Fast Algorithms and Integral Equation Methods
CS598APK

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Fall 2022
Outline

Introduction

Dense Matrices and Computation

Tools for Low-Rank Linear Algebra

Rank and Smoothness

Near and Far: Separating out High-Rank Interactions

Outlook: Building a Fast PDE Solver

Going Infinite: Integral Operators and Functional Analysis

Singular Integrals and Potential Theory

Boundary Value Problems

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What’s the point of this class?

- Starting point: Large-scale scientific computing
- Many popular numerical algorithms: $O(n^\alpha)$ for $\alpha > 1$
  (Think Matvec, Matmat, Gaussian Elimination, LU, ...)
- Build a set of tools that lets you cheat: Keep $\alpha$ small
  (Generally: probably not–Special purpose: possible!)
- Final goal: Extend this technology to yield PDE solvers
- But: Technology applies in many other situations
  - Many-body simulation
  - Stochastic Modeling
  - Image Processing
  - ‘Data Science’ (e.g. Graph Problems)
- This is class is about an even mix of math and computation
Survey

- Home dept
- Degree pursued
- Longest program ever written
  - in Python?
- Research area
- Interest in PDE solvers

contains:
- Class outline
- Assignments
- Piazza
- Grading
- Video
Why study this at all?

- Finite difference/element methods are inherently ill-conditioned and tricky to get high accuracy with.
- Build up a toolset that does not have these flaws.
- Plus: An interesting/different analytical and computational point of view.
  - If you’re not going to use it to solve PDEs, it (or the ideas behind it) will still help you gain insight.
FD/FEM: Issues

Idea of these methods:

1. Take differential equations
2. Discretize derivatives
3. Make linear system
4. Solve

So what’s wrong with doing that?
Discretizing Derivatives: Issues?
Discretizing Derivatives: Issues?

Result: The better we discretize (the more points we use), the worse the condition number gets.

Demo: Conditioning of Derivative Matrices
To be fair: Multigrid works around that (by judiciously using fewer points!)
But there’s another issue that’s not fixable.

Q: Are these problems real?

So this class is about starting fresh with methods that (rigorously!) don’t have these flaws!
Both multigrid and fast/IE schemes ultimately are $O(N)$ in the number of degrees of freedom $N$. 
Open Source <3

These notes (and the accompanying demos) are open-source!

Bug reports and pull requests welcome:
https://github.com/inducer/fast-alg-ie-notes

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Matvec: A Slow Algorithm

Matrix-vector multiplication: our first ‘slow’ algorithm. $O(N^2)$ complexity.

$$\beta_i = \sum_{j=1}^{N} A_{ij} \alpha_j$$

Assume $A$ dense.
Matrices and Point Interactions

$$A_{ij} = G(x_i, y_j)$$

Does that actually change anything?
Matrices and Point Interactions

\[ A_{ij} = G(x_i, y_j) \]

Graphically, too:
Matrices and point Interactions

\[
\psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j) \phi(y_j)
\]

This feels different.

Q: Are there enough matrices that come from globally defined G to make this worth studying?
Point Interaction Matrices: Examples (I)
Point Interaction Matrices: Examples (II)
So yes, there are indeed lots of these things.
Integral Operators

Why did we go through the trouble of rephrasing matvecs as

\[ \psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j)\varphi(y_j) \]
Cheaper Matvecs

\[ \psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j) \varphi(y_j) \]

So what can we do to make evaluating this cheaper?
Fast Dense Matvecs

Consider

\[ A_{ij} = u_i v_j, \]

let \( u = (u_i) \) and \( v = (v_j) \).

Can we compute \( Ax \) quickly? (for a vector \( x \))
Fast Dense Matvecs (II)

\[ A = u_1 v_1^T + \cdots + u_K v_K^T \]

Does this generalize? What is \( K \) here?
Low-Rank Point Interaction Matrices

Usable with low-rank complexity reduction?

\[ \psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j) \varphi(y_j) \]
Numerical Rank

What would a *numerical* generalization of ‘rank’ look like?
Eckart-Young-Mirsky Theorem

Theorem (Eckart-Young-Mirsky)

SVD $A = U\Sigma V^T$. If $k < r = \text{rank}(A)$ and

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T,$$

then

$$\min_{\text{rank}(B) = k} |A - B|_2 = |A - A_k|_2 = \sigma_{k+1}.$$ 

Q: What’s that error in the Frobenius norm?
So in principle that’s good news:

- We can find the numerical rank.
- We can also find a factorization that reveals that rank (!)

Demo: Rank of a Potential Evaluation Matrix (Attempt 2)
Constructing a tool

There is still a slight downside, though.
Representation

What does all this have to do with (right-)preconditioning?
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- Low-Rank Approximation: Error Control
- Reducing Complexity

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Rephrasing Low-Rank Approximations

SVD answers low-rank-approximation (‘LRA’) question. But: too expensive. First, rephrase the LRA problem:
Using LRA bases

If we have an LRA basis $Q$, can we compute an SVD?
Finding an LRA basis

How would we *find* an LRA basis?
Giving up optimality

What problem should we actually solve then?
Recap: The Power Method

How did the power method work again?
How do we construct the LRA basis?

Put randomness to work:
Tweaking the Range Finder (I)

Can we accelerate convergence?
Tweaking the Range Finder (II)

What is one possible issue with the power method?
Assumptions on $\Omega$ are pretty weak—can use more or less anything we want. → Make it so that we can apply the matvec $A\Omega$ in $O(n \log \ell)$ time. How? Pick $\Omega$ as a carefully-chosen subsampling of the Fourier transform.
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If we use the randomized range finder, how close do we get to the optimal answer?

**Theorem**

For an $m \times n$ matrix $A$, a target rank $k \geq 2$ and an oversampling parameter $p \geq 2$ with $k + p \leq \min(m, n)$, with probability $1 - 6 \cdot p^{-p}$,

$$\left| A - QQ^T A \right|_2 \leq \left( 1 + 11 \sqrt{k + p \sqrt{\min(m, n)}} \right) \sigma_{k+1}.$$  

(given a few more very mild assumptions on $p$)

[Halko/Tropp/Martinsson ‘10, 10.3]

**Message:** We can probably (!) get away with oversampling parameters as small as $p = 5$. 
A-posteriori and Adaptivity

The result on the previous slide was \textit{a-priori}. Once we're done, can we find out ‘how well it turned out’?
Adaptive Range Finding: Algorithm
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Rank-revealing/pivoted QR

Sometimes the SVD is too good (aka expensive)–we may need less accuracy/weaker promises, for a significant decrease in cost.
Using RRQR for LRA
Interpolative Decomposition (ID): Definition

Would be helpful to know *columns of* $A$ *that contribute ‘the most’ to the rank.*

(orthogonal transformation like in QR ’muddies the waters’)


ID: Computation

How do we construct this (from RRQR): (short/fat case)

Q: What is $P$, in terms of the RRQR?
What does row selection mean for the LRA?

[Martinsson, Rokhlin, Tygert '06]
Slight tradeoff here: what?

How would we use the ID in the context of the range finder?

Demo: Interpolative Decomposition
What does the ID buy us?

Name a property that the ID has over other factorizations.

All our randomized tools have two stages:

1. Find ONB of approximate range
2. Do actual work only on approximate range

Complexity?

What is the impact of the ID?
Leveraging the ID for SVD (I)

Build a low-rank SVD with row extraction.
Leveraging the ID for SVD (II)

In what way does this give us an SVD of $A$?
Q: Why did we need to do the row QR?
Where are we now?

- We have observed that we can make matvecs faster if the matrix has low-ish numerical rank.
- In particular, it seems as though if a matrix has low rank, there is no end to the shenanigans we can play.
- We have observed that some matrices we are interested in (in some cases) have low numerical rank (cf. the point potential example).
- We have developed a toolset that lets us obtain LRAs and do useful work (using SVD as a proxy for “useful work”) in $O(N \cdot K^\alpha)$ time (assuming availability of a cheap matvec).

Next stop: Get some insight into why these matrices have low rank in the first place, to perhaps help improve our machinery even further.
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- Multipole Expansions
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- Proxy Expansions

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Punchline

What do (numerical) rank and smoothness have to do with each other?

Even shorter punchline?
Smoothing Operators

If the operations you are considering are *smoothing*, you can expect to get a lot of mileage out of low-rank machinery.

What types of operations are smoothing?

Now: Consider some examples of smoothness, with justification.

How do we judge smoothness?
Recap: Multivariate Taylor
How can we estimate the error in a Taylor expansion?
Now suppose that we had an estimate that
\[ \left| \frac{f^{(p)}(c)}{p!} h^p \right| \leq \alpha^p. \]
Connect Taylor and Low Rank

Can Taylor help us establish low rank of an interaction?
Compute a Taylor expansion of a 2D Laplace point potential.
Why is it interesting to consider Taylor expansions of Laplace point potentials?
Taylor on Potentials (II)
Taylor on Potentials (III)

Which of these is the most dangerous (largest) term?
→ Hard to say. They all contain the same number of powers of components of $y$.

What's a bound on it? Let $R = \sqrt{y_1^2 + y_2^2}$.

$$\left| \frac{5040y_1}{(y_2^2 + y_1^2)^4} \right| \leq C \left| \frac{y_1}{R^8} \right| \leq C \frac{1}{R^7}.$$

'Generalize' this bound:

$$|D^p \psi| \leq C_p \left\{ \begin{array}{ll} \log(R) & |p| = 0 \\ R^{-|p|} & |p| > 0 \end{array} \right.$$  

Appears true at least from the few $p$ we tried. (Actually is true.) $C_p$ is a 'generic constant'—its value could change from one time it’s written to the next.
Taylor on Potentials (IV)

What does this mean for the convergence of the Taylor series as a whole?
Lesson: As long as

\[ \frac{\max_i |x_i - c|_2}{\min_j |y_j - c|_2} = \frac{r}{R} < 1, \]

the Taylor series converges.
A few remarks:

▶ We have just invented one specific example of what we will call a *local expansion* (of a potential \( \psi \)).

▶ The abstract idea of a *local expansion* is that:
  
  ▶ it converges on the interior of a ball as long as the closest source is outside that ball,
  
  ▶ The error in approximating the potential by a truncated (at order \( k \)) local expansion is

\[
C_p \left( \frac{r}{R} \right)^{k+1} = \left( \frac{\text{dist}(c, furthest target)}{\text{dist}(c, closest source)} \right)^{k+1}
\]
Local expansions as a Computational Tool

Low rank makes evaluating interactions cheap(er). Do local expansions help with that goal?
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Taylor on Potentials, Again

Stare at that Taylor formula again.
Multipole Expansions (I)

At first sight, it doesn’t look like much happened, but mathematically/geometrically, this is a very different animal. **First Q:** When does this expansion converge?
The abstract idea of a *multipole expansion* is that:

- it converges on the exterior of a ball as long as the furthest source is closer to the center than the closest target,
- The error in approximating the potential by a truncated (at order \( k \)) local expansion is

\[
\left( \frac{\text{dist}(\mathbf{c}, \text{furthest source})}{\text{dist}(\mathbf{c}, \text{closest target})} \right)^{k+1}.
\]

The multipole expansion converges everywhere outside the circle! (Possibly: slowly, if the targets are too close— but it does!)
If our particle distribution is like in the figure, then a multipole expansion is a computationally useful thing. If we set

- $S = \#\text{sources},$
- $T = \#\text{targets},$
- $K = \#\text{terms in expansion},$

then the cost \textit{without} the expansion is $O(ST)$, whereas the cost \textit{with} the expansion is $O(SK + KT)$.

If $K \ll S, T$, then that’s going from $O(N^2)$ to $O(N)$.

The rank (\#terms) of the multipole expansion is the same as above for the local expansion.

\textbf{Demo:} Multipole/local expansions
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Taylor on Potentials: Low Rank?

Connect this to the numerical rank observations:
On Rank Estimates

So how many terms do we need for a given precision $\varepsilon$?

Demo: Checking rank estimates
Estimated vs Actual Rank

Our rank estimate was off by a power of $\log \varepsilon$. What gives?
Taylor and PDEs

Look at $\partial_x^2 G$ and $\partial_y^2 G$ in the multipole demo again. Notice anything?
Being Clever about Expansions

How could one be clever about expansions? (i.e. give examples)
Expansions for Helmholtz

How do expansions for other PDEs arise?

DLMF 10.23.6 shows ‘Graf’s addition theorem’:

\[ H_0^{(1)}(\kappa \| x - y \|_2) = \sum_{\ell=-\infty}^{\infty} \left( H_\ell^{(1)}(\kappa \| y - c \|_2) e^{i\ell\theta'} + J_\ell(\kappa \| x - c \|_2) e^{-i\ell\theta} \right) \]

where \( \theta = \angle(x - c) \) and \( \theta' = \angle(x' - c) \).

