# MATH 393C: Fast Methods in Scientific Computing 

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## The potential evaluation map

In this lecture, we will look more carefully at the map that given a source distribution $q$ in a ("source") domain $\Omega_{\mathrm{S}}$ evaluates the potential in a ("target") domain $\Omega_{\mathrm{t}}$ :

$$
[A q](\boldsymbol{x})=\int_{\Omega_{\mathrm{s}}} \phi(\boldsymbol{x}-\boldsymbol{y}) q(\boldsymbol{y}) d A(\boldsymbol{y}), \quad \boldsymbol{x} \in \Omega_{\mathrm{t}}
$$

We will cover two cases in detail:

1. Laplace: $\phi(\boldsymbol{x})=\log |\boldsymbol{x}|$.
2. Helmholtz: $\phi(\boldsymbol{x})=H_{0}^{(1)}(\kappa|\boldsymbol{x}|)$.

The discussion will more generally apply to elasticity, Stokes, the equations of elasticity, time-harmonic Maxwell, etc.

Themes:

- The effective "rank of interaction".
- Loss of information.
- Techniques for "compressing" the interaction.

Let us start with a Laplace problem (for me, it helps to think of it as electro-statics). Suppose we are given two "well-separated" domains $\Omega_{\mathrm{s}}$ and $\Omega_{\mathrm{t}}$.
There are $m$ sources in $\Omega_{\mathrm{s}}$ inducing $n$ potentials in $\Omega_{\mathrm{t}}$.


Let $\mathbf{A}$ denote the $m \times n$ matrix with entries

$$
\mathbf{A}(i, j)=\log \left|\boldsymbol{x}_{i}-\boldsymbol{y}_{j}\right|
$$

Given a vector $\mathbf{q} \in \mathbb{R}^{n}$ of source strengths, we seek a vector of potentials $\mathbf{f} \in \mathbb{R}^{m}$, where

$$
\underset{m \times 1}{\mathbf{f}}=\underset{m \times n}{\mathbf{A}} \underset{n \times 1}{\mathbf{q}}
$$

Using direct evaluation, the cost is $O(m n)$.
$\mathbf{A}$ is the $m \times n$ matrix with entries

$$
\mathbf{A}(i, j)=\log \left|\boldsymbol{x}_{i}-\boldsymbol{y}_{j}\right| .
$$

We seek to evaluate

$$
\mathbf{q} \mapsto \mathbf{f}=\mathbf{A q} .
$$



Target locations $\left\{\boldsymbol{x}_{i}\right\}_{i-1}^{m}$

$\mathbf{A}$ is the $m \times n$ matrix with entries

$$
\mathbf{A}(i, j)=\log \left|\boldsymbol{x}_{i}-\boldsymbol{y}_{j}\right| .
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Target locations $\left\{\boldsymbol{x}_{i}\right\}^{m}$


Multipole Expansion: We showed that we can separate variables in the kernel,

$$
\log |\boldsymbol{x}-\boldsymbol{y}|=\sum_{p=0}^{\infty} B_{p}(\boldsymbol{x}) C_{p}(\boldsymbol{y})
$$

Using polar coordinates,

$$
\boldsymbol{x}-\boldsymbol{c}_{\mathrm{s}}=r e^{i \theta}, \quad \text { and } \quad \boldsymbol{y}-\boldsymbol{c}_{\mathrm{s}}=r^{\prime} e^{i \theta^{\prime}}
$$

the functions $B_{p}$ and $C_{p}$ can (for instance) be

$$
\begin{aligned}
B_{0}(\boldsymbol{x}) & =\log r, & C_{0}(\boldsymbol{y}) & =1 \\
B_{2 p-1}(\boldsymbol{x}) & =-\frac{\sin (p \theta)}{p r^{p}} & C_{2 p-1}(\boldsymbol{y}) & =\left(r^{\prime}\right)^{p} \sin \left(p \theta^{\prime}\right) \\
B_{2 p}(\boldsymbol{x}) & =-\frac{\cos (p \theta)}{p r^{p}} & C_{2 p-1}(\boldsymbol{y}) & =\left(r^{\prime}\right)^{p} \cos \left(p \theta^{\prime}\right)
\end{aligned}
$$

