

An Introduction to Fast Direct Solvers for Acoustic Scattering

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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>



Srinath Kailasa
GitHub: skailasa



Manas Rachh
GitHub: mrachh

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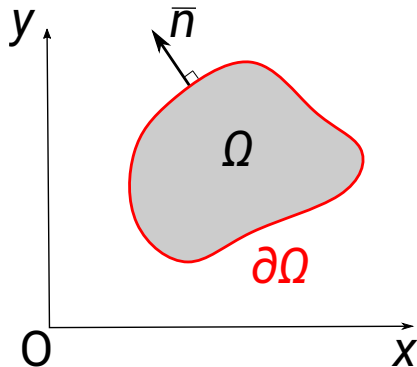
Fast Direct Solvers

Future Directions

Motivation I

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

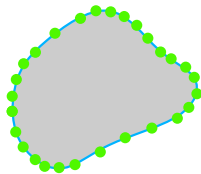
$$(\Delta + k^2)u^s = 0$$



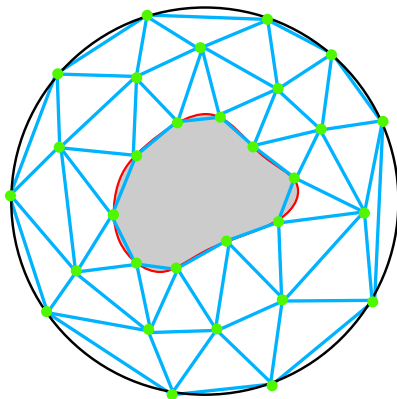
Motivation II

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

BEM



FEM



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

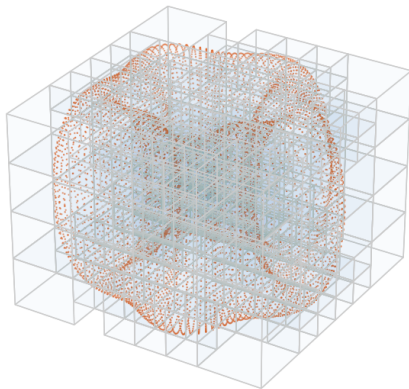
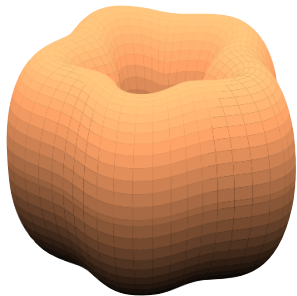
- Multilevel methods (e.g. \mathcal{H} and \mathcal{H}^2 matrices) for fast matvecs and inversion (Hackbusch, 1999), (Hackbusch and Khoromskij 2000).
- 'Semi-Analytic' Kernel Independent Fast Multipole Methods - based on kernel evaluations rather than analytical multipole series expansions of kernel.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

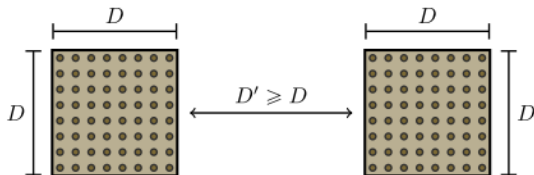
2020s ...

Intuition Behind Fast Solvers I



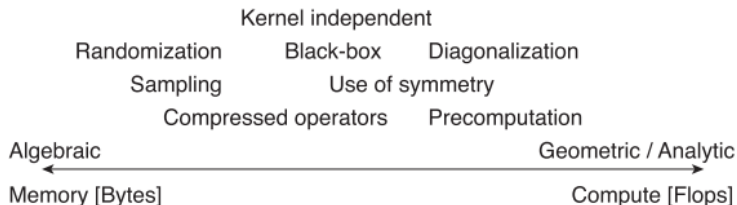
Sources evenly spaced on the surface of a 'wiggly torus'

Intuition Behind Fast Solvers II



Two 'well separated' quadtree boxes (Minden et. al 2017)

From Analytic to Algebraic Fast Algorithms



Compute/Memory trade-off between analytical and algebraic fast-algorithms, (Yokota et. al 2016)

Fast Direct Solvers for Matrix Inversion

Aim to invert dense matrices that arise from discretisations where low-rank approximation applies faster than $O(N^3)$. In $O(N)$ of we can.