Can apply same family of tricks as with Taylor to derive multipole/local expansions.
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Actual expansions cheaper than LA approaches. Can this be fixed? Compare costs for this situation:
The Proxy Trick

**Idea:** Skeletonization using Proxies

**Demo:** Skeletonization using Proxies

**Q:** What error do we expect from the proxy-based multipole/local ‘expansions’?
Why Does the Proxy Trick Work?

In particular, how general is this? Does this work for any kernel?
Where are we now? (I)

Summarize what we know about interaction ranks.

- We know that far interactions with a smooth kernel have low rank. (Because: short Taylor expansion suffices)
- If
  \[ \psi(x) = \sum_j G(x, y_j) \varphi(y_j) \]
  satisfies a PDE (e.g. Laplace), i.e. if \( G(x, y_j) \) satisfies a PDE, then that low rank is even lower.
- Can construct interior (‘local’) and exterior (‘multipole’) expansions (using Taylor or other tools).
- Can lower the number of terms using the PDE.
- Can construct LinAlg-workalikes for interior (‘local’) and exterior (‘multipole’) expansions.
- Can make those cheap using proxy points.
Where are we now? (II)

So we can compute interactions where sources are distant from targets (i.e. where the interaction is low rank) quite quickly.

Problem: In general, that’s not the situation that we’re in.

But: Most of the targets are far away from most of the sources.

(⇔ Only a few sources are close to a chosen ‘close-knit’ group of targets.)

So maybe we can do business yet—we just need to split out the near interactions to get a hold of the far ones (which (a) constitute the bulk of the work and (b) can be made cheap as we saw.)
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Preliminaries: Convolution

$$(f \ast g)(x) = \int_{\mathbb{R}} f(\xi)g(x - \xi) \, d\xi.$$  

- Convolution with shifted $\delta$ is the same as shifting the function;  
  $$[f \ast (\xi \mapsto \delta(\xi - a))](x) = f(x - a)$$  
- Convolution is linear (in both arguments) and commutative.
Preliminaries: Fourier Transform

\[ \mathcal{F}(f)(\omega) = \int_{\mathbb{R}} f(x) e^{-2\pi i \omega x} \, dx \]

- Convolution turns into multiplication: \( \mathcal{F}\{f \ast g\} = \mathcal{F}f \cdot \mathcal{F}g \),
- A single \( \delta \) turns into: \( \mathcal{F}\{\delta(x - a)\}(\omega) = e^{-i a \omega} \)
- And a “train” of \( \delta \)s turns into:

\[
\mathcal{F}\left\{ \sum_{\ell \in \mathbb{Z}} \delta(x - \ell) \right\}(\omega) = \sum_{k \in \mathbb{Z}} \delta(\omega - 2\pi k).
\]

What is \( \mathcal{F}\{f(x - a)\} \)?

See e.g. [Décoret ‘04].
Simple and Periodic: Ewald Summation

Want to evaluate potential from an infinite periodic grid of sources:

\[ \psi(x) = \sum_{m \in \mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(x, y_j + m) \varphi(y_j) \]
Lattice Sums: Convergence

Q: When does this have a right to converge?
Ewald Summation: Dealing with Smoothness

\[
\psi(x) = \sum_{i \in \mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(x, y_j + i) \varphi(y_j)
\]

Clear: a discrete convolution. Would like to make use of the fact that the Fourier transform turns convolutions into products. How?
Ewald Summation: Screens
Ewald Summation: Field Splitting

We can split the computation (from the perspective of a unit cell target) as follows:
Ewald Summation: Summation (1D for simplicity)

Interesting bit: How to sum $G_{LR}$. 
In practice: Fourier transforms carried out discretely, using FFT.

- Additional error contributions from interpolation
  (small if screen smooth enough to be well-sampled by mesh)
- $O(N \log N)$ cost (from FFT)
- Need to choose evaluation grid (‘mesh’)
- Resulting method called Particle-Mesh-Ewald (‘PME’)

Ewald Summation: Remarks
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Barnes-Hut: Putting Multipole Expansions to Work

nil
Barnes-Hut: The Task At Hand

Want: All-pairs interaction.

Caution:
- In these (stolen) figures: targets sources
- Here: targets and sources
Barnes-Hut: Putting Multipole Expansions to Work

nil
Barnes-Hut: Putting Multipole Expansions to Work

nil
Barnes-Hut: Box Targets

For sake of discussion, choose one ‘box’ as targets.
Q: For which boxes can we then use multipole expansions?
Barnes-Hut: Putting Multipole Expansions to Work

il
Barnes-Hut: Accuracy

With this computational outline, what’s the accuracy?

Q: Does this get better or worse as dimension increases?
Barnes-Hut (Single-Level): Computational Cost

What’s the cost of this algorithm?
Barnes-Hut Single Level Cost: Observations
Box Splitting

nil
Level Count

How many levels?
Want to evaluate all the source interactions with the targets in the box.

Q: What would be good sizes for source boxes? What’s the requirement?
Data from which of these boxes could we bring in using multipole expansions? Does that depend on the type of expansion? (Taylor/special function vs skeletons)
What properties do these boxes have?

Simple observation: The further, the bigger.
Barnes-Hut: Box Properties
Barnes-Hut: Well-separated-ness

Which boxes in the tree should be allowed to contribute via multipole?
Barnes-Hut: Revised Cost Estimate

Which of these boxes are well-separated from one another?

nil

What is the cost of evaluating the target potentials, assuming that we know the multipole expansions already?
Barnes-Hut: Revised Cost Estimate
nil

Summarize the algorithm (so far) and the associated cost.
Barnes-Hut: Next Revised Cost Estimate

Summarize the algorithm (so far) and the associated cost.
How could this process be sped up?
Observation: The amount of work does not really decrease as we go up the tree: Fewer boxes, but more particles in each of them. But we already compute multipoles to summarize lower-level boxes. . .
To get a new ‘big’ multipole from a ‘small’ multipole, we need a new mathematical tool.
Barnes-Hut: Translations
Cost of Multi-Level Barnes-Hut
Observation: Multipole evaluation remains as the single most costly bit of this algorithm.  *Fix?*

Idea: Exploit the tree structure also in performing this step. If ‘upward’ translation of multipoles helped earlier, maybe ‘downward’ translation of *local* expansions can help now.
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Come up with an algorithm that computes the interaction in the figure.
Using Multipole-to-Local

Come up with an algorithm that computes the interaction in the figure.
Using Multipole-to-Local: Next Level

nil

Assuming we retain information from the previous level, how can we obtain a valid local expansion on the target box?
Using Multipole-to-Local: Next Level

Assuming we retain information from the previous level, how can we obtain a valid local expansion on the target box?
Define ‘Interaction List’

For a box $b$, the interaction list $I_b$ consists of all boxes $b'$ so that
The Fast Multipole Method (‘FMM’)

Upward pass

1. Build tree
2. Compute interaction lists
3. Compute lowest-level multipoles from sources
4. Loop over levels $\ell = L - 1, \ldots, 2$:
   4.1 Compute multipoles at level $\ell$ by $\text{mp} \rightarrow \text{mp}$

Downward pass

1. Loop over levels $\ell = 2, 3, \ldots, L - 1$:
   1.1 Loop over boxes $b$ on level $\ell$:
      1.1.1 Add contrib from $I_b$ to local expansion by $\text{mp} \rightarrow \text{loc}$
      1.1.2 Add contrib from parent to local exp by $\text{loc} \rightarrow \text{loc}$

2. Evaluate local expansion and direct contrib from 9 neighbors.

Overall algorithm: Now $O(N)$ complexity.

Note: $L$ levels, numbered $0, \ldots, L - 1$. Loop indices above inclusive.
What about adaptivity?

Figure credit: Carrier et al. (‘88)
What about adaptivity?

Figure credit: Carrier et al. ('88)
Adaptivity: what changes?
Make a list of cases:
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What about solving?

Likely computational goal: Solve a linear system $Ax = b$. How do our methods help with that?
A Matrix View of Low-Rank Interaction

Only *parts of the matrix are low-rank*! What does this look like from a matrix perspective?
(Recursive) Coordinate Bisection (RCB)
Block-separable matrices

\[ A = \begin{bmatrix}
D_1 & A_{12} & A_{13} & A_{14} \\
A_{21} & D_2 & A_{23} & A_{24} \\
A_{31} & A_{32} & D_3 & A_{34} \\
A_{41} & A_{42} & A_{43} & D_4
\end{bmatrix} \]

where \( A_{ij} \) has low rank: How to capture rank structure?
Saw: If $A$ comes from a kernel for which Green’s formula holds, then the same skeleton will work for all of space, for a given set of sources/targets. What would the resulting matrix look like?
Rank and Proxies

Unlike FMMs, partitions here do not include “buffer” zones of near elements. What are the consequences?
Block-Separable Matrices

A *block-separable matrix* looks like this:

\[
A = \begin{bmatrix}
D_1 & P_1\tilde{A}_{12}\Pi_2 & P_1\tilde{A}_{13}\Pi_3 & P_1\tilde{A}_{14}\Pi_4 \\
P_2\tilde{A}_{21}\Pi_1 & D_2 & P_2\tilde{A}_{23}\Pi_3 & P_2\tilde{A}_{24}\Pi_4 \\
P_3\tilde{A}_{31}\Pi_1 & P_3\tilde{A}_{32}\Pi_2 & D_3 & P_3\tilde{A}_{34}\Pi_4 \\
P_4\tilde{A}_{41}\Pi_1 & P_4\tilde{A}_{42}\Pi_2 & P_4\tilde{A}_{43}\Pi_3 & D_4
\end{bmatrix}
\]

Here:

- \(\tilde{A}_{ij}\) smaller than \(A_{ij}\)
- \(D_i\) has full rank (not necessarily diagonal)
- \(P_i\) shared for entire row
- \(\Pi_i\) shared for entire column

**Q:** Why is it called that?
Block-Separable Matrix: Questions

Q: Why is it called that?

Q: How expensive is a matvec?

Q: How about a solve?
BSS Solve (I)

Use the following notation:

\[
B = \begin{bmatrix}
0 & P_1 \tilde{A}_{12} & P_1 \tilde{A}_{13} & P_1 \tilde{A}_{14} \\
\tilde{A}_{21} & 0 & P_2 \tilde{A}_{23} & P_2 \tilde{A}_{24} \\
\tilde{A}_{31} & \tilde{A}_{32} & 0 & P_3 \tilde{A}_{34} \\
\tilde{A}_{41} & \tilde{A}_{42} & \tilde{A}_{43} & 0
\end{bmatrix}
\]

and

\[
D = \begin{bmatrix}
D_1 \\
D_2 \\
D_3 \\
D_4
\end{bmatrix}, \quad \Pi = \begin{bmatrix}
\Pi_1 \\
\Pi_2 \\
\Pi_3 \\
\Pi_4
\end{bmatrix}.
\]

Then \( A = D + B \Pi \) and

\[
\begin{bmatrix}
D & B \\
-\Pi & \text{Id}
\end{bmatrix}
\begin{bmatrix}
\tilde{x} \\
x
\end{bmatrix}
= \begin{bmatrix}
b \\
0
\end{bmatrix}
\]

is equivalent to \( Ax = b \).
Q: What are the matrix sizes? The vector lengths of $x$ and $\tilde{x}$?

Now work towards doing just a ‘coarse’ solve on $\tilde{x}$, using, effectively, the \ Schur complement. Multiply first row by $\Pi D^{-1}$, add to second:
Focus in on the second row:

$$(\text{Id} + \Pi D^{-1} B)\tilde{x} = \Pi D^{-1} b$$

Every non-zero entry in $\Pi D^{-1} B$ looks like

Define a diagonal entry:
Next, left-multiply \((\text{Id} + \Pi D^{-1} B)\) by \(\text{diag}(\tilde{A}_{ii})\):
What have we achieved?

- Instead of solving a linear system of size

\[(N_{L0\text{ boxes}} \cdot m) \times (N_{L0\text{ boxes}} \cdot m)\]

we solve a linear system of size

\[(N_{L0\text{ boxes}} \cdot K) \times (N_{L0\text{ boxes}} \cdot K),\]

which is cheaper by a factor of \((K/m)^3\).

- We are now only solving on the skeletons.

(Figure credit: G. Martinsson)
Hierarchically Block-Separable

To get to $O(N)$, realize we can \textit{recursively}

- group skeletons
- eliminate more variables.

Where does this process start?
Hierarchically Block-Separable

In order to get $O(N)$ complexity, could we apply this procedure recursively?

(Figure credit: G. Martinsson)
Hierarchically Block-Separable

- Using this hierarchical grouping gives us \textit{Hierarchically Block-Separable (HBS)} matrices.
- If you have heard the word \textit{H-matrix} and \textit{H$^2$-matrix}, the ideas are very similar. Differences:
  - \textit{H-family} matrices don’t typically use the ID (instead often use \textit{Adaptive Cross Approximation} or \textit{ACA})
  - \textit{H$^2$} does target clustering (like FMM), \textit{H} does not (like Barnes-Hut)
The most decrease in ‘volume’ happens in the off-diagonal part of the matrix. → Rightfully so!