Upon truncation, we have $|\log | \boldsymbol{x}-\boldsymbol{y}\left|-\sum_{p=0}^{k} B_{p}(\boldsymbol{x}) C_{p}(\boldsymbol{y})\right| \lesssim(\sqrt{2} / 3)^{k / 2}$.
$\mathbf{A}$ is the $m \times n$ matrix



$$
\mathbf{q} \mapsto \mathbf{f}=\mathbf{A q} .
$$



Multipole Expansion: The precise form of the factors is not directly relevant for the discussion at hand, so to keep the notation uncluttered, let us simply write the approximation as

$$
\log |\boldsymbol{x}-\boldsymbol{y}| \approx \sum_{p=1}^{k} B_{p}(\boldsymbol{x}) C_{p}(\boldsymbol{y})
$$

Note that we truncated the expansion after $k$ terms, incurring an error $\approx(\sqrt{2} / 3)^{k / 2}$.
(We changed the summation index to start at 1, too.)
$\mathbf{A}$ is the $m \times n$ matrix



$$
\mathbf{q} \mapsto \mathbf{f}=\mathbf{A q} .
$$



Multipole Expansion: Recall the $k$ term multipole expansion:

$$
\begin{equation*}
\log |\boldsymbol{x}-\boldsymbol{y}| \approx \sum_{p=1}^{k} B_{p}(\boldsymbol{x}) C_{p}(\boldsymbol{y}) \tag{1}
\end{equation*}
$$

An approximation (1) is called a separation of variables, and directly leads to a low-rank factorization

$$
\mathbf{A} \approx \mathbf{B} \mathbf{C} .
$$

$$
m \times n \quad m \times k k \times n
$$

where $\mathbf{B}$ has entries $\mathbf{B}(i, p)=B_{p}\left(\boldsymbol{x}_{i}\right)$ and $\mathbf{C}$ has entries $\mathbf{C}(p, j)=C_{p}\left(\boldsymbol{y}_{j}\right)$.


Reduction in cost: From mn flops to $2 k(m+n)$ flops, where $k \sim \log (1 / \varepsilon)$.

Suppose $\mathbf{A}$ is a given $m \times n$ matrix.
Question: What is the theoretically "best" factorization of $\mathbf{A}$ for any given $\varepsilon$ ?
Answer: Consider the singular value decomposition (SVD) of $\mathbf{A}$ :

$$
\begin{aligned}
& \mathbf{A} \approx \mathbf{U} \quad \mathbf{D} \quad \mathbf{V}^{*} \text {. } \\
& m \times n \quad m \times r r \times r r \times n
\end{aligned}
$$

where $r=\min (m, n)$ and where
$\mathbf{U}=\left[\begin{array}{llll}\mathbf{u}_{1} & \mathbf{u}_{2} & \cdots & \mathbf{u}_{r}\end{array}\right] \quad$ is a matrix holding the "left singular vectors" $\mathbf{u}_{i}$,
$\mathbf{V}=\left[\mathbf{v}_{1} \mathbf{v}_{2} \cdots \mathbf{v}_{r}\right] \quad$ is a matrix holding the "right singular vectors" $\mathbf{v}_{i}$,
$\mathbf{D}=\operatorname{diag}\left(\sigma_{1}, \sigma_{2}, \ldots, \sigma_{r}\right)$ is a diagonal matrix holding the "singular values" $\sigma_{i}$.
Let $\|\cdot\|$ denote a matrix norm and let $e_{k}$ denote the minimal error in a rank- $k$ factorization

$$
e_{k}=\min \left\{\left\|\mathbf{A}-\mathbf{A}_{k}\right\|: \mathbf{A}_{k} \text { has rank } k\right\}
$$

