An Fast Direct Solver for Helmholtz with Proxy Compression

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Team

My Research Focus:

1. High Performance & Scientific Computing
2. Fast algorithms for Integral Equations
3. Software Engineering

Find our Software on GitHub:
https://github.com/betckegroup
https://github.com/fastalgorithms

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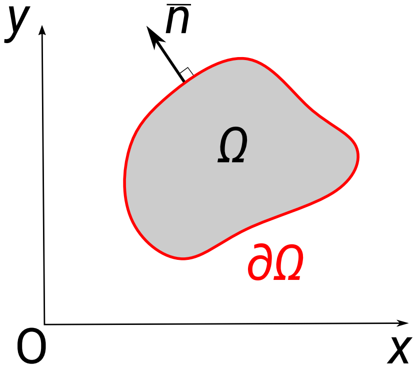
Motivation I

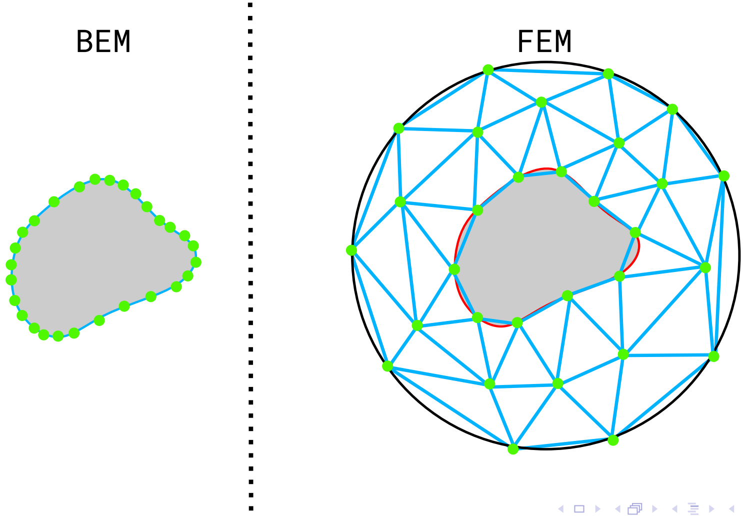
Consider a simple exterior scattering problem in 2D, where we can impose different boundary conditions.

$$(\Delta + k^2)u^s = 0$$



Motivation II

$$(\Delta + k^2)u^s = 0$$



Motivation III

- BEM gives us dense matrices
- Computational cost of naively applying to a vector is $O(N^2)$, matrix-vector product or 'matvec'.
- Computational cost of naively inverting is $O(N^3)$, e.g LU, Gaussian Elimination, QR etc.

Can we take advantage of the properties of our equation to do better than this? Yes! $\rightarrow$ fast algorithms can, in the best case, reduce the application **and** inversion cost to just $O(N)$.

Fast Algorithms I

Fast algorithms enable:

1. Fast particle simulation, e.g. electrostatics and gravitation - the original application!
2. Fast iterative methods for PDEs, e.g. Krylov subspace methods. an $O(N)$ matvec giving a final complexity of $O(N \cdot n_{\text{iter}})$.
3. $O(N)$ Fast direct solvers for matrix inversion, better than iterative methods for problems that involve multiple right hand sides.
4. Time-dependent problems, can solve a fixed geometry at each time step.
5. Can solve a geometry that undergoes low-rank perturbations.

Fast Algorithms II

Late 1980s

- 'Analytic' Fast Multipole Methods - based on analytical multipole series expansions of kernel. $O(N)$ matvec for Laplace, Helmholtz, Stokes (Greengard and Rokhlin, 1987)

1990s/2000s

- Multilevel methods (e.g. $\mathcal{H}$ and $\mathcal{H}^2$ matrices) for fast matvecs and inversion (Hackbusch, 1999), (Hackbusch and Khoromskij 2000).
- 'Semi-Analytic' Kernel Independent Fast Multipole Methods - based on kernel evaluations rather than analytical multipole series expansions of kernel. Easier to write generic software implementations. (Ying et al, 2004)

2010s

- FMM software implementations that can process up to $O(10^6)$ of points per second (Malhotra and Biros, 2015)
- Fast direct solvers and software for 2D and 3D problems (Ambikasaran and Darve, 2014), (Minden et al., 2017)

2020s ...

From Analytic to Algebraic Fast algorithms

Drawbacks of analytic FMM, and analytic fast algorithms. Give sketch of semi-analytic methods, and what might be accomplished by a fully algebraic method.