All matrices are block-diagonal, except for the highest-level matrix—but that is small!
Recap: Fast Fourier Transform

The *Discrete Fourier Transform (DFT)* is given by:

\[
X_k = \sum_{n=0}^{N-1} x_n e^{-\frac{2\pi i}{N} nk} \quad (k = 0, \ldots, N - 1)
\]

The foundation of the *Fast Fourier Transform (FFT)* is the factorization:

\[
X_k = \sum_{m=0}^{N/2-1} x_{2m} e^{-\frac{2\pi i}{N/2} mk} + e^{-\frac{2\pi i}{N} k} \sum_{m=0}^{N/2-1} x_{2m+1} e^{-\frac{2\pi i}{N/2} mk}.
\]

- DFT of even-indexed part of \(x_n\)
- DFT of odd-indexed part of \(x_n\)
FFT: Data Flow

Perhaps a little bit like a butterfly?
Claim:

The [numerical] rank of the normalized Fourier transform with kernel $e^{i\gamma xt}$ is bounded by a constant times $\gamma$, at any fixed precision $\epsilon$.

(i.e. rank is bounded by the area of the rectangle swept out by $x$ and $t$) [O’Neil et al. ‘10]

**Demo:** Butterfly Factorization (Part I)
Recompression: Making use of Area-Bounded Rank

How do rectangular submatrices get expressed so as to reveal their constant rank?
Observations

**Demo:** Butterfly Factorization (Part II)

For which types of matrices is the Butterfly factorization guaranteed accurate?

For which types of \( n \times n \) matrices does the butterfly lead to a reduction in cost?

Explore the limit cases of the characterization.
Observations: Cost

What is the cost (in the reduced-cost case) of the matvec?

Comments?
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PDEs: Simple Ones First, More Complicated Ones Later

**Laplace**
\[ \triangle u = 0 \]

- Steady-state \( \partial_t u = 0 \) of wave propagation, heat conduction
- Electric potential \( u \) for applied voltage
- Minimal surfaces/“soap films”
- \( \nabla u \) as velocity of incompressible flow

**Helmholtz**
\[ \triangle u + k^2 u = 0 \]

- Assume time-harmonic behavior \( \tilde{u} = e^{\pm i\omega t} u(x) \) in time-domain wave equation:
  \[ \partial_t^2 \tilde{u} = \triangle \tilde{u} \]
- Sign in \( \tilde{u} \) determines direction of wave: Incoming/outgoing if free-space problem
- **Applications**: Propagation of sound, electromagnetic waves
 aka. *Free space Green’s Functions*

How do you assign a precise meaning to the statement with the $\delta$-function?
Green’s Functions

Why care about Green’s functions?

What is a non-free-space Green’s function? I.e. one for a specific domain?
Green’s Functions (II)

Why not just use domain Green’s functions?

What if we don’t know a Green’s function for our PDE... at all?
Fundamental Solutions

Laplace

\[ G(x) = \begin{cases} \frac{1}{-2\pi} \log |x| & \text{2D} \\ \frac{1}{4\pi \ |x|} & \text{3D} \end{cases} \]

\[ \frac{\partial}{\partial x} G(x) \]

Helmholtz

\[ G(x) = \begin{cases} \frac{i}{4} H^1_0(k |x|) & \text{2D} \\ \frac{1}{4\pi} \frac{e^{ik |x|}}{|x|} & \text{3D} \end{cases} \]

\[ \frac{\partial}{\partial x} G(x) \]
Layer Potentials (I)

\[
(S_k \sigma)(x) := \int_{\Gamma} G_k(x - y)\sigma(y)ds_y
\]

\[
(S'_k \sigma)(x) := n \cdot \nabla_x PV \int_{\Gamma} G_k(x - y)\sigma(y)ds_y
\]

\[
(D_k \sigma)(x) := PV \int_{\Gamma} n \cdot \nabla_y G_k(x - y)\sigma(y)ds_y
\]

\[
(D'_k \sigma)(x) := n \cdot \nabla_x f.p. \int_{\Gamma} n \cdot \nabla_y G_k(x - y)\sigma(y)ds_y
\]

- \(G_k\) is the Helmholtz kernel \((k = 0 \rightarrow \text{Laplace})\)
- Operators—map function \(\sigma\) on \(\Gamma\) to...
  - ...function on \(\mathbb{R}^n\)
  - ...function on \(\Gamma\) (in particular)
Layer Potentials (II)

- Alternate ("standard") nomenclature:
  
<table>
<thead>
<tr>
<th>Ours</th>
<th>Theirs</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>V</td>
</tr>
<tr>
<td>D</td>
<td>K</td>
</tr>
<tr>
<td>S'</td>
<td>K'</td>
</tr>
<tr>
<td>D'</td>
<td>T</td>
</tr>
</tbody>
</table>

- $S''$ (and higher) analogously

- Called layer potentials:
  
  - $S$ is called the single-layer potential
  - $D$ is called the double-layer potential

- (Show pictures using pytential/examples/layerpot.py, observe continuity properties.)
How does this actually solve a PDE?

Solve a (interior Laplace Dirichlet) BVP, $\partial \Omega = \Gamma$

$$\triangle u = 0 \quad \text{in } \Omega, \quad u|_{\Gamma} = f|_{\Gamma}.$$ 

1. Pick representation:
   $$u(x) := (S\sigma)(x)$$

2. Take (interior) limit onto $\Gamma$:
   $$u|_{\Gamma} = S\sigma$$

3. Enforce BC:
   $$u|_{\Gamma} = f$$

4. Solve resulting linear system:
   $$S\sigma = f$$

   (quickly—using the methods we’ve developed: It is precisely of the form that suits our fast algorithms!)

5. Obtain PDE solution in $\Omega$ by evaluating representation
Observations:

- One can choose representations relatively freely. Only constraints:
  - Can I get to the solution with this representation?
    - I.e. is the solution I’m looking for represented?
  - Is the resulting integral equation solvable?

Q: How would we know?
Some representations lead to better integral equations than others. The one above is actually terrible (both theoretically and practically). Fix above: Use $u(x) = D\sigma(x)$ instead of $u(x) = S\sigma(x)$.

Q: How do you tell a good representation from a bad one?

Need to actually evaluate $S\sigma(x)$ or $D\sigma(x)$…

Q: How?

→ Need some theory
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Norms

Definition

(Norm) A norm $\| \cdot \|$ maps an element of a vector space into $[0, \infty)$. It satisfies:

- $\| x \| = 0 \iff x = 0$
- $\| \lambda x \| = |\lambda| \| x \|$
- $\| x + y \| \leq \| x \| + \| y \|$ (triangle inequality)

Can create norm from inner product: $\| x \| = \sqrt{\langle x, x \rangle}$
Name some function spaces with their norms.
Convergence

Name some ways in which a sequence can ‘converge’.
**Operators**

$X, Y$: Banach spaces, $A : X \rightarrow Y$ linear operator

**Definition (Operator norm)**

$\|A\| := \sup\{\|Ax\| : x \in X, \|x\| = 1\}$

**Theorem**

$\|A\|$ bounded $\iff$ $A$ continuous

Other facts?

- What does ‘linear’ mean here?
- Is there a notion of ‘continuous at $x$’ for linear operators?
Operators: Examples

Which of these is bounded as an operator on functions on the real line?
- Multiplication by a scalar
- “Left shift”
- Fourier transform
- Differentiation
- Integration
- Integral operators
## Integral Equations: Zoology

<table>
<thead>
<tr>
<th>Volterra</th>
<th>Fredholm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\int_a^x k(x, y)f(y)dy = g(x)$</td>
<td>$\int_G k(x, y)f(y)dy = g(x)$</td>
</tr>
</tbody>
</table>

### Questions:
- **First row**: First or second kind?
- **Second row**: Volterra or Fredholm?
- Matrix (i.e. finite-dimensional) analogs?
- What can happen in 2D/3D?
- Factor allowable in front of the identity?
- Why even talk about ‘second-kind operators’?
  - Throw a $+\delta(x - y)$ into the kernel, back to looking like first kind. So?
  - Is the identity in $(I + K)$ crucial?
Complex analysis is *full* of integral operators:

- **Cauchy’s integral formula:**

\[
 f(a) = \frac{1}{2\pi i} \oint_{\gamma} \frac{1}{z-a} f(z) \, dz
\]

- **Cauchy’s differentiation formula:**

\[
 f^{(n)}(a) = \frac{n!}{2\pi i} \oint_{\gamma} \frac{1}{(z-a)^{n+1}} f(z) \, dz
\]
Theorem (Continuous kernel ⇒ bounded)

$G \subset \mathbb{R}^n$ closed, bounded ("compact"), $K \in C(G^2)$. Let

$$(A\phi)(x) := \int_G K(x, y)\phi(y)dy.$$  

Then

$$||A||_\infty = \max_{x \in G} \int_G |K(x, y)|dy.$$ 

Show ‘$\leq$’.
Solving Integral Equations

Given

\[(A\phi)(x) := \int_G K(x, y)\phi(y)dy,\]

are we allowed to ask for a solution of

\[(\text{Id} + A)\phi = g?\]
Attempt 1: The Neumann series

Want to solve

\[ \varphi - A\varphi = (I - A)\varphi = g. \]

Formally:

\[ \varphi = (I - A)^{-1}g. \]

What does that remind you of?
Theorem

\[ A : X \to X {\text{ Banach, }} \|A\| < 1 \ (I - A)^{-1} = \sum_{k=0}^{\infty} A^k \text{ with} \]

\[ \|(I - A)^{-1}\| \leq 1/(1 - \|A\|). \]

- How does this rely on completeness/Banach-ness?
- There's an iterative procedure hidden in this.
  (Called Picard Iteration. Cf: Picard-Lindelöf theorem.)
  
  **Hint:** How would you compute \( \sum_k A^k f \)?

**Q:** Why does this fall short?
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Compact Sets

Definition (Precompact/Relatively compact)

\[ M \subseteq X \text{ precompact} : \iff \text{all sequences } (x_k) \subseteq M \text{ contain a subsequence converging in } X \]

Definition (Compact/‘Sequentially complete’)

\[ M \subseteq X \text{ compact} : \iff \text{all sequences } (x_k) \subseteq M \text{ contain a subsequence converging in } M \]

- Precompact \(\implies\) bounded
- Precompact \(\iff\) bounded (finite dim. only!)
Compact Sets (II)

Counterexample to ‘precompact $\Leftrightarrow$ bounded’? ($\infty$ dim)
Compact Operators

\[ X, Y: \text{Banach spaces} \]

**Definition (Compact operator)**

\( T : X \to Y \) is *compact* \( \iff T(\text{bounded set}) \text{ is precompact.} \)

**Theorem**

- \( T, S \) compact \( \Rightarrow \alpha T + \beta S \) compact
- One of \( T, S \) compact \( \Rightarrow S \circ T \) compact
- \( T_n \) all compact, \( T_n \to T \) in operator norm \( \Rightarrow T \) compact

**Questions:**

- Let \( \dim T(X) < \infty \). Is \( T \) compact?
- Is the identity operator compact?
Intuition about Compact Operators

- Compact operator: As finite-dimensional as you’re going to get in infinite dimensions.
- Not clear yet—but they are moral (∞-dim) equivalent of a matrix having low numerical rank.
- Are compact operators continuous (≡bounded)?
- What do they do to high-frequency data?
- What do they do to low-frequency data?
Let $G \subset \mathbb{R}^n$ be compact.

**Theorem (Arzelà-Ascoli)**

$U \subset C(G)$ is precompact iff it is bounded and equicontinuous.

**Equicontinuous** means:

**Continuous** means:
Arzelà-Ascoli: Proof Sketch
Arzelà-Ascoli (II)

Intuition?

“Uniformly continuous”?

When does uniform continuity happen?

(Note: Kress LIE 2nd ed. defines ‘uniform equicontinuity’ in one go.)
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Integral Operators are Compact

Theorem (Continuous kernel $\Rightarrow$ compact [Kress LIE 2nd ed. Thm. 2.20])

$G \subset \mathbb{R}^m$ compact, $K \in C(G^2)$. Then

$$(A\phi)(x) := \int_G K(x, y)\phi(y)dy.$$ 

is compact on $C(G)$.

Use A-A. (a statement about compact sets) What is there to show?

Pick $U \subset C(G)$. $A(U)$ bounded?