Theorem (Eckart-Young): The minimal error is

$$
\begin{aligned}
& e_{k}=\sigma_{k+1} \\
& e_{k}=\sqrt{\sigma_{k+1}^{2}+\sigma_{k+2}^{2}+\cdots+\sigma_{r}^{2}}
\end{aligned}
$$

when the spectral norm is used when the Frobenius norm is used and the minimal error is attained for the SVD truncated to the first $k$ terms

$$
e_{k}=\left\|\mathbf{A}-\sum_{j=1}^{k} \mathbf{u}_{j} \sigma_{j} \mathbf{v}_{j}^{*}\right\|=\left\|\mathbf{A}-\mathbf{U}_{k} \mathbf{D}_{k} \mathbf{V}_{k}^{*}\right\|
$$

$\mathbf{A}$ is the $m \times n$ matrix



$$
\mathbf{q} \mapsto \mathbf{f}=\mathbf{A q} .
$$



Optimal factorization - SVD: Compute the SVD of A, and pick $k$ such that $\sigma_{k+1} \leq \varepsilon$. Set $\mathbf{B}=\mathbf{U}_{k}$ and $\mathbf{C}=\mathbf{D}_{k} \mathbf{V}_{k}^{*}$. Then

$$
\underset{m \times n}{ } \underset{m \times k}{ } \mathbf{A} \underset{k \times n}{ }
$$

is the theoretically most economical factorization of $\mathbf{A}$.
However, the SVD is not quite ideal:

- All factors are determined numerically - expensive!
- The factors $\mathbf{B}$ and $\mathbf{C}$ depend on the precise geometry.

> You have to custom-build all translation operators.

We will next describe a factorization that is almost optimal, and is also easy and economical to work with.

## The Interpolative Decomposition (ID):

Let $\mathbf{A}$ be an $m \times n$ matrix of (precise) rank $k$. Then $\mathbf{A}$ admits a factorization

$$
\begin{gathered}
\mathbf{A}_{m \times n}=\mathbf{A}^{(\text {skel })} \quad \mathbf{V}^{*}, \\
m \times k k \times n
\end{gathered}
$$

where

1. $\mathbf{A}^{(\text {skel })}=\mathbf{A}(:, \tilde{l})$ consists of $k$ columns of $\mathbf{A}$.
2. V contains a $k \times k$ identity matrix.
3. No entry of $\mathbf{V}$ has magnitude greater than 1 (so $\mathbf{V}$ is reasonably well-conditioned). How do you construct an ID in practice?

- Computing an ID that satisfies (3) is (in general) very hard.
- If we relax condition (3) slightly, and require only that, say, $\max _{i j}|\mathbf{V}(i, j)| \leq 1.1$, then it can be done efficiently [1996, Gu \& Eisenstat].
- In practice, simply performing Gram-Schmidt on the columns works great.

After $k$ steps of column pivoted QR, we have

$$
\mathbf{A}(:, I)=\mathbf{Q}\left[\begin{array}{ll}
\mathbf{R}_{11} & \mathbf{R}_{12}
\end{array}\right]=\underbrace{\mathbf{Q} \mathbf{R}_{11}}_{=\mathbf{A}^{(\mathrm{sk}}(\underline{)})} \underbrace{\left[\begin{array}{ll}
\boldsymbol{I} & \mathbf{R}_{11}^{-1} \mathbf{R}_{12}
\end{array}\right]}_{=\mathbf{V}^{*}} .
$$

- If $\mathbf{A}$ does not have exact rank $k$, but its singular values decay rapidly, then the ID resulting from Gram-Schmidt satisfies $\left\|\mathbf{A}-\mathbf{A}^{(\text {skel })} \mathbf{V}^{*}\right\| \approx \sigma_{k+1}$.
$\mathbf{A}$ is the $m \times n$ matrix



$$
\mathbf{q} \mapsto \mathbf{f}=\mathbf{A q} .
$$

We seek to evaluate

Interpolative decomposition (ID): Performing G-S on the columns of A, we obtain

$$
\begin{gathered}
\mathbf{A} \approx \mathbf{A}^{(\text {skel })} \quad \mathbf{V}^{*} \\
m \times n \quad m \times k k \times n
\end{gathered}
$$

where $\mathbf{A}^{(\text {skel })}=\mathbf{A}(:, \tilde{l})$ consists of $k$ columns of $\mathbf{A}$.


