expansions for boxes at Max Level) and sum up directly contributions of sources in the neighborhood of receivers

1. Evaluate R-exp

2. Direct summation
Wideband FMM


Present

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Truncation numbers

\[ p_{\text{low}} = \frac{1}{\ln \delta} \ln \frac{1}{\epsilon (1 - \delta^{-1})^{3/2}} + 1, \]

\[ p_{\text{high}} = k a + \frac{1}{2} \left( 3 \ln \frac{1}{\epsilon} \right)^{2/3} (k a)^{1/3}, \]

\[ p = \left( p_{\text{low}}^4 + p_{\text{high}}^4 \right)^{1/4}. \]
Translation methods and algorithm complexity

- Matrix based translations are performed via the RCR-decomposition (Rotation-Coaxial translation-back Rotation), that has complexity $O(p^3)$ for $p^2$ representations.
- Conversion from representations via expansion coefficients to (and back) is performed with complexity $O(p^3)$.
- All other steps of the algorithm have complexity $O(p^2)$ or $O((kD)^2)$. Number of levels is $O(\log N)$.
- Overall complexity is $O((kD)^2 + \alpha(\varepsilon) ((kD)^3)$ with $\alpha<10^3$.
fGMRES and FMM-based preconditioning

- Ideal preconditioner $M$ for solution of equation $Ax=c$ is $M=A^{-1}$
- Approximate right preconditioner can be obtained via a program which solves $Ay=b$ for given $b$ with a matrix approximating $A$
- This can be achieved using a few steps of unpreconditioned GMRES (inner iteration loop), while more accurate approximation of $A$ is used in the outer loop of the fGMRES
- FMM speed substantially depends on the accuracy
- Low accuracy FMM can provide fast enough preconditioning

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Tests for sphere

Typicall configuration:
Comparing with analytical solution, which is available

Incident wave

ka=30
Preconditioning

Neumann problem:
$ka=50$ ($kD=173$), mesh: 202,808 panels, 101,402 vertices, overall accuracy: $5e-4$,
Time for mat-vec product in the outer loop: 9.75 sec, in the inner loop: 1.4 sec.
Overall solution time: unpreconditioned ~ 1200 sec, preconditioned: ~ 400 sec
(4 core PC, OMP parallelized algorithm)

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Spurious modes

\[ \theta \]

\[ ka=9.424778 \]

Green's Identity

Burton-Miller

Analytical

N=15002
M=30000

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Scaling with $kD$

In numerical experiments $kD$ varied in range $0.0001 \leq kD \leq 500$
For the largest $kD$ mesh contained 1,500,002 vertices and 3,000,000 panels
Comparison with data available in the literature


$k_D=435$, Robin problem, impedance=$10-10i$

<table>
<thead>
<tr>
<th># elements</th>
<th>N (unknowns)</th>
<th>T (s)</th>
<th>M (GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tong et al (1 core)</td>
<td>1,046,528</td>
<td>1,046,528</td>
<td>54,267</td>
</tr>
<tr>
<td>Present (1) (4 core)</td>
<td>1,130,988</td>
<td>565,496</td>
<td>3,820</td>
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<tr>
<td>Present (2) (4 core)</td>
<td>2,096,688</td>
<td>1,048,346</td>
<td>7,762</td>
</tr>
</tbody>
</table>
Complex shapes

N_{\text{vert}} = 54,945
N_{\text{elem}} = 109,882

N_{\text{vert}} = 65,539
N_{\text{elem}} = 132,072

N_{\text{vert}} = 520,192
N_{\text{elem}} = 1,038,336

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Recently this method was incorporated into commercial products

(Fantalgo, LLC: BEM/FMM)
(ESI group: VA One)
Conclusion

- Practical acoustical scattering problems require wideband computations for \( kD \) in range \( 10^{-4}-10^3 \) and meshes with up to millions elements.
- Such problems can be solved by contemporary PCs which employ advanced algorithms, such as FMM and use advantage of multicore architectures.
- FMM based preconditioning enable speed up of solution several times and substantially reduce memory.
- Use of Burton-Miller (or combined) BIE is important to handle nearly resonance cases and high frequency modes (substantially accelerate convergence).
- Algorithm is scaled in complexity as \((kD)^{2.4}\) or so at large \(kd\leq 500\).
- It is important to provide stabilization of some numerical procedures for the present algorithm. Additional research is needed to obtain stable methods for high \(kd\).
Thank you!