$A(U)$ equicontinuous?
Weakly singular

\( G \subset \mathbb{R}^n \) compact

**Definition (Weakly singular kernel)**

- \( K \) defined, continuous everywhere except at \( x = y \)
- There exist \( C > 0, \alpha \in (0, n] \) such that

\[
|K(x, y)| \leq C|x - y|^{\alpha-n} \quad (x \neq y)
\]

**Theorem (Weakly singular kernel \( \Rightarrow \) compact [Kress LIE 2nd ed. Thm. 2.22])**

\( K \) weakly singular. Then

\[
(A\phi)(x) := \int_G K(x, y)\phi(y)dy.
\]

is compact on \( C(G) \), where \( \text{cl}(G^o) = G \).
Outline the proof of ‘Weakly singular kernel $\Rightarrow$ compact’.
Weakly singular (on surfaces)

\( \Omega \subset \mathbb{R}^n \) bounded, open, \( \partial \Omega \) is \( C^1 \) (what does that mean?)

**Definition (Weakly singular kernel (on a surface))**

- \( K \) defined, continuous everywhere except at \( x = y \)
- There exist \( C > 0, \alpha \in (0, n - 1] \) such that

\[
|K(x, y)| \leq C|x - y|^{\alpha-n+1} \quad (x, y \in \partial \Omega, \ x \neq y)
\]

**Theorem (Weakly singular kernel \( \Rightarrow \) compact [Kress LIE 2nd ed. Thm. 2.23])**

\( K \) weakly singular on \( \partial \Omega \). Then \( (A\phi)(x) := \int_{\partial \Omega} K(x, y)\phi(y)dy \) is compact on \( C(\partial \Omega) \).

Q: Has this estimate gotten worse or better?
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Riesz Theory (I)

Still trying to solve

\[ L\phi := (I - A)\phi = \phi - A\phi = f \]

with \( A \) compact.

Theorem (First Riesz Theorem [Kress, Thm. 3.1])

\[ N(L) \text{ is finite-dimensional.} \]

Questions:

- What is \( N(L) \) again?
- Why is this good news?
Riesz First Theorem: Proof Outline

Show it.
A compact. Then:

- \((I - A)\) injective \iff \((I - A)\) surjective
  - It's either bijective or neither s nor i.
- If \((I - A)\) is bijective, \((I - A)^{-1}\) is bounded.

Rephrase for solvability:

Key shortcoming?
Riesz Theory: Boundedness Proof Outline

Assuming \((I - A)\) is bijective, show that \((I - A)^{-1}\) is bounded.
Hilbert spaces

Hilbert space: Banach space with a norm coming from an *inner product*:

\[(\alpha x + \beta y, z) =?\]
\[(x, \alpha y + \beta z) =?\]
\[(x, x)?\]
\[(y, x) =?\]

Is \(C^0(G)\) a Hilbert space?

Name a Hilbert space of functions.
Continuous and Square-Integrable

Can we carry over $C^0(G)$ boundedness/compactness results to $L^2(G)$?

$X, Y$ normed spaces with a scalar product so that $|⟨\phi, \psi⟩| \leq ∥\phi∥∥\psi∥$ for $\phi, \psi \in X$.

**Theorem (Lax dual system [Kress LIE 3rd ed. Thm. 4.13])**

Let $U \subseteq X$ be a subspace and let $A : X \to Y$ and $B : Y \to X$ be bounded linear operators with

$$A\phi, \psi⟩ = ⟨\phi, B\psi⟩ \quad (\phi \in U, \psi \in Y).$$

Then $A : U \to Y$ is bounded with respect to $∥⋅∥_s$ induced by the scalar product and $∥A∥^2_s \leq ∥A∥∥B∥$.

Based on this, it is also possible to carry over compactness results.
Adjoint Operators

Definition (Adjoint operator)

A* called adjoint to A if

\[(Ax, y) = (x, A^*y)\]

for all \(x, y\).

Facts:

- \(A^*\) unique
- \(A^*\) exists
- \(A^*\) linear
- \(A\) bounded \(\Rightarrow\) \(A^*\) bounded
- \(A\) compact \(\Rightarrow\) \(A^*\) compact
Adjoint Operator: Observations?

What is the adjoint operator in finite dimensions? (in matrix representation)

What do you expect to happen with integral operators?

Adjoint of the single-layer?

Adjoint of the double-layer?
Fredholm Alternative

Theorem (Fredholm Alternative [Kress LIE 2nd ed. Thm. 4.14])

A : X → X compact. Then either:

- I − A and I − A* are bijective

  or:

- \( \dim N(I − A) = \dim N(I − A^*) \)
- \( (I − A)(X) = N(I − A^*)^\perp \)
- \( (I − A^*)(X) = N(I − A)^\perp \)

Seen these statements before?
Fundamental Theorem of Linear Algebra
Fredholm Alternative in IE terms

Translate to language of integral equation solvability:
Fredholm Alternative: Further Thoughts

What about symmetric kernels \((K(x, y) = K(y, x))\)?

Where to get uniqueness?
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  - Compactness
  - Integral Operators
  - Riesz and Fredholm
    A Tiny Bit of Spectral Theory

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Spectral Theory: Terminology

A : X → X bounded, λ is a ... value:

**Definition (Eigenvalue)**

There exists an element \( \phi \in X, \phi \neq 0 \) with \( A\phi = \lambda \phi \).

**Definition (Regular value)**

The “resolvent” \((\lambda I - A)^{-1}\) exists and is bounded.

Can a value be regular and “eigen” at the same time?

What’s special about \( \infty\)-dim here?
Resolvent Set and Spectrum

**Definition (Resolvent set)**

\[ \rho(A) := \{ \lambda \text{ is regular} \} \]

**Definition (Spectrum)**

\[ \sigma(A) := \mathbb{C} \setminus \rho(A) \]
Theorem

$A : X \to X$ compact linear operator, $X$ $\infty$-dim.

Then:

- $0 \in \sigma(A)$ (show!)
- $\sigma(A) \setminus \{0\}$ consists only of eigenvalues
- $\sigma(A) \setminus \{0\}$ is at most countable
- $\sigma(A)$ has no accumulation point except for 0
Spectral Theory of Compact Operators: Proofs

Show the first part.

Show second part.
Spectral Theory of Compact Operators: Implications

Rephrase last two: how many eigenvalues with $|\cdot| \geq R$?

Recap: What do compact operators do to high-frequency data?

Don't confuse $I - A$ with $A$ itself!
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Recap: Layer potentials

\[(S\sigma)(x) := \int_{\Gamma} G(x - y)\sigma(y)\,ds_y\]

\[(S'\sigma)(x) := PV \hat{n} \cdot \nabla_x \int_{\Gamma} G(x - y)\sigma(y)\,ds_y\]

\[(D\sigma)(x) := PV \int_{\Gamma} \hat{n} \cdot \nabla_y G(x - y)\sigma(y)\,ds_y\]

\[(D'\sigma)(x) := f.p. \hat{n} \cdot \nabla_x \int_{\Gamma} \hat{n} \cdot \nabla_y G(x - y)\sigma(y)\,ds_y\]

**Definition (Harmonic function)**

\[\nabla u = 0\]

Where are layer potentials harmonic?
On the double layer again

Is the double layer *actually* weakly singular? Recap:

**Definition (Weakly singular kernel)**

- $K$ defined, continuous everywhere except at $x = y$
- There exist $C > 0$, $\alpha \in (0, n - 1]$ such that

\[
|K(x, y)| \leq C|x - y|^{\alpha-n+1} \quad (x, y \in \partial \Omega, \ x \neq y)
\]
Actual Singularity in the Double Layer

\[
\frac{\partial}{\partial x} \log(|0 - x|) = \frac{x}{x^2 + y^2}
\]

- Singularity with approach on \( y = 0 \)?
- Singularity with approach on \( x = 0 \)?
Cauchy Principal Value

But I don’t want to integrate across a singularity! → punch it out.

Problem: Make sure that what’s left over is well-defined

\[
\int_{-1}^{1} \frac{1}{x} \, dx?
\]
Principal Value in $n$ dimensions

Integration Contour

Again: Symmetry matters!

What about even worse singularities?
Recap: Layer potentials

\[(S\sigma)(x) := \int_{\Gamma} G(x - y)\sigma(y)ds_y\]

\[(S'\sigma)(x) := \text{PV} \hat{n} \cdot \nabla_x \int_{\Gamma} G(x - y)\sigma(y)ds_y\]

\[(D\sigma)(x) := \text{PV} \int_{\Gamma} \hat{n} \cdot \nabla_y G(x - y)\sigma(y)ds_y\]

\[(D'\sigma)(x) := f.p. \hat{n} \cdot \nabla_x \int_{\Gamma} \hat{n} \cdot \nabla_y G(x - y)\sigma(y)ds_y\]

Important for us: Recover ‘average’ of interior and exterior limit without having to refer to off-surface values.
Green’s Theorem

Ω bounded

Theorem (Green’s Theorem [Kress LIE 2nd ed. Thm 6.3])

$$\int_\Omega u \triangle v + \nabla u \cdot \nabla v = \int_{\partial \Omega} u (\hat{n} \cdot \nabla v) \, ds$$

$$\int_\Omega u \triangle v - v \triangle u = \int_{\partial \Omega} u (\hat{n} \cdot \nabla v) - v (\hat{n} \cdot \nabla u) \, ds$$

If $\triangle v = 0$ and $u = 1$, then

$$\int_{\partial \Omega} \hat{n} \cdot \nabla v = ?$$
Green’s Formula

What if $\triangle v = 0$ and $u = G(|y - x|)$ in Green’s second identity?

$$\int_{\Omega} u\triangle v - v\triangle u = \int_{\partial\Omega} u(\hat{n} \cdot \nabla v) - v(\hat{n} \cdot \nabla u)ds$$

Can you write that more briefly?
Green’s Formula (Full Version)

\( \Omega \) bounded

**Theorem (Green’s Formula \[Kress \text{ LIE} \, 2\text{nd ed. Thm 6.5}\])**

*If \( \triangle u = 0 \), then*

\[
(S(\hat{n} \cdot \nabla u) - Du)(x) = \begin{cases} 
    u(x) & x \in \Omega, \\
    \frac{u(x)}{2} & x \in \partial\Omega, \\
    0 & x \notin \Omega.
\end{cases}
\]
Green’s Formula and Cauchy Data

Suppose I know ‘Cauchy data’ \((u|_{\partial \Omega}, \hat{n} \cdot \nabla u|_{\partial \Omega})\) of \(u\). What can I do?

What if \(\Omega\) is an exterior domain?

What if \(u = 1\)? Do you see any practical uses of this?
Mean Value Theorem

Theorem (Mean Value Theorem [Kress LIE 2nd ed. Thm 6.7])

If $\Delta u = 0$, $u(x) = \int_{B(x,r)} u(y) dy = \int_{\partial B(x,r)} u(y) dy$

Define $\int$?

Trace back to Green’s Formula (say, in 2D):
Maximum Principle

Theorem (Maximum Principle [Kress LIE 2nd ed. 6.9])

If $\triangle u = 0$ on compact set $\bar{\Omega}$:

$u$ attains its maximum on the boundary.

Suppose it were to attain its maximum somewhere inside an open set... 

What do our constructed harmonic functions (layer potentials) do there?
Green’s Formula at Infinity: Statement

\( \Omega \subseteq \mathbb{R}^n \) bounded, \( C^1 \), connected boundary, \( \triangle u = 0 \) in \( \mathbb{R}^n \setminus \Omega \), \( u \) bounded

Theorem (Green’s Formula in the exterior [Kress LIE 3rd ed. Thm 6.11])

\[
(S_{\partial \Omega}(\hat{n} \cdot \nabla u) - D_{\partial \Omega}u)(x) + PV u_{\infty} = u(x)
\]

for some constant \( u_{\infty} \). Only for \( n = 2 \),

\[
u_{\infty} = \frac{1}{2\pi r} \int_{|y|=r} u(y) ds_y.
\]

Realize the power of this statement:
We will focus on $\mathbb{R}^3$. WLOG assume $0 \in \Omega$. Let $M = \| u \|_{L^\infty(\mathbb{R}^n \setminus \bar{\Omega})}$. First, show $\| \nabla u \| \leq 6M/\|x\|$ for $x \geq R_0$. 

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Let $x \in \mathbb{R}^3 \setminus \bar{\Omega}$. Let $r$ be such that $\bar{\Omega} \subset B(x, r)$. Apply Green’s formula on bounded domains to $B(x, r) \setminus \bar{\Omega}$:

$$(S_{\partial \Omega}(\partial_n u) - D_{\partial \Omega} u)(x) + (S_{\partial B(x, r)}(\partial_n u) - D_{\partial B(x, r)} u)(x) = u(x).$$

Show $S_{\partial B(x, r)}(\partial_n u) \to 0$ as $r \to \infty$: 
Green’s Formula at Infinity: Proof (3/4)

It remains to bound the term

\[ D_{\partial B(x,r)} u(x) = \frac{4\pi}{r^2} \int_{\partial B(x,r)} u(y) dS_y. \]

Can we transplant that ball to the origin in some sense?
Observe
\[ \left| \frac{4\pi}{r^2} \int_{\partial B(0,r)} u(y) dS_y \right| \leq 4\pi M. \]

Consider the sequence
\[ \mu_n := \frac{4\pi}{r_n^2} \int_{\partial B(0,r_n)} u(y) dS_y. \]

Because of its boundedness and sequential compactness of the bounding interval, out of a sequence of radii \( r_n \), we can pick a subsequence so that \( (\mu_{n(k)}) \) converges. Call the limit \( u_\infty \).
Can we use this to bound $u$ as $x \to \infty$?
Consider the behavior of the kernel as $r \to \infty$. Focus on 3D for simplicity. (But 2D holds also.)