The nodes marked in red above are the nodes marked by the index vector $\tilde{I}$.
The interaction of $\Omega_{\mathrm{s}}$ with the outside is through the original kernel function.
$\mathbf{A}$ is the $m \times n$ matrix



$$
\mathbf{q} \mapsto \mathbf{f}=\mathbf{A q} .
$$



Interpolative decomposition (ID): Let's do G-S on the rows of $\mathbf{A}$ as well

$$
\begin{gathered}
\mathbf{A} \approx \underset{m \times n}{m \times k} \mathbf{A}^{(\text {skel })} \quad \mathbf{V}^{*} \\
m \times k \times n
\end{gathered}
$$

where $\mathbf{A}^{(\text {skel })}=\mathbf{A}\left(\tilde{l}_{\mathrm{t}}, \tilde{I}_{\mathrm{s}}\right)$ is a $k \times k$ sub-matrix of $\mathbf{A}$.


Approximation errors as a function of the rank $k$.
Interaction potential is Laplace, $\mathbf{A}(i, j)=\log \left|\mathbf{x}_{i}-\boldsymbol{y}_{j}\right|$.


The 20 skeleton points required for (relative) accuracy $\varepsilon=10^{-12}$. Interaction potential is Laplace, $\mathbf{A}(i, j)=\log \left|\boldsymbol{x}_{i}-\boldsymbol{y}_{j}\right|$.


Conclusions from experiments:

- The SVD and ID are comparable in effectiveness.
(In our case! When the singular values decay slowly, this is not true.)
- The multipole expansion requires more terms.

But, the comparison is not quite fair - the multipole expansion is valid for any source point that is well-separated.

Question: Can we find skeleton points that "work" for any well-separated target point?


First observe that we do not need to consider "every" potential target point.
Let $u$ denote the potential caused by the source points: $u(\boldsymbol{x})=\sum_{j=1}^{n} q_{j} \log \left|\boldsymbol{x}-\boldsymbol{y}_{j}\right|$.
Now suppose that we can accurately reconstruct $u$ on the green square shown:


Observe that $u$ is harmonic (i.e. $-\Delta u=0$ ) outside the green square.
Since the Laplace problem has a unique solution, we know that if we correctly reproduce $u$ on the green square, then it is correctly reproduced everywhere outside the square.


Let $\left\{\boldsymbol{y}_{j}\right\}_{j=1}^{n}$ be sources in the small red box.
Let $\left\{\boldsymbol{x}_{i}\right\}_{i=1}^{m}$ be targets on the large blue box.
Let $\mathbf{A}$ be the matrix with elements $\mathbf{A}(i, j)=\log \left|\boldsymbol{x}_{i}-\boldsymbol{y}_{j}\right|$.
Perform Gram-Schmidt on the columns of $\mathbf{A}$,


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Perform Gram-Schmidt on the columns of $\mathbf{A}$,

$$
\begin{gathered}
\mathbf{A} \approx \mathbf{A}^{(\text {skel })} \quad \mathbf{V}^{*} \\
m \times n \quad m \times k k \times n
\end{gathered}
$$

We know that (to within precision $\varepsilon$ ), this skeleton is valid at any well-separated point. For $\varepsilon=10^{-12}$, we now have $k=45$. It as $k=20$ for the two-box geometry.

One concern remains: So far, we've looked at a given distribution of source locations. The skeleton points chosen are not "universal".

To address this issue, we will henceforth investigate the continuum operator $A$ :

$$
f(\boldsymbol{x})=[A q](\boldsymbol{x})=\int_{\Omega_{\mathrm{s}}} \log |\boldsymbol{x}-\boldsymbol{y}| q(\boldsymbol{y}) d \boldsymbol{y}, \quad \boldsymbol{x} \in \Omega_{\mathrm{t}}
$$

which maps a source distribution $q$ in a source domain $\Omega_{\mathrm{S}}$ to a potential $f$ in a target domain $\Omega_{\mathrm{t}}$.