Algebraic Fast Algorithms for Matrix Inversion

Fast direct solvers, overview of what they are trying to accomplish, and of course the major pros and cons.

Summary

Summarise the motivation for fast algorithms, and briefly discuss their other applications outside of integral equations.

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FMM-LU: A fast direct solver for BIEs

Introduce motivation behind FMM-LU (RS-S).

Proxy Compression I

Proxy Compression II

Helmholtz - Sound Hard I

Let's consider the exterior acoustic scattering problem in 3D, with sound-hard boundary conditions, for low-frequencies.

$$(\Delta + k^2)u^s(x) = 0, \;\; x \in \mathbb{R}^3 \setminus \Omega$$
$$\frac{\partial u^s}{\partial n} = -\frac{\partial u^i}{\partial n}, \;\; \text{on } \Gamma$$

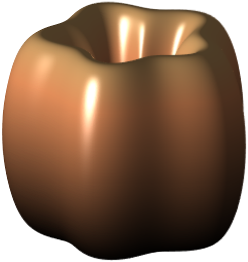


Figure 1: 'Wiggly Torus', test geometry

Helmholtz - Sound Hard II

Using a regularised representation, form a boundary integral equation.

$$u^s(x) = (\mathcal{D}_k \circ \mathcal{S}_K - i\eta\mathcal{S}_k)\mu(x), \;\; x \in \mathbb{R}^3 \setminus \Omega$$

$$\left(i\eta(\frac{1}{2}\mathcal{I} - \mathcal{D}_k') - \frac{1}{4}I + (\mathcal{D}_k')^2 \right) \mu(x) = g$$

Helmholtz - Sound Hard III

Using a Calderon Identity, can form a system of equations, which we proceed to discretise.

$$\mathcal{T}_k \circ \mathcal{S}_k = -\frac{1}{4}\mathcal{I} + (\mathcal{D}'_k)^2$$

$$\begin{pmatrix} (\frac{i\eta}{2} - \frac{1}{4})\mathcal{I} - i\eta\mathcal{D}'_k & \mathcal{D}'_k \\ \mathcal{D}'_k & -\mathcal{I} \end{pmatrix} \begin{pmatrix} \mu \\ \theta \end{pmatrix} = \begin{pmatrix} g \\ 0 \end{pmatrix}$$

Helmholtz - Sound Hard, Numerical Results I

Experiment where density is generated by 50 random charged placed inside the torus.

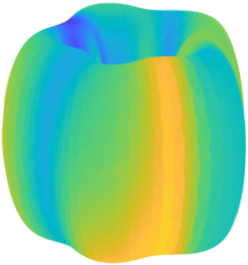
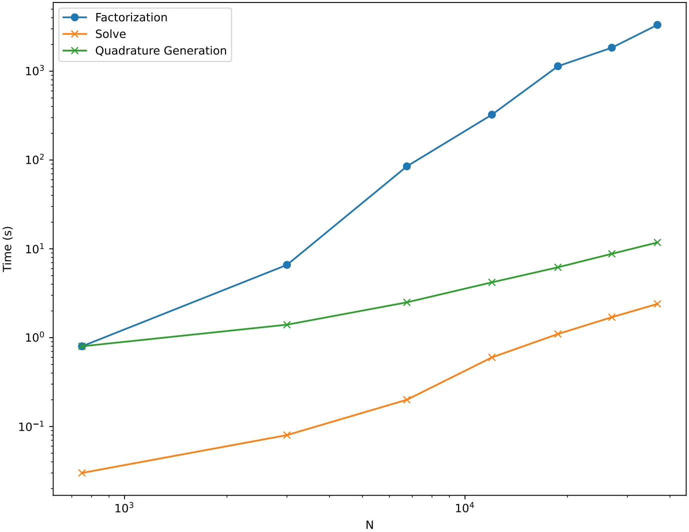


Figure 2: Real component of density solved for $p = 4$, $N_{\text{patch}} = 200$ $N = 3000$.

Helmholtz - Sound Hard, Numerical Results II



Helmholtz - Transmission

Towards Maxwell

$$
\begin{aligned}
\nabla \times \nabla \times e - k^2 e = 0, &\quad x \in \mathbb{R}^3 \setminus \Omega \\
e \times \nu = 0, &\quad x \in \Gamma
\end{aligned}
$$

+Silver Muller Radiation Condition

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Future Directions

1. Complete a first FDS for Maxwell.
2. Unification of software landscape for fast solvers in Rust.