How about $u$’s derivatives?
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Jump relations:

\[ S_\mu \]

\[ S'_\mu \]

\[ r \]

\[ \mu \]

\[ \Gamma \]
Jump Relations: Mathematical Statement

Let \([X] = X_+ - X_-\). (Normal points towards "+"="exterior".)

**Theorem (Jump Relations [Kress LIE 2nd ed. Thm. 6.14, 6.17,6.18])**

\[
\lim_{x \to x_0^\pm} (S' \sigma) = \left( S' \mp \frac{1}{2} I \right) (\sigma)(x_0) \quad \Rightarrow \quad [S' \sigma] = -\sigma
\]

\[
\lim_{x \to x_0^\pm} (D \sigma) = \left( D \mp \frac{1}{2} I \right) (\sigma)(x_0) \quad \Rightarrow \quad [D \sigma] = \sigma
\]

Truth in advertising: Assumptions on \(\Gamma\)?
Jump Relations: Proof Sketch for SLP

Sketch the proof for the single layer.
Jump Relations: Proof Sketch for DLP

Sketch proof for the double layer.
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**Boundary Value Problems**

Laplace

Helmholtz

Calderón identities

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## Boundary Value Problems: Overview

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<tr>
<th></th>
<th><strong>Dirichlet</strong></th>
<th><strong>Neumann</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Int.</strong></td>
<td>( \lim_{x \to \partial \Omega^-} u(x) = g )</td>
<td>( \lim_{x \to \partial \Omega^-} \hat{n} \cdot \nabla u(x) = g )</td>
</tr>
<tr>
<td></td>
<td>+ unique</td>
<td>+ may differ by constant</td>
</tr>
<tr>
<td><strong>Ext.</strong></td>
<td>( \lim_{x \to \partial \Omega^+} u(x) = g )</td>
<td>( \lim_{x \to \partial \Omega^+} \hat{n} \cdot \nabla u(x) = g )</td>
</tr>
<tr>
<td></td>
<td>( u(x) = \begin{cases} O(1) &amp; 2D \ o(1) &amp; 3D \end{cases} \text{ as }</td>
<td>x</td>
</tr>
<tr>
<td></td>
<td>+ unique</td>
<td>+ unique</td>
</tr>
</tbody>
</table>

with \( g \in C(\partial \Omega) \).

What does \( f(x) = O(1) \) mean? (and \( f(x) = o(1) \)?)
Uniqueness Proofs

Dirichlet uniqueness: why?

Neumann uniqueness: why?
Uniqueness: Remaining Points

Truth in advertising: Missing assumptions on $\Omega$?

What’s a DtN map?

Next mission: Find IE representations for each.
Uniqueness of Integral Equation Solutions

Theorem (Nullspaces [Kress LIE 2nd ed. Thm 6.20])

- $\mathcal{N}(I/2 - D) = \mathcal{N}(I/2 - S') = \{0\}$
- $\mathcal{N}(I/2 + D) = \text{span}\{1\}, \mathcal{N}(I/2 + S') = \text{span}\{\psi\}$, where $\int \psi \neq 0$. 
IE Uniqueness: Proofs (1/3)

Show $N(I/2 - D) = \{0\}$. 
Show $N(I/2 - S') = \{0\}$. 
IE Uniqueness: Proofs (3/3)

Show $N(I/2 + D) = \text{span}\{1\}$.

What conditions on the RHS do we get for int. Neumann and ext. Dirichlet?

→ “Clean” Existence for 3 out of 4.
Patching up Exterior Dirichlet

Problem: \( N(I/2 + S') = \{ \psi \} \ldots \) do not know \( \psi \). Use different kernel:

\[
\hat{n} \cdot \nabla_y G(x, y) \rightarrow \hat{n} \cdot \nabla_y G(x, y) + \frac{1}{|x|^{n-2}}
\]

Note: Singularity only at origin! (assumed \( \in \Omega \))

- 2D behavior? 3D behavior?
- Still a solution of the PDE? Compact?
- Jump condition? Exterior limit? Deduce \( u = 0 \) on exterior.
  - Consider \( \partial_n G = O(1/r^{n-1}) \).
- \( |x|^{n-2} u(x) = ? \) as \( |x| \to \infty \)?
- Thus \( \int \phi = 0 \). Contribution of the second term?
- \( \phi/2 + D\phi = 0 \), i.e. \( \phi \in N(I/2 + D) = ? \)
- Existence/uniqueness?
→ Existence for 4 out of 4.
Domains with Corners

What’s the problem?  *(Hint: Jump condition for constant density)*
Domains with Corners (II)

At corner $x_0$: (2D)

$$\lim_{x \to x_0 \pm} = \int_{\partial \Omega} \hat{n} \cdot \nabla_y G(x, y) \phi(y) ds_y \pm \frac{1}{2} \frac{\langle \text{opening angle on } \pm \text{ side} \rangle}{\pi} \phi$$

→ non-continuous behavior of potential on $\Gamma$ at $x_0$

What space have we been living in? How do we fix this mess?

Numerically: Needs consideration, can drive up cost through refinement.
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Where does Helmholtz come from?

Derive the Helmholtz equation from the wave equation $\partial_t^2 U = c^2 \triangle U$. Q: 
What is $c$?
Helmholtz vs. Yukawa

Helmholtz Equation

- $\Delta u + k^2 u(x) = 0$
- Indefinite operator
- Oscillatory solution
- Difficult to solve, especially for large $k$

Yukawa Equation

- $-\Delta u + k^2 u(x) = 0$
- Positive definite operator
- Smooth solutions
- ‘Screened Coulomb’ interaction
- Generally quite simple to solve
The prototypical Helmholtz BVP: A Scattering Problem

Ansatz:

$$u^{\text{tot}} = u + u^{\text{inc}}$$

Solve for scattered field $u$. 
Helmholtz: Some Physics

Physical quantities:

- Velocity potential: \( U(x, t) = u(x)e^{-i\omega t} \)
  (fix phase by e.g. taking real part)
- Velocity: \( v = \frac{1}{\rho_0} \nabla U \)
- Pressure: \( p = -\partial_t U = i\omega ue^{-i\omega t} \)
  - Equation of state: \( p = f(\rho) \)

What’s \( \rho_0 \)?

What happens to a pressure BC as \( \omega \to 0 \)?
Helmholtz: Boundary Conditions

Interfaces between media: What’s continuous?

- **Sound-soft**: Scatterer “gives”
  - Pressure remains constant in time
  - \( u = f \) → Dirichlet

- **Sound-hard**: Scatterer “does not give”
  - Pressure varies, same on both sides of interface
  - \( \hat{n} \cdot \nabla u = 0 \) → Neumann

- **Impedance**: Some pressure translates into motion
  - Scatterer “resists”
  - \( \hat{n} \cdot \nabla u + ik\lambda u = 0 \) → Robin (\( \lambda > 0 \))

- **Sommerfeld** radiation condition: allow only outgoing waves (\( n \)-dim)
  \[
  r^{\frac{n-1}{2}} \left( \frac{\partial}{\partial r} - ik \right) u(x) \to 0 \quad (r \to \infty)
  \]

Many interesting BCs → many IEs! :)
Unchanged from Laplace

Theorem (Green’s Formula [Colton/Kress IAEST Thm 2.1])

If $\triangle u + k^2 u = 0$, then

$$(S(\hat{n} \cdot \nabla u) - Du)(x) = \begin{cases} 
  u(x) & x \in D \\
  \frac{u(x)}{2} & x \in \partial D \\
  0 & x \not\in D 
\end{cases}$$

$$
\lim_{x \to x_0 \pm} (S'u) = \left( S' \mp \frac{1}{2} I \right) (u)(x_0) \quad \Rightarrow \quad [S'u] = -u
$$

$$
\lim_{x \to x_0 \pm} (Du) = \left( D \mp \frac{1}{2} I \right) (u)(x_0) \quad \Rightarrow \quad [Du] = u
$$

$[Su] = 0$

$[D'u] = 0$
Unchanged from Laplace

Why is singular behavior (esp. jump conditions) unchanged?

Why does Green’s formula survive?
Resonances

$-\Delta$ on a bounded (interior) domain with homogeneous Dirichlet/Neumann BCs has countably many real, positive eigenvalues. What does that have to with Helmholtz?

Why could it cause grief?
Helmholtz: Boundary Value Problems

Find \( u \in C(\bar{D}) \) with \( \Delta u + k^2 = 0 \) such that

**Dirichlet**

<table>
<thead>
<tr>
<th>Int. ( \lim_{x \to \partial D^-} u(x) = g ) unique (−resonances)</th>
</tr>
</thead>
</table>

**Neumann**

<table>
<thead>
<tr>
<th>Ext. ( \lim_{x \to \partial D^+} u(x) = g ) Sommerfeld unique</th>
</tr>
</thead>
</table>

with \( g \in C(\partial D) \).

Find layer potential representations for each.
Patching up resonances

**Issue:** Ext. IE inherits non-uniqueness from ‘adjoint’ int. BVP

**Fix:** Tweak representation [Brakhage/Werner ‘65, ...] (also called the CFIE or combined field integral equation)

\[ u = D\phi - i\alpha S\phi \]

(\(\alpha\): tuning knob \(\rightarrow\) 1 is fine, \(\sim k\) better for large \(k\))
Patching up resonances: CFIE (1/3)
Patching up resonances: CFIE (2/3)
Patching up resonances: CFIE (3/3)
Helmholtz Uniqueness

Uniqueness for remaining IEs similar:
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A word about $D'$

Show that $D'$ is self-adjoint. [Kress LIE 3rd ed. Sec 7.6]
Towards Calderón

Show that \((S\varphi, D'\psi) = ((S' + I/2)\varphi, (D - I/2)\psi)\).

\((\varphi, SD'\psi)\)?
Calderón Identities: Summary

- $SD' = D^2 - I/4$
- $D'S = S'^2 - I/4$

Also valid for Laplace (jump relation same after all!)

Why do we care?
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  Integral Equation Discretizations
  Integral Equation Discretizations: Nyström
  Integral Equation Discretizations: Projection

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Going General: More PDEs
Numerics: What do we need?

- Discretize curves and surfaces
  - Interpolation
  - Grid management
  - Adaptivity
- Discretize densities
- Discretize integral equations
  - Nyström, Collocation, Galerkin
- Compute integrals on them
  - “Smooth” quadrature
  - Singular quadrature
- Solve linear systems
Constructing Discrete Function Spaces

Floating point numbers (Degrees of Freedom or DoFs) ↔ Functions

Discretization relies on three things:
▶ Base/reference domain
▶ Basis of functions
▶ Meaning of DoFs

Related finite element concept: Ciarlet triple

Discretization options for a curve?
What do the DoFs mean?

Common DoF choices:

- Point values of function
- Point values of (directional?) derivatives
- Basis coefficients
- Moments

Often: useful to have both “modes”, “nodes”, jump back and forth
Why high order?

Order $p$: Error bounded as $|u_h - u| \leq C h^p$

Thought experiment:

<table>
<thead>
<tr>
<th>First order</th>
<th>Fifth order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,000 DoFs $\approx 1,000$ triangles</td>
<td>1,000 DoFs $\approx 66$ triangles</td>
</tr>
<tr>
<td>Error: 0.1</td>
<td>Error: 0.1</td>
</tr>
<tr>
<td>Error: 0.01 $\rightarrow$ ?</td>
<td>Error: 0.01 $\rightarrow$ ?</td>
</tr>
</tbody>
</table>

Complete the table.

Remarks:
- Want $p \geq 3$ available.
- **Assumption**: Solution sufficiently smooth
- Ideally: $p$ chosen by user
What is an Unstructured Mesh?

Why have an unstructured mesh?

What is the trade-off in going unstructured?

Demo: CAD software
## Fixed-order vs Spectral

<table>
<thead>
<tr>
<th>Fixed-order</th>
<th>Spectral</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Number of DoFs</strong> $n$</td>
<td><strong>Number of DoFs</strong> $n$</td>
</tr>
<tr>
<td>$\sim$</td>
<td>$\sim$</td>
</tr>
<tr>
<td>Number of ‘elements’</td>
<td>Number of modes resolved</td>
</tr>
<tr>
<td>Error $\sim \frac{1}{n^p}$</td>
<td>Error $\sim \frac{1}{C^n}$</td>
</tr>
</tbody>
</table>

**Examples?**
- ▶ Piecewise Polynomials
- ▶ Global Fourier
- ▶ Global Orth. Polynomials

What assumptions are buried in each of these?
Fixed-order vs Spectral

What should the DoFs be?