Let $\left\{\boldsymbol{x}_{i}, v_{i}\right\}_{i=1}^{m}$ be a quadrature for the target domain, and let $\left\{\boldsymbol{y}_{j}, w_{j}\right\}_{j=1}^{n}$ be a quadrature for the source domain.
Let the vector $\mathbf{f}$ have entries $\mathbf{f}(i)=\sqrt{v_{i}} f\left(\boldsymbol{x}_{i}\right)$ so that $\|f\|_{L^{2}\left(\Omega_{\mathrm{t}}\right)} \approx\|\mathbf{f}\|_{\ell^{2}}$.
Let the vector $\mathbf{q}$ have entries $\mathbf{q}(j)=\sqrt{w_{j}} q\left(\boldsymbol{y}_{j}\right)$ so that $\|q\|_{L^{2}\left(\Omega_{s}\right)} \approx\|\mathbf{q}\|_{\ell^{2}}$.
Finally, let $\mathbf{A}$ be the $m \times n$ matrix with entries $\mathbf{A}(i, j)=\sqrt{v_{i}} \log \left|\boldsymbol{x}_{i}-\boldsymbol{y}_{j}\right| \sqrt{w_{j}}$.
Then the singular values/vectors of $\mathbf{A}$ are accurate approximations of the singular values/vectors of $A$.

Observe that when $\Omega_{\mathrm{s}}$ and $\Omega_{\mathrm{t}}$ are not "too close," the kernel $\log |\boldsymbol{x}-\boldsymbol{y}|$ is smooth.

Example: Two concentric circles - ideal for multipole expansion.


Sources in a disc of radius 0.5, targets on a circle of radius 1.5.

Example: Two concentric circles - ideal for multipole expansion.


Sources in a disc of radius 0.5, targets on a circle of radius 1.5. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=44$.

Example: Two concentric circles - ideal for multipole expansion.


Errors. For this geometry, $E_{\text {mpole }}=E_{\text {svd }}$ exactly!

Example: Two concentric circles - now much tighter.


Sources in a disc of radius 0.5, targets on a circle of radius 0.75 .

Example: Two concentric circles - now much tighter.


Sources in a disc of radius 0.5, targets on a circle of radius 1.5. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=81$.

Example: Two concentric circles - now much tighter.


Errors. For this geometry, $E_{\text {mpole }}=E_{\text {svd }}$ exactly!
(The weirdness at the end reflects the discretization error.)

Example: Two squares - realistic FMM geometry.


Sources in a box of side length 1, targets on a box of side length 3.

Example: Two squares - realistic FMM geometry.


Sources in a box of side length 1, targets on a box of side length 3. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=47$.

## Example: Two squares - realistic FMM geometry.



Errors.

Example: Two squares - now tighter.


Sources in a box of side length 1, targets on a box of side length 1.6.

Example: Two squares - now tighter.


Sources in a box of side length 1, targets on a box of side length 1.6. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=108$.

## Example: Two squares - now tighter.



Sources in a box of side length 1, targets on a box of side length 1.6.

Example: Two squares - now even tighter.


Sources in a box of side length 1, targets on a box of side length 1.2.

Example: Two squares - now even tighter.


Sources in a box of side length 1, targets on a box of side length 1.2. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=260$.

## Example: Two squares - now even tighter.



Sources in a box of side length 1, targets on a box of side length 1.2.

Example: A piece of a contour.


## Example: A piece of a contour.



Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=25$.

## Example: A piece of a contour.



Skeletonization can be performed for $\Omega_{\mathrm{S}}$ and $\Omega_{\mathrm{T}}$ of various shapes.


Rank $=29$ at $\varepsilon=10^{-10}$.


Rank $=48$ at $\varepsilon=10^{-10}$.

Adjacent boxes can be skeletonized.


Rank $=46$ at $\varepsilon=10^{-10}$.


## Benefits:

- The rank is typically very close to optimal.
- The projection and interpolation are well-conditioned.
- An inexpensive local computation (e.g. Gram-Schmidt) determines:
- The $k$ skeleton points.
- Matrices U and V.
- The map $\mathbf{A}^{\text {skel }}$ has the same kernel as $\mathbf{A}$.
(We loosely say that "the physics of the problem is preserved".)
- The skeleton points can be determined either as generic points valid for any source distribution, or as a subset of a given set of points. In the latter case $\mathbf{U}$ and $\mathbf{V}$ contain $k \times k$ identity matrices.
- Interaction between adjacent boxes can be compressed (no buffering is required).