- Low rank assumption fails for high-frequency Helmholtz.
- Rank scaling even worse in 2D and 3D problems.
- Most approaches have been algebraic.
- Our approach is also algebraic, with some niceties, that help us tackle a (low-frequency) 3D Helmholtz scattering problem.



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FMM-LU: A fast direct solver for BIEs

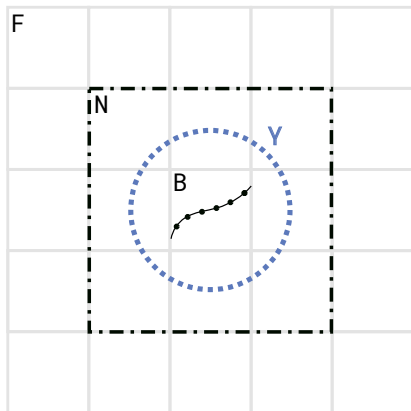
- An algebraic FDS that is based on Recursive Strong Skeletonization (RS-S) (Minden et. al, 2017).
- Computes an approximate factorization into block triangular matrices and a block diagonal matrix, ready for $O(N)$ inversion and application.
- RS-S can be accelerated with the 'proxy compression' trick.
- FMM-LU extends RS-S with quadratures that can handle oscillatory kernels and multiscale geometries.

Contributions

- Formulation of proxy trick for acoustic scattering problems.
- Results from numerical experiments for sound-hard acoustic scattering.

Proxy Compression I

$$A_{\mathcal{F}\mathcal{B}} = B_{\mathcal{F}\gamma} C_{\gamma\mathcal{B}}$$



Proxy Compression II

$$A_{\mathcal{F}B} = \begin{bmatrix} A_{QB} \\ A_{PB} \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & B_{\mathcal{P}\gamma} \end{bmatrix} \begin{bmatrix} A_{QB} \\ C_{\gamma B} \end{bmatrix} \quad (1)$$

Proxy Compression III

$$\begin{bmatrix} A_{QB} \\ C_{\gamma B} \end{bmatrix} = \begin{bmatrix} A_{QS} \\ C_{\gamma S} \end{bmatrix} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} \quad (2)$$

Where S and R are the skeleton and redundant points respectively.
Plugging back into our expression (1),

$$A_{FB} = \begin{bmatrix} I & 0 \\ 0 & B_{P\gamma} \end{bmatrix} \begin{bmatrix} A_{QS} \\ C_{\gamma S} \end{bmatrix} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} \quad (3)$$

$$= \begin{bmatrix} A_{QS} \\ B_{P\gamma} C_{\gamma S} \end{bmatrix} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} \quad (4)$$

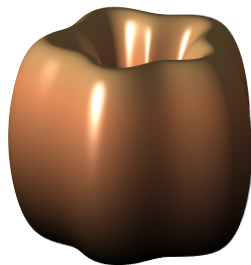
$$= A_{FS} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} \quad (5)$$

Helmholtz - Sound Hard I

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

$$(\Delta + k^2)u^s(x) = 0, \quad x \in \mathbb{R}^3 \setminus \Omega$$

$$\frac{\partial u^s}{\partial n} = -\frac{\partial u^i}{\partial n}, \quad \text{on } \Gamma$$



'Wiggly Torus', test geometry

Helmholtz - Sound Hard II

Using a regularised representation, form a boundary integral equation.

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

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

Helmholtz - Sound Hard III

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

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

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

Formulating Proxy Trick I

A double-layer potential, due to some unknown density ψ , supported on τ ,

$$v(x) = \int_{\Gamma \cap B} \frac{\partial \Phi(x, y)}{\partial n(y)} \psi(y) ds(y) := \mathcal{D}\psi, \quad x \in \mathbb{R}^m \setminus \tau \quad (6)$$

solves the Helmholtz equation everywhere it's valid.