What’s the difficulty with purely modal discretizations?
Vandermonde Matrices

\[
\begin{bmatrix}
  x_0^0 & x_0^1 & \cdots & x_0^n \\
  x_1^0 & x_1^1 & \cdots & x_1^n \\
  \vdots & \vdots & \ddots & \vdots \\
  x_n^0 & x_n^1 & \cdots & x_n^n \\
\end{bmatrix}
\begin{bmatrix}
  a_0 \\
  a_1 \\
  \vdots \\
  a_n \\
\end{bmatrix}
= ?
\]
Generalized Vandermonde Matrices

\[
\begin{bmatrix}
\phi_0(x_0) & \phi_1(x_0) & \cdots & \phi_n(x_0) \\
\phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_n(x_1) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_0(x_n) & \phi_1(x_n) & \cdots & \phi_n(x_n)
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
\vdots \\
a_n
\end{bmatrix}
= ?
\]
Generalized Vandermonde Matrices

\[
\begin{bmatrix}
\phi_0(x_0) & \phi_1(x_0) & \cdots & \phi_n(x_0) \\
\phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_n(x_1) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_0(x_n) & \phi_1(x_n) & \cdots & \phi_n(x_n)
\end{bmatrix}
\]

MODAL COEFFS = NODAL COEFFS

- Node placement? **Demo:** Interpolation node placement
- Vandermonde conditioning? **Demo:** Vandermonde conditioning
- What about multiple dimensions?
  - **Demo:** Visualizing the 2D PKDO Basis
  - **Demo:** 2D Interpolation Nodes
Common Operations

(Generalized) Vandermonde matrices simplify common operations:

- Modal ↔ Nodal ("Global interpolation")
  - Filtering
  - Up-/Oversampling
- Point interpolation (Hint: solve using $V^T$)
- Differentiation
- Indefinite Integration
- Inner product
- Definite integration
Unstructured Mesh

- Design a data structure to represent this
- Compute normal vectors
- Compute area
- Compute integral of a function
- How is the function represented?

**Demo:** Working with Unstructured Meshes
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Integral Equation Discretizations: Overview

\[ \phi(x) - \int_{\Gamma} K(x, y)\phi(y)\,dy = f(y) \]

<table>
<thead>
<tr>
<th>Nyström</th>
<th>Projection</th>
</tr>
</thead>
<tbody>
<tr>
<td>▶ Approximate integral by quadrature: ( \int_{\Gamma} f(y),dy \rightarrow \sum_{k=1}^{n} \omega_k f(y_k) )</td>
<td>▶ Consider residual: ( R := \phi - A\phi - f )</td>
</tr>
<tr>
<td>▶ Evaluate quadrature’d IE at quadrature nodes, solve</td>
<td>▶ Pick projection ( P_n ) onto finite-dimensional subspace ( P_n\phi := \sum_{k=1}^{n} \langle \phi, v_k \rangle w_k \rightarrow ) DOFs ( \langle \phi, v_k \rangle )</td>
</tr>
<tr>
<td></td>
<td>▶ Solve ( P_n R = 0 )</td>
</tr>
</tbody>
</table>
Projection/Galerkin

- Equivalent to projection: Test IE with test functions
- Important in projection methods: sub-space (e.g. of $C(\Gamma)$)

Name some generic discrete projection bases.

Collocation and Nyström: the same?

Are projection methods implementable?
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Nyström Discretizations (1/4)

Nyström consists of two distinct steps:

1. Approximate integral by quadrature:

   \[ \varphi_n(x) - \sum_{k=1}^{n} \omega_k K(x, y_k) \varphi_n(y_k) = f(x) \]  

2. Evaluate quadrature’d IE at quadrature nodes, solve discrete system

   \[ \varphi_j^{(n)} - \sum_{k=1}^{n} \omega_k K(x_j, y_k) \varphi_k^{(n)} = f(x_j) \]  

with \( x_j = y_j \) and \( \varphi_j^{(n)} = \varphi_n(x_j) = \varphi_n(y_j) \)

Is version (1) solvable?
Nyström Discretizations (2/4)

What’s special about (2)?

Solution density also only known at point values. But: can get approximate continuous density. How?

Assuming the IE comes from a BVP. Do we also only get the BVP solution at discrete points?
Nyström Discretizations (3/4)

Does (1) ⇒ (2) hold?

Does (2) ⇒ (1) hold?
What good does that do us?

Does Nyström work for first-kind IEs?
Convergence for Nyström (1/2)

Increase number of quadrature points $n$:
Get sequence $(A_n)$
Want $A_n \to A$ in some sense
What senses of convergence are there for sequences of functions $f_n$?

What senses of convergence are there for sequences of operators $A_n$?
Convergence for Nyström (2/2)

Will we get norm convergence \( \| A_n - A \|_\infty \to 0 \) for Nyström? \([\text{Kress LIE 2nd ed. Thm. 12.8}]\)

Is functionwise convergence good enough?
Compactness-Based Convergence

$X$ Banach space (think: of functions)

**Theorem (Not-quite-norm convergence [Kress LIE 2nd ed. Cor 10.4])**

$A_n : X \to X$ bounded linear operators, functionwise convergent to $A : X \to X$

Then convergence is uniform on compact subsets $U \subset X$, i.e.

$$\sup_{\phi \in U} \| A_n \phi - A \phi \| \to 0 \quad (n \to \infty)$$

How is this different from norm convergence?
Collective Compactness

Set $\mathcal{A}$ of operators $A : X \to X$

**Definition (Collectively compact)**

$\mathcal{A}$ is called *collectively compact* if and only if for $U \subset X$ bounded, $\mathcal{A}(U)$ is relatively compact.

What was relative compactness (=precompactness)?
Is each operator in the set $\mathcal{A}$ compact?

Is collective compactness the same as “every operator in $\mathcal{A}$ is compact”?
Collective Compactness: Questions (2/2)

When is a sequence collectively compact?

Is the limit operator of such a sequence compact?

How can we use the two together?
Making use of Collective Compactness

$X$ Banach space, $A_n : X \to X$, $(A_n)$ collectively compact, $A_n \to A$ functionwise.

**Corollary (Post-compact convergence [Kress LIE 3rd ed. Cor 10.11])**

- $\| (A_n - A)A \| \to 0$
- $\| (A_n - A)A_n \| \to 0$
  ($n \to \infty$)
Anselone’s Theorem

\((I - A)^{-1}\) exists, with \(A : X \to X\) compact, \((A_n) : X \to X\) collectively compact and \(A_n \to A\) functionwise.

**Theorem (Nyström error estimate [Kress LIE 3rd ed. Thm 10.12])**

For sufficiently large \(n\), \((I - A_n)\) is invertible and

\[
\|\phi_n - \phi\| \leq C(\|(A_n - A)\phi\| + \|f_n - f\|)
\]

\[
C = \frac{1 + \| (I - A)^{-1} A_n \|}{1 - \| (I - A)^{-1} (A_n - A) A_n \|}
\]

\(I + (I - A)^{-1} A = ?\)
Define approximate inverse $B_n = I + (I - A)^{-1}A_n$.

How good of an inverse is it?

\[
\text{Id} \approx? \quad B_n(I - A_n) \\
= (I + (I - A)^{-1}A_n)(I - A_n) \\
= [I + (I - A)^{-1}A_n] - [A_n + (I - A)^{-1}A_nA_n] \\
= [I + (I - A)^{-1}A_n] - [(I - A)^{-1}(I - A)A_n + (I - A)^{-1}A_nA_n] \\
= [I + (I - A)^{-1}A_n] - [(I - A)^{-1}I A_n - (I - A)^{-1}AA_n + (I - A)^{-1}A_nA_n] \\
= I + (I - A)^{-1}AA_n - (I - A)^{-1}A_nA_n \\
= I + (I - A)^{-1}(A - A_n)A_n = I - S_n \\
= I - S_n
\]
Anselone’s Theorem: Proof (II)

Want $S_n \to 0$ somehow. Prior result gives us $\|(A - A_n)A_n\| \to 0$. 
Anselone’s Theorem: Proof (III)
Nyström: *specific to I + compact*. Why?
We assumed collective compactness. Do we have that? Assume

$$\sum |\text{quad. weights for } n \text{ points}| \leq C \quad \text{(independent of } n) \quad (3)$$
Nyström: Collective Compactness

Also assumed functionwise uniform convergence, i.e. $\|A_n\phi - A\phi\| \to 0$ for each $\phi$. 
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Projection Method

$X$ Banach space, $U \subset X$ nontrivial subspace, $A : X \to Y$ injective, $X_n \subset X$, $Y_n \subset Y$, $\dim X_n = n$, $\dim Y_n = n$, $P_n : ? \to ?$

- $P$ is a projection $\iff P|_U = \text{Id} \iff P^2 = P$
- $\|P\| \geq 1$
- Orthogonal projectors: $\|P\| = 1$
- Interpolators (“collocation projection”): Also projections
- **Projection method**: $P_n A \phi_n = P_n f$ (#)

Define convergence:
Assumptions on the Approximation Spaces

What’s needed of $X_n$ so that it can even approximate the solution?
Norm Convergence of Inverses

X, Y Banach spaces, A : X → Y bounded, A\(^{-1}\) bounded

Theorem (Norm Convergence of Inverses [Kress LIE 3rd ed. Thm. 10.1])

If \(\|A_n - A\| \to 0\) as \(n \to \infty\). Then for sufficiently large \(n\), \(A_n^{-1}\) exists and is bounded by

\[
\|A_n^{-1}\| \leq \frac{\|A^{-1}\|}{1 - \|A^{-1}(A_n - A)\|}.
\]

For \(A\varphi = f\) and \(A_n\varphi_n = f_n\), we have the estimate

\[
\|\varphi_n - \varphi\| \leq \frac{\|A^{-1}\|}{1 - \|A^{-1}(A_n - A)\|} \left[\|(A_n - A)\varphi\| + \|f_n - f\|\right].
\]
Norm Convergence of Inverses: Proof

Prove the result:
Write out the projected version of the second-kind equation $\varphi - A\varphi = f$: 

$$\varphi - A\varphi = f$$
Error Estimate for Second Kind Projection

$X$ Banach, $A : X \rightarrow X$ compact, $I - A$ injective

**Theorem (Second Kind Projection Estimate [Kress LIE 3rd ed. Thm. 13.10])**

Assume $\|P_nA - A\| \rightarrow 0$ ($n \rightarrow \infty$). Then for sufficiently large $n$,

$$\varphi_n - P_nA\varphi_n = P_nf$$

is uniquely solvable for all $f \in X$, and we have $\|\varphi_n - \varphi\| \leq M \|P_n\varphi - \varphi\|$ for $M$ a constant depending on $A$. 

Error Estimate for Second Kind Projection: Proof

Prove the result:
In actual numerical use, we’re not solving

\[ \varphi_n - P_n A \varphi_n = P_n f \]

but

\[ \tilde{\varphi}_n - P_n A_n \tilde{\varphi}_n = P_n f_n, \]

where

- \( A_n \) approximates \( A \),
- \( f_n \) approximates \( f \).
Perturbations of Projection Methods for Second Kind: Estimate

\( X \) Banach, \( A : X \to X \) compact, \( I - A \) injective

**Theorem (SK Projection Perturbation [Kress LIE 3rd ed. Cor. 13.11])**

Assume that functionwise \( P_n A_n - P_n A \to 0 \) and \( \| P_n A_n - P_n A \| \to 0 \) \((n \to \infty)\). Then for sufficiently large \( n \) \( \tilde{\varphi}_n - P_n A_n \tilde{\varphi}_n = P_n f_n \) is uniquely solvable and for some positive constant \( M \),

\[
\| \tilde{\varphi}_n - \varphi \| \leq M (\| P_n \varphi - \varphi \| + \| (P_n A_n - P_n A) \varphi_n \| + \| P_n (f_n - f) \|).
\]
Problem: Singular behavior at corner points. Density may blow up. Can the density be convergent in the $\| \cdot \|_\infty$ sense? Conditioning of the discrete system? GMRES will flail and break, because it sees $\ell^2 \sim l^\infty \sim L^\infty$ convergence.

Make GMRES ‘see’ $L^2$ convergence by redefining density DOFs:

$$\overline{\sigma}_h := \begin{bmatrix} \sqrt{\omega_1} \sigma(x_1) \\ \vdots \\ \sqrt{\omega_n} \sigma(x_n) \end{bmatrix} = \sqrt{\omega} \sigma_h$$

So $\overline{\sigma}_h \cdot \overline{\sigma}_h =$?