Before closing this topic, let us briefly consider the Helmholtz problem.
Recall that the Helmholtz equation is associated with the classical wave equation

$$
\begin{equation*}
-v^{2} \Delta \phi=-\frac{\partial^{2} \phi}{\partial t^{2}} \tag{2}
\end{equation*}
$$

where $v$ is the wave-speed. Assume $\phi(\boldsymbol{x}, t)=u(\boldsymbol{x}) e^{i \omega t}$. Then (2) turns into

$$
\begin{equation*}
-v^{2} \Delta u=\omega^{2} u \tag{3}
\end{equation*}
$$

We define the "wave number" as $\kappa=\omega / v$, and can then write (3) as

$$
\begin{equation*}
-\Delta u-\kappa^{2} u=0 \tag{4}
\end{equation*}
$$

A typical "free-space" problem for the Helmholtz equation could read

$$
\left\{\begin{align*}
-\Delta u(\boldsymbol{x})-\kappa^{2} u(\boldsymbol{x}) & =q(\boldsymbol{x}), & & \boldsymbol{x} \in \mathbb{R}^{2}  \tag{5}\\
\frac{\partial u(\boldsymbol{x})}{\partial|\boldsymbol{x}|}-i \kappa u(\boldsymbol{x}) & =O\left(\frac{1}{|\boldsymbol{x}|}\right) & & |\boldsymbol{x}| \rightarrow \infty
\end{align*}\right.
$$

where the condition "at infinity" is called a "radiation condition."
We typically consider $u$ to be a complex valued potential.
The fundamental solution is $H_{0}^{(1)}(\kappa|\boldsymbol{x}|)$, so the solution to (5) is

$$
u(\boldsymbol{x})=\int_{\mathbb{R}^{2}} H_{0}^{(1)}(\kappa|\boldsymbol{x}-\boldsymbol{y}|) q(\boldsymbol{y}) d \boldsymbol{y}
$$

Plots of the fundamental solution $H_{0}^{(1)}(|\boldsymbol{x}|)=J_{0}(|\boldsymbol{x}|)+i Y_{0}(|\boldsymbol{x}|)$.


Real part
$J_{0}$


Negative imaginary part

$$
-Y_{0}
$$

Plots of the fundamental solution $H_{0}^{(1)}(|\boldsymbol{x}|)=J_{0}(|\boldsymbol{x}|)+i Y_{0}(|\boldsymbol{x}|)$.
Now zoom in to the origin:


Real part

$$
J_{0}
$$



Negative imaginary part

$$
-Y_{0}
$$

Logarithmic singularity at the origin!

Example of solution of the Helmholtz equation $-\Delta u-\kappa^{2} u=g$
Suppose we are given point charges $\left\{q_{j}\right\}_{j=1}^{5}$ in a "source domain" $\Omega_{s}$.
We are interested in the potential in a "target domain" $\Omega_{\mathrm{t}}$.
Helmholtz problem. Side of boxes $=0.80$ lambda


The source domain $\Omega_{\mathrm{S}}(\mathrm{red})$ and the target domain $\Omega_{\mathrm{t}}$ (blue).

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Real part of field generated by the sources (truncated - the peaks go to infinity).

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## Example of solution of the Helmholtz equation $-\Delta u-\kappa^{2} u=g$

Suppose we are given point charges $\left\{q_{j}\right\}_{j=1}^{5}$ in a "source domain" $\Omega_{s}$. We are interested in the potential in a "target domain" $\Omega_{\mathrm{t}}$. Now for larger $\kappa$ !

Helmholtz problem. Side of boxes $=6.37$ lambda


Real part of field generated by the sources (truncated - the peaks go to infinity).

## Example of solution of the Helmholtz equation $-\Delta u-\kappa^{2} u=g$

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Helmholtz problem. Side of boxes $=6.37$ lambda


Absolute value of field generated by the sources (truncated - the peaks go to infinity).

