A Fast Direct Solver for Helmholtz Problems

Srinath Kailasa [1,2] Manas Rachh [2]

[1] Department of Mathematics, University College London

[2] Centre for Computational Mathematics, Flatiron Institute

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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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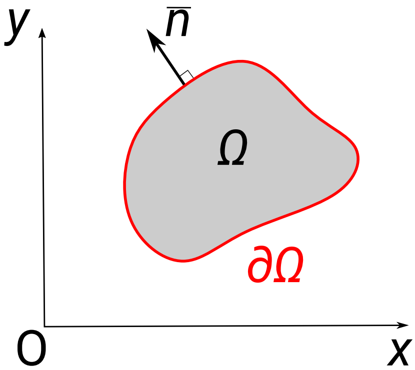
Motivation I

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

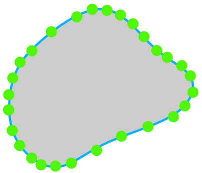
$$(\Delta + k^2)u^s = 0$$



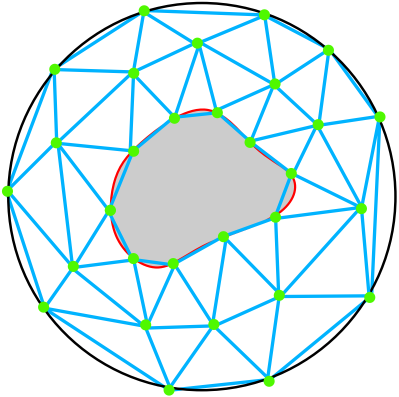
Motivation II

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

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

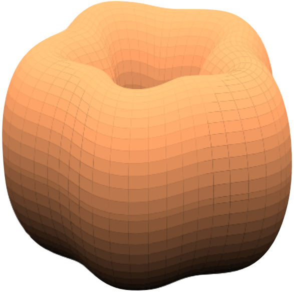
- Multilevel methods (e.g. $\mathcal{H}$ and $\mathcal{H}^2$ matrices) for fast matvecs and inversion (Hackbusch, 1999), (Hackbusch and Khoromskij 2000).
- ‘Semi-Analytic’ Kernel Independent Fast Multipole Methods - based on kernel evaluations rather than analytical multipole series expansions of kernel.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

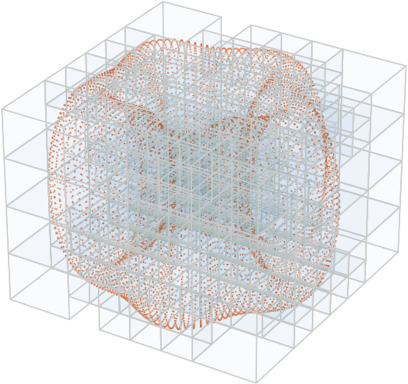
2010s

- 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 ...

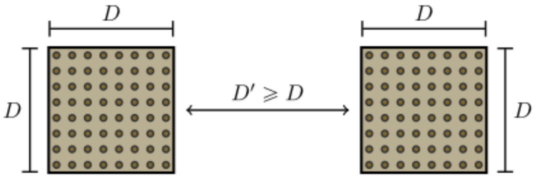
Intuition Behind Fast Solvers I





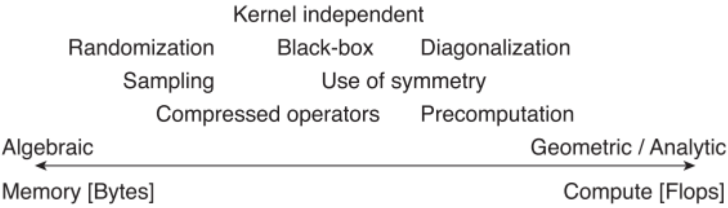
Sources evenly spaced on the surface of a ‘wiggly torus’