Also fixes system conditioning! Why?
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‘Off-the-shelf’ ways to compute integrals

How do I compute an integral of a nasty singular kernel?
Symbolic integration

Why not Gaussian?
Numerically distinct scenarios:

- Near-Singular quadrature
  - Integrand nonsingular
  - But may locally require lots of
  - Adaptive quadrature works, but...

- Singular quadrature
  - Integrand singular
  - Conventional quadrature fails
Kussmaul-Martensen quadrature

Theorem (A special integral [Kress LIE Lemma 8.21])

\[
\frac{1}{2\pi} \int_0^{2\pi} \log \left( 4 \sin^2 \frac{t}{2} \right) e^{imt} dt = \begin{cases} 
0 & m = 0, \\
-\frac{1}{|m|} & m = \pm 1, \pm 2 \ldots .
\end{cases}
\]

Why is that exciting?

**Demo:** Kussmaul-Martensen quadrature
Singularity Subtraction

\[ \int \langle \text{Thing } X \text{ you would like to integrate} \rangle = \int \langle \text{Thing } Y \text{ you } \textit{can} \text{ integrate} \rangle + \int \langle \text{Difference } X - Y \text{ which is easy to integrate (numerically)} \rangle \]

Give a typical application.

Drawbacks?
High-Order Corrected Trapezoidal Quadrature

- Conditions for new nodes, weights
  $\rightarrow$ linear algebraic system, dep. on $n$
  to integrate
  $\langle\text{smooth}\rangle \cdot \langle\text{singular}\rangle + \langle\text{smooth}\rangle$

- Allowed singularities: $|x|^\lambda$ (for $|\lambda| < 1$), $\log|x|$

- Generic nodes and weights for log singularity

- Nodes and weights copy-and-pasteable from paper

[Kapur, Rokhlin ‘97]

Alpert ‘99 conceptually similar:
Generalized Gaussian

- “Gaussian”:
  - Integrates $2n$ functions exactly with $n$ nodes
  - Positive weights
- Clarify assumptions on system of functions (“Chebyshev system”) for which Gaussian quadratures exist
- When do (left/right) singular vectors of integral operators give rise to Chebyshev systems?
  - In many practical cases!
- Find nodes/weights by Newton’s method
  - With special starting point
- Very accurate
- Nodes and weights for download

[Yarvin/Rokhlin ‘98]
Singularity cancellation: Polar coordinate transform

\[
\int \int_{\partial \Omega} K(x, y) \phi(y) \, ds_y \\
= \\
\int_0^R \int_{x+r \in \partial \Omega \cap \partial B(x, r)} K(x, x + r) \phi(x + r) d\langle \text{angles} \rangle \, r \, dr \\
= \\
\int_0^R \int_{x+r \in \partial \Omega \cap \partial B(x, r)} K_{\text{less singular}}(x, x + r) \frac{1}{r} \phi(x + r) d\langle \text{angles} \rangle \, r \, dr
\]

where \( K_{\text{less singular}} = K \cdot r \).
Quadrature on Triangles

Problem: Singularity can sit anywhere in triangle → need lots of quadrature rules (one per target)
Quadrature on Triangles

Problem: Singularity can sit *anywhere* in triangle
→ need *lots* of quadrature rules (one per target)
Kernel regularization

Singularity makes integration troublesome: *Get rid of it!*

\[ \cdots \frac{\pi}{\sqrt{(x - y)^2}} \rightarrow \cdots \frac{\pi}{\sqrt{(x - y)^2 + \epsilon^2}} \]

Use Richardson extrapolation to recover limit as \( \epsilon \rightarrow 0 \).
(May also use geometric motivation: limit along line towards singular point.)

Primary drawbacks:
- Low-order accurate
- Need to make \( \epsilon \) smaller (i.e. kernel more singular) to get better accuracy

Can take many forms—for example:
- Convolve integrand to smooth it
  \((\rightarrow \text{remove/weaken singularity})\)
- Extrapolate towards no smoothing

Related: [Beale/Lai ‘01]
Acceleration and Quadature

How can singular quadrature and FMM acceleration be made compatible?
FMMs and other Layer Potentials

How does an FMM evaluate a double layer?

How does an FMM evaluate $S'$?

What effect does this have on accuracy?
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Layer Potential Evaluation: Some Intuition
QBX: Idea

Expansion center

Potential from expansion

Target point $x$

"Naive" potential

Curve $\Gamma$

Source quad. nodes $x'$

$log_{10}(\text{Error})$
QBX: An Experiment

\[ p = 3, \quad N = 80 \]

<table>
<thead>
<tr>
<th>log_{10}(Error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0</td>
</tr>
<tr>
<td>5.4</td>
</tr>
<tr>
<td>4.8</td>
</tr>
<tr>
<td>4.2</td>
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<tr>
<td>0.6</td>
</tr>
<tr>
<td>0.0</td>
</tr>
</tbody>
</table>

\begin{align*}
\text{log}_{10}(\text{Error})
\end{align*}

\[ p = 12, \quad N = 240 \]

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>12.0</td>
</tr>
<tr>
<td>10.5</td>
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<td>3.0</td>
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<tr>
<td>1.5</td>
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<tr>
<td>0.0</td>
</tr>
</tbody>
</table>

\begin{align*}
\text{log}_{10}(\text{Error})
\end{align*}
QBX: An Experiment

$p = 3, N = 80$

$p = 6, N = 80$

$p = 12, N = 80$

$p = 12, N = 240$
QBX: An Experiment

$p = 3, \quad N = 80$

$p = 6, \quad N = 80$

$p = 12, \quad N = 80$
QBX: An Experiment

$p = 3, N = 80$

$p = 6, N = 80$

$p = 12, N = 80$

$p = 12, N = 240$
Graf’s addition theorem

\[ H(1)_{\pm \infty} \left( k | x - x' | \right) = H(1)_{\pm \infty} \left( k | x - c | \right) e^{i l \theta'} J_{l} \left( k | x - c | \right) e^{-i l \theta} \]

Requires:

\[ |x - c| < |x' - c| \] ("local expansion")
Graf’s addition theorem requires: $|x - c| < |x' - c|$ (“local expansion”)

\[
H_0^{(1)}(k|x - x'|) = \sum_{l=-\infty}^{\infty} H_l^{(1)}(k|x' - c|) e^{i l \theta'} J_l(k|x - c|) e^{-i l \theta}
\]
Compute layer potential on the disk as

\[ S_k\sigma(x) = \sum_{l=-\infty}^{\infty} \alpha_l J_l(k \rho) e^{-il\theta} \]

with

\[ \alpha_l = \frac{i}{4} \int_{\Gamma} H_l^{(1)}(k|x' - c|) e^{il\theta'} \sigma(x') \, dx' \quad (l = -\infty, \ldots, \infty) \]

\( S\sigma \) is a smooth function up to \( \Gamma \).
Compute layer potential on the disk as

\[ S_k \sigma(x) = \sum_{l=-p}^{p} \alpha_l J_l(k \rho) e^{-il\theta} \]

with

\[ \alpha_l = \frac{i}{4} T_N \left( \int_{\Gamma} H_l^{(1)}(k|x'| - c|) e^{il\theta'} \sigma(x') \, dx' \right) \quad (l = -\infty, \ldots, \infty) \]

\( S \sigma \) is a smooth function up to \( \Gamma \).
Quadrature by Expansion (QBX)

\[
\text{Error} \leq \left( C \left\lbrack r^{p+1} \right\rbrack \text{Truncation error} + C \left\lbrack \left( \frac{h}{r} \right)^q \right\rbrack \text{Quadrature error} \right) \|\sigma\|
\]

[K, Barnett, Greengard, O’Neil JCP ‘13]
Achieving high order

\[
\text{Error} \leq \left( C \underbrace{r^{p+1}}_{\text{Truncation error}} + C \underbrace{\left( \frac{h}{r} \right)^q}_{\text{Quadrature error}} \right) \| \sigma \|
\]

Two approaches:

- **Asymptotically convergent**: \( r = \sqrt{h} \)
  - \( \checkmark \) Error \( \to 0 \) as \( h \to 0 \)
  - \( \times \) Low order: \( h^{(p+1)/2} \)

- **Convergent with controlled precision**: \( r = 5h \)
  - \( \times \) Error \( \not\to 0 \) as \( h \to 0 \)
  - \( \checkmark \) High order: \( h^{p+1} \) to controlled precision \( \epsilon := (1/5)^q \)
Other layer potentials

Can’t just do single-layer potentials:

\[ \alpha^D_\ell = \frac{i}{4} \int_{\Gamma} \frac{\partial}{\partial \hat{n}_{x'}} H^{(1)}_\ell(k|x' - c|) e^{i\ell\theta'} \mu(x') \, dx'. \]

Even easier for target derivatives (S’ et al.): Take derivative of local expansion.

Analysis says: Will lose an order.

Slight issue: QBX computes one-sided limits.

Fortunately: Jump relations are known—e.g.

\[ (PV)D^* \mu(x)|_{\Gamma} = \lim_{x^\pm \to x} D \mu(x^\pm) \mp \frac{1}{2} \mu(x). \]

Alternative: Two-sided average → Preferred because of conditioning
Understanding Truncation Behavior

Let $\Gamma = \partial \Omega^-$ be piecewise $C^2$ with no inward facing cusps. Let $\Psi$ be the exterior Riemann map that maps the exterior $\Omega^+$ onto the exterior of the unit disk.

**Theorem (A basis of QBX-exact densities)**

A function on the interior $f : \Omega^- \to \mathbb{R}$ is a harmonic polynomial of degree $n$ if and only if $f$ has the representation $f = D\varphi$ and the associated double-layer density function $\varphi$ takes the form

$$\varphi(z) = \sum_{k=0}^{n} \lambda_k \cos(k\theta(z) + \mu_k), \quad z \in \Gamma$$

for some set of real coefficients $\lambda_k, \mu_k$, where $\theta(w) = \text{arg} \Psi(w)$ is the boundary correspondence.

[Wala, K '18]
QBX and Conformal Mapping

Require: A smooth Jordan boundary $\Gamma$, with 0 in the interior.
Require: A boundary sign $s$: +1 for exterior, −1 for interior.
Ensure: Computes the boundary correspondence $\theta$.

Stage 1
Solve the following integral equation for the density $\sigma$, for all $\zeta \in \Gamma$:

\[
\begin{align*}
\zeta &= \left( \mathcal{D} - \frac{1}{2} \right) \sigma(\zeta) \quad \text{if } s = +1 \\
\bar{\zeta}^{-1} &= \left( \mathcal{D} + \int + \frac{1}{2} \right) \sigma(\zeta) \quad \text{if } s = -1.
\end{align*}
\]

Stage 2
Let $\tilde{\sigma}(\zeta) = \sigma(\zeta) + \frac{s}{2\pi i} \int_{\Gamma} \frac{\sigma(y)}{y} dy \ (\zeta \in \Gamma)$.

Stage 3
Let $\theta(\zeta) = \arg \left( -s \frac{\tilde{\sigma}(\zeta)}{|\tilde{\sigma}(\zeta)|} \right) \ (\zeta \in \Gamma)$. 

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  A Bag of Quadrature Tricks
  Quadrature by expansion (‘QBX’)
  **QBX Acceleration**
  Reducing Complexity through better Expansions
  Results: Layer Potentials
  Results: Poisson

Going General: More PDEs
Local QBX: Viewing QBX as a Local Correction

What happens if one attempts to use QBX quadrature as a ’local correction’?
QBX + FMM: A straightforward coupling

QBX expansion

QBX center

Box local expansion

Γ
### Accuracy vs FMM/QBX orders: Straightforward (2D)

<table>
<thead>
<tr>
<th>$(1/2)^{p_{\text{FMM}}+1}$</th>
<th>$p_{\text{FMM}}$</th>
<th>$p_{\text{QBX}} = 3$</th>
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<tr>
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$\ell_{\infty}$ error in Green’s formula $S(\partial_n u) - D(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish $\gamma_{65}$, using the conventional QBX FMM algorithm. 3250 Gauss-Legendre panels, with 33 nodes per panel.
Recap: Local Expansions of Potentials

Truncation Error \( \sim \left( \frac{\text{furthest target}}{\text{closest source}} \right)^{p+1} \)
QBX + FMM: Sources of Inaccuracy
Possible Expansion Sequences

- Source → Multipole($p$) → QBX-Local($q$)
- Source → Local($p$) → QBX-Local($q$)
- Source → Multipole($p$) → Local($p$) → QBX-Local($q$)
Translation chains for QBX

\[
\begin{align*}
\text{log}_{10} |\ell_{3,\text{direct}} - \ell_{8,\rightarrow 8, M2L(8)}| \\
\%
\end{align*}
\]
Translation chains for QBX

\[
\log_{10} |l_3, \text{direct} - l_{3, \rightarrow 15, M2L(15)}| \%
\]
Expansions of Expansions?