## Example of solution of the Helmholtz equation $-\Delta u-\kappa^{2} u=g$

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Helmholtz problem. Side of boxes $=6.37$ lambda


Absolute value of field generated by the sources (truncated - the peaks go to infinity).

Superficially, almost everything we've discussed for the Laplace case carries right over to the Helmholtz case.

For instance, there is a "multipole expansion." Set

$$
\begin{aligned}
& S_{n}(\boldsymbol{x})=H_{n}^{(1)}(\kappa r) e^{-i n \theta} \\
& R_{n}(\boldsymbol{x})=J_{n}(\kappa r) e^{i n \theta} .
\end{aligned}
$$

Then

$$
H_{0}^{(1)}(\kappa|\boldsymbol{x}-\boldsymbol{y}|)=\sum_{n=-\infty}^{\infty} S_{n}(\boldsymbol{x}) R_{n}(\boldsymbol{y}), \quad \text { when }|\boldsymbol{x}|>|\boldsymbol{y}| .
$$

## Example: Two squares - Helmholtz — small wave number.

The geometry: Source region has side $=0.875$ lambda


Sources in a box of side length 0.9 $\lambda$, targets on a box of side length 2.6 $\lambda$.

Example: Two squares - Helmholtz — small wave number.

Skeleton points: eps=1.0e-12 k=49 side of source box $=0.875$ lambda


Sources in a box of side length 0.9 $\lambda$, targets on a box of side length 2.6 $\lambda$. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=49$.

Example: Two squares - Helmholtz - small wave number.


Sources in a box of side length $0.9 \lambda$, targets on a box of side length $2.6 \lambda$.

Example: Two squares - Helmholtz - medium wave number.

The geometry: Source region has side $=8.117$ lambda


Sources in a box of side length 8.1 $\lambda$, targets on a box of side length 24.4 $\lambda$.

Example: Two squares - Helmholtz - medium wave number.

Skeleton points: eps=1.0e-12 k=118 side of source box $=8.117$ lambda


Sources in a box of side length 8.1 $\lambda$, targets on a box of side length 24.4 $\lambda$. Skeleton to precision $\varepsilon=10^{-12}$, which requires $k=118$.
Observe how many points are now internal - they used to cluster along the boundary.

Example: Two squares - Helmholtz - medium wave number.


Sources in a box of side length 8.1 $\lambda$, targets on a box of side length 24.4 $\lambda$.

## Complications with the Helmholtz problem:

1. Decay of singular values starts happening only for sub-wave-length scales.

For geometries that are "large" in terms of wave-lengths, rank considerations alone will be not be sufficient.
2. Resonances are possible. Consider for instance the Dirichlet boundary value problem:

$$
\left\{\begin{aligned}
-\Delta u(\boldsymbol{x})-\kappa^{2} u(\boldsymbol{x}) & =0, & & \boldsymbol{x} \in \Omega \\
u(\boldsymbol{x}) & =f(\boldsymbol{x}), & & \boldsymbol{x} \in \partial \Omega
\end{aligned}\right.
$$

where $\Omega$ is a "simple" finite domain. There exist a sequence of wave-numbers $0 \leq \kappa_{1} \leq \kappa_{2} \leq \kappa_{3} \leq \cdots$ for which the BVP is ill-posed. These are the numbers for which $\kappa_{j}^{2}$ is an eigenvalue of $-\Delta$. At these "resonant wave-numbers" there exist non-trivial solutions for $f=0$.

This creates complications in setting up proxy charges (need two layers, or use both monopoles and dipoles, e.g.).
3. While the Laplace equation has a simple "maximum principle" (a harmonic function attains its max on the boundary), the Helmholtz equation is more complicated.
4. Etc.

Similar schemes have been proposed by many researchers:

1993 - C.R. Anderson<br>1995-C.L. Berman<br>1996 - E. Michielssen, A. Boag<br>1999-J. Makino<br>2004 - L. Ying, G. Biros, D. Zorin<br>A mathematical foundation:<br>1996 - M. Gu, S. Eisenstat