It's normal derivative wrt targets, does not.

$$\frac{\partial v}{\partial n(x)} = \frac{\partial}{\partial n(x)} \int_{\Gamma \cap B} \frac{\partial \Phi(x, y)}{\partial n(y)} \psi(y) ds(y) := \mathcal{T}\psi, \quad x \in \Gamma \cap \mathcal{F} \quad (7)$$

Formulating Proxy Trick II

However, we can separate out the normal part of the derivative,

$$\frac{\partial v}{\partial n(x)} = n(x) \cdot \nabla_x \int_{\Gamma \cap B} \frac{\partial \Phi(x, y)}{\partial n(y)} \psi(y) ds(y) := n \cdot w \quad (8)$$

The function

$$w(x) = \nabla_x \int_{\Gamma \cap B} \frac{\partial \Phi(x, y)}{\partial n(y)} \psi(y) ds(y) := \nabla_x \mathcal{D}\psi \quad (9)$$

Does satisfy our PDE, everywhere.

Formulating Proxy Trick III

Consider an associated boundary value problem for just a single component of \tilde{w} that satisfies,

$$(\Delta + k^2)\tilde{w} = 0, \quad x \in \mathbb{R}^m \setminus D \quad (10)$$

$$\tilde{w} = w_1(x) \quad (11)$$

$$\text{A radiation condition at } \infty \quad (12)$$

A combined field representation might be nice, as we know it has good properties,

$$\tilde{w} = (\mathcal{D} - ik\mathcal{S})_{\mathcal{F}_\gamma} \mu \quad (13)$$

Formulating Proxy Trick IV

Forming the boundary integral equation, and plugging back into the representation for \tilde{w} ,

$$\tilde{w} = (\mathcal{D} - ik\mathcal{S})_{\mathcal{F}\gamma} \left(\frac{1}{2}\mathcal{I} + \mathcal{D} - ik\mathcal{S} \right)_{\gamma\gamma}^{-1} w_1 \quad (14)$$

$$= (\mathcal{D} - ik\mathcal{S})_{\mathcal{F}\gamma} \left(\frac{1}{2}\mathcal{I} + \mathcal{D} - ik\mathcal{S} \right)_{\gamma\gamma}^{-1} \nabla_1 \mathcal{D}_{\gamma B} \psi_\gamma \quad (15)$$

$$\equiv B_{\mathcal{F}\gamma} C_{\gamma B} \psi_\gamma \quad (16)$$

where we identify,

$$C_{\gamma B} = \nabla_1 \mathcal{D}_{\gamma B} \quad (17)$$

Formulating Proxy Trick V

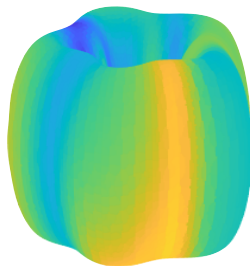
We end up having to compress

$$[\nabla_1 \mathcal{D}_{\gamma B}, \nabla_2 \mathcal{D}_{\gamma B}, \nabla_3 \mathcal{D}_{\gamma B}] \quad (18)$$

for the outgoing problem.

Helmholtz - Sound Hard, Numerical Results I

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



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

Helmholtz - Sound Hard, Numerical Results II

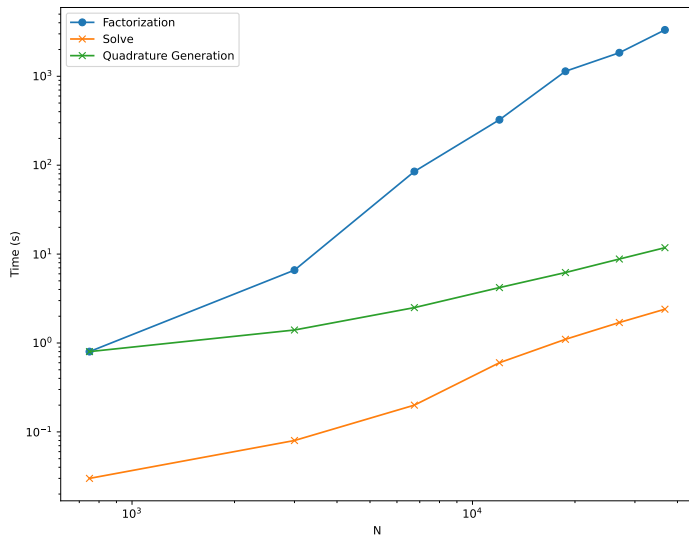


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1. Extend FMM-LU to Transmission problem (scalar)
2. Extend to Maxwell scattering (vector)