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

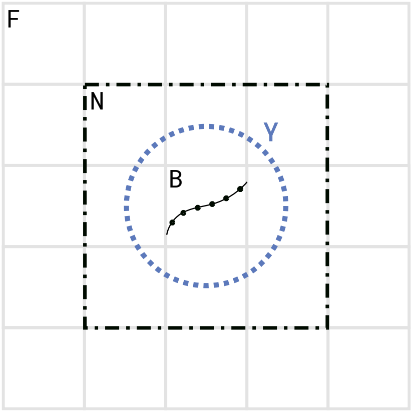
- An algebraic FDS that is based on Recursive Strong Skeletonization (RS-S) (Minden et. al, 2017).
- Computes an approximate factorization into block triangular matrices and a block diagonal matrix, ready for $O(N)$ inversion and application.
- RS-S can be accelerated with the 'proxy compression' trick.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

$$A_{\mathcal{F}B} = \begin{bmatrix} A_{\mathcal{Q}B} \\ A_{\mathcal{P}B} \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & B_{\mathcal{P}\gamma} \end{bmatrix} \begin{bmatrix} A_{\mathcal{Q}B} \\ C_{\gamma B} \end{bmatrix} \tag{1}$$

Proxy Compression III

$$\begin{bmatrix} A_{\mathcal{Q}B} \\ C_{\gamma B} \end{bmatrix} = \begin{bmatrix} A_{\mathcal{Q}S} \\ C_{\gamma S} \end{bmatrix} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} \tag{2}$$

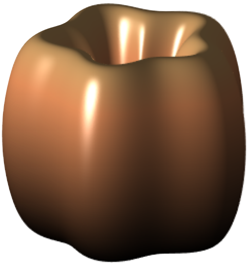
Where S and R are the skeleton and redundant points respectively. Plugging back into our expression (1),

$$\begin{aligned} A_{\mathcal{F}B} &= \begin{bmatrix} I & 0 \\ 0 & B_{\mathcal{P}\gamma} \end{bmatrix} \begin{bmatrix} A_{\mathcal{Q}S} \\ C_{\gamma S} \end{bmatrix} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} && (3) \\ &= \begin{bmatrix} A_{\mathcal{Q}S} \\ B_{\mathcal{P}\gamma} C_{\gamma S} \end{bmatrix} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} && (4) \\ &= A_{\mathcal{F}S} \begin{bmatrix} T_{SR} & 1 \end{bmatrix} && (5) \end{aligned}$$

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.

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

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

Helmholtz - Sound Hard III

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

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

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

Formulating Proxy Trick I

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

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

solves the Helmholtz equation everywhere it's valid.
It's normal derivative wrt targets, does not.

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

Formulating Proxy Trick II

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

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

The function

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

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,

$$(\Delta + k^2)\tilde{w} = 0, \;\; x \in \mathbb{R}^m \setminus D \tag{10}$$
$$\tilde{w} = w_1(x) \tag{11}$$
$$\text{A radiation condition at } \infty \tag{12}$$

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

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

Formulating Proxy Trick IV

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

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

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

$$\equiv B_{\mathcal{F}\gamma} C_{\gamma B}\psi_\gamma \tag{16}$$

where we identify,

$$C_{\gamma B} = \nabla_1 \mathcal{D}_{\gamma B} \tag{17}$$

Formulating Proxy Trick V

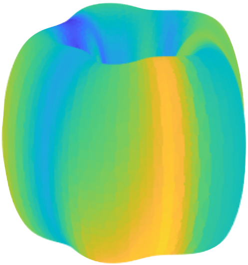
We end up having to compress

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

for the outgoing problem.

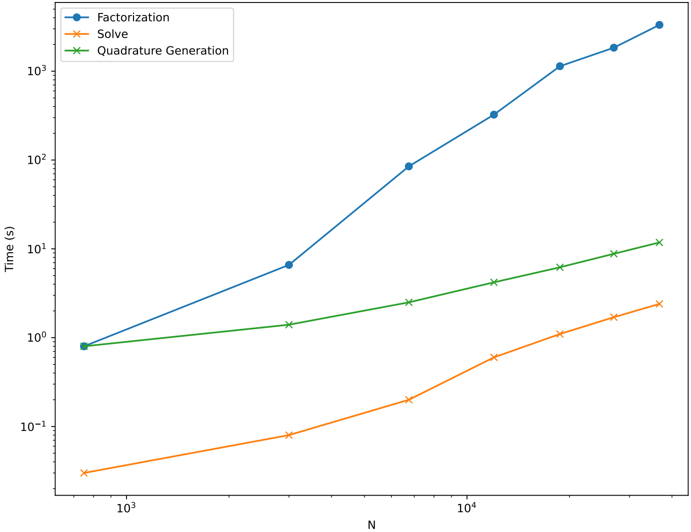
Helmholtz - Sound Hard, Numerical Results I

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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Future Directions

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