Truncation Error \( \sim \left( \frac{\text{furthest target}}{\text{closest source}} \right)^{p+1} \)

This holds for point evaluations of a single expansion.

Question: Can we generalize it to hold when forming expansions of expansions?
**Lemma**

Let $c, r > 0$. Suppose that a single unit strength charge is placed at $z_0$, with $|z_0| \geq (c + 1)r$. Suppose that $y, z \in \overline{B}(0, r)$. If $|z| < r$ and $|y - z| \leq r - |z|$, the potential $\phi$ due to the charge is described by a power series

$$\phi(y) = \sum_{k=0}^{\infty} \beta_k (y - z)^k.$$  

Fix the intermediate local order $p \geq 0$. For $n \geq 0$, let

$$\tilde{\beta}_n = \frac{1}{n!} \frac{d^n}{dz^n} \left( \sum_{k=0}^{p} \frac{\phi^{(k)}(0)}{k!} z^k \right).$$

Fix the local expansion order $q \geq 0$. Define $\alpha = 1/(1 + c)$. Then

$$\left| \sum_{k=0}^{q} \beta_k (y - z)^k - \sum_{k=0}^{q} \tilde{\beta}_k (y - z)^k \right| \leq \left( \frac{q + 1}{p + 1} \right) \left( \frac{\alpha^{p+1}}{1 - \alpha} \right).$$

[Wala, K ‘18a – arxiv:1801.04070]
Example: Local($p$) → Local($q$) Truncation Error (2D Lap.)

**Lemma**

Let $c, r > 0$. Suppose that a single unit strength charge is placed at $z_0$, with $|z_0| \geq (c + 1)r$. Suppose that $y, z \in \overline{B}(0, r)$. If $|z| < r$ and $|y - z| \leq r - |z|$, the potential $\phi$ due to the charge is described by a power series

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[Wala, K ‘18a – arxiv:1801.04070]
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Fix the local expansion order $q > 0$. Define

$$\text{Truncation Error} \sim \left( \frac{\text{furthest target}}{\text{closest source}} \right)^{p+1}.$$
A Glimpse of Expansion Technology

- M/L expansions typically work by separation of variables
  - In angular + radial coordinates
- Basis for capturing the angular dependency in 3D?
- Known: Expanded potential solves PDE
- So: Expansion fully specified if known on surface of sphere
  - (Interior Dirichlet BVP, e.g.)
  - Radial dependency: find ODE, straightforward to evaluate
Expansions on the Surface of a Sphere

- Generalizing to $n$ dimensions: (we care about $d = 2, 3$)
  \[ S^{d-1} = \{ x \in \mathbb{R}^d : \|x\| = 1 \} \]

- A polynomial $p : \mathbb{R}^d \to \mathbb{C}$ is homogeneous of degree $k$ if $p$ satisfies $p(rx) = r^k p(x)$ for all $x \in \mathbb{R}^d$.

- Space of spherical harmonics $\mathbb{Y}_n^d$: restrictions to the unit sphere $S^{d-1}$ of the harmonic ($\triangle p = 0$), homogeneous polynomials of degree $n$.

- Fourier-Laplace series:
  \[ \mathcal{F}_p f(\xi) = \sum_{n=0}^{p} \mathcal{P}_n f(\xi), \quad \xi \in S^{d-1}, \]

  where $\mathcal{P}_n[:]$ is an orthogonal projection onto $\mathbb{Y}_n^d$. 

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Proposition (Norm of the Fourier-Laplace partial sum)

Let \( f \in C(\mathbb{S}^{d-1}) \). Then a constant \( \Lambda_{n,d} > 0 \) exists such that

\[
\| \mathcal{F}_n f \|_\infty \leq \Lambda_{p,d} \| f \|_\infty,
\]

where, in dimensions \( d = 2 \) and \( d = 3 \),

\[
\Lambda_{p,2} = \frac{4}{\pi^2} \log p + O(1),
\]

\[
\Lambda_{p,3} = 2 \sqrt{\frac{2p}{\pi}} + o(\sqrt{p}),
\]

asymptotically as \( p \to \infty \).

[Rivlin ‘69], [Gronwall 1911]
Expansions of Expansions: M2QBXL

\[ \mathcal{M}_c^p[\mathcal{K}_s] \]

\[ \mathcal{L}^q_{c'}[\mathcal{M}_c^p[\mathcal{K}_s]] \]

\[ \overline{B(c, r)} \]

\[ \overline{B(0, R)} \]
Let $R > 0$ and $\rho > r > 0$. Consider a closed ball of radius $r$ centered at $c$, with $\|c\| = R + \rho$, containing a unit-strength source $s$. Also, let a ball of radius $R$ centered at the origin contain points $t$ and $c'$ satisfying $\|c\| \leq R$ and $\|t - c'\| \leq R - \|c'\|$.

Then, in the situation of the previous slide:

$$|\mathcal{L}_{c'}^{q}[\mathcal{K}_s](t) - \mathcal{L}_{c}^{q}[\mathcal{M}^{p}_{c}[\mathcal{K}_s]](t)| \leq \Lambda_{q,d} \left\| (\mathcal{K}_s - \mathcal{M}^{p}_{c}[\mathcal{K}_s]) |_{B(0,R)} \right\|_{\infty}.$$
Translation Chains for QBX

Rigorous truncation error bounds for local expansions for scenarios QBX locals *near* box locals:
Targets with Extent: Target Confinement Regions

QBX center ‘not in’ box

QBX center ‘in’ box
M2L Convergence Factor with 2-Away, TCF (3D)

3D, $t_f = 0.9$: Conv. factor $\approx 0.77$
Theorem (GIGAQBX FMM for Laplace (2D/3D))

Let the center \( c \) be owned by the box \( b \) and let \( t \) be a target associated with the center \( c \). Assuming that \( 0 \leq t_f \leq 6/\sqrt{d} - 2 \), and defining the constants

\[
\omega = \frac{\sqrt{d}(1 + t_f)}{6 - \sqrt{d}}, \quad A = \sum_{i=1}^{N_S} |w_i|,
\]

and letting \( D \) be the minimum box width in the tree, the (absolute) acceleration error in the GIGAQBX FMM is bounded as follows:

\[
\| L_q^c[\phi](t) - G_c^{p,q}[\phi](t) \| \leq \begin{cases} 
A\Lambda_{q,2}^p \max \left( \frac{1 - \sqrt{2}}{3} \left( \frac{\sqrt{2}}{3} \right)^{p+1}, \frac{1}{1-\omega} \omega^{p+1} \right), & d = 2, \\
A\Lambda_{q,3}^p \max \left( \frac{1}{3 - \sqrt{3}} \left( \frac{\sqrt{3}}{3} \right)^{p+1}, \frac{1}{6-2\sqrt{3}-\sqrt{3}t_f} \omega^{p+1} \right), & d = 3.
\end{cases}
\]

[Wala-K '19—in prep.]
Theorem (GIGAQBX FMM for Laplace (2D/3D))

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$$\|L_q^c[\phi](t) - G_{q,c}[\phi](t)\| \leq \begin{cases} A\Lambda_{q,2} \max (1, t_f) & \text{for } \sqrt{d} = 2, \\ A\Lambda_{q,3} \max (1, t_f) \frac{3}{D} \max (1, t_f) & \text{for } \sqrt{d} = 3. \end{cases}$$

[Wala-K ‘19—in prep.]

“GIGAQBX”:

- Consider sized targets (QBX expansions)
- Introduce a Target Confinement Rule
- Some M2P and P2L must be direct
- Targets in Non-Leaf Boxes
- Two-Box Separation
Interaction Lists
### Complexity (3D, Point-and-Shoot)

<table>
<thead>
<tr>
<th>Modeled Operation Count</th>
<th>What</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NL$</td>
<td>Build tree</td>
</tr>
<tr>
<td>$N_S p_{FMM}^2 + N_B p_{FMM}^3$</td>
<td>Form M, Upward pass</td>
</tr>
<tr>
<td>$(27(N_C + N_S) n_{\text{max}} + N_C M_C) p_{\text{QBX}}^2$</td>
<td>List 1: P2QBXL</td>
</tr>
<tr>
<td>$875 N_B p_{FMM}^3$</td>
<td>List 2: M2L</td>
</tr>
<tr>
<td>$N_C M_C q^2 + 124 L N_S n_{\text{max}} p_{\text{QBX}}^2$</td>
<td>List 3: P2QBXL+M2QBXL</td>
</tr>
<tr>
<td>$375 N_B n_{\text{max}} p_{FMM}^2 + 250 N_C n_{\text{max}} p_{\text{QBX}}^2$</td>
<td>List 4: P2QBXL+P2L</td>
</tr>
<tr>
<td>$8 N_B p_{FMM}^3$</td>
<td>Downward</td>
</tr>
<tr>
<td>$N_C p_{FMM}^3$</td>
<td>L2QBXL</td>
</tr>
<tr>
<td>$N_T p_{\text{QBX}}^2$</td>
<td>QBXL2P</td>
</tr>
</tbody>
</table>
Complexity (3D)

**Theorem**

Assume that $p_{FMM} = O(\|\log \epsilon\|)$, and that $p_{QBX} \leq p_{FMM}$. For a fixed value of $n_{\text{max}}$, using a level-restricted octree and with $t_f < \sqrt{3} - 1$, the cost in modeled flops of the evaluation stage of the GIGAQBX FMM is

$$O((N_C + N_S + N_B)\|\log \epsilon\|^3 + N_C M_C \|\log \epsilon\|^2 + N_T \|\log \epsilon\|^2).$$

Assuming that the particle distribution satisfies $N_B = O(N)$ and $M_C = O(1)$, the worst-case modeled cost using a level-restricted octree and $t_f < \sqrt{3} - 1$ is linear in $N$.

[Wala-K ‘18]
Curve Interaction Lists
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- QBX Acceleration
  - Reducing Complexity through better Expansions

  Results: Layer Potentials
  Results: Poisson

Going General: More PDEs
Spherical Harmonic Expansions: Notation

- $s$: source point
- $t$: target point
- $c$: expansion center
- $a = t - c$
- $b = s - c$
- $\gamma$: angle between $a$ and $b$
- $p$: expansion order
Expansion of Laplace potential in 3D:

\[
\frac{(4\pi)^{-1}}{\|a - b\|} = \sum_{n=0}^{\infty} \frac{1}{2n + 1} \frac{\|a\|^n}{\|b\|^{n+1}} \sum_{m=-n}^{n} Y^n_m(\theta_a, \phi_a) Y_n^{-m}(\theta_b, \phi_b)
\]

Valid for $|a| < |b|$.

**Total cost:** $O((p + 1)^2(N + M))$ (for $M$ targets, $N$ sources)
Spherical Harmonic Expansions: An Identity

By Legendre addition theorem

\[ P_n(\cos \gamma) = \frac{1}{2n + 1} \sum_{m=-n}^{n} Y_n^m(\theta_a, \phi_a) Y_n^{-m}(\theta_b, \phi_b) \]

\( P_n \) are Legendre polynomials

Results in line expansion (or ‘target-specific expansion’):

\[ \left( \frac{4\pi}{||a - b||} \right)^{-1} = \sum_{n=0}^{\infty} \frac{||a||^n}{||b||^{n+1}} P_n(\cos \gamma) \]

**Total cost:** \( O((p + 1)NM) \)

First use in ‘local’ QBX: [Siegel, Tornberg ’17]

**Downside:** Sources/targets no longer separated.
Details

- QBX [K et al ‘13]: Unifies toolset for quad. and accel.
- QBX FMM [Rachh et al ‘16]: Geometry proc., first fast alg.
- Truncation Result [Wala, K ‘18]: Exact density basis
- GIGAQBX 2D [Wala, K ‘18]: Guaranteed-Accuracy Accel.
- GIGAQBX 3D [Wala, K ‘18]: $\ell^2$ TC, improved geom. proc.
- GIGAQBX-TS [Wala, K ‘19]: Reduce accel. cost
- Fourier-Laplace bounds [Wala, K ‘19–in prep.]: 2D/3D analysis
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Layer Potentials: Accuracy (2D GIGAQBX)

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$\ell^\infty$ error in Green’s formula $S(\partial_n u) - D(u) = u/2$, scaled by $1/\|u\|_{\infty}$, for the 65-armed starfish $\gamma_{65}$, using the GIGAQBX FMM algorithm. 3250 Gauss-Legendre panels, with 33 nodes per panel.
## Layer Potentials: Accuracy (2D Straightforward)

\[ (1/2)^{p_{FMM}+1} \begin{array}{cccccc}
\hline
p_{FMM} & p_{QBX} = 3 & p_{QBX} = 5 & p_{QBX} = 7 & p_{QBX} = 9 \\
\hline
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5e-7 & 20 & 4.35e-6 & 1.31e-5 & 8.99e-5 & 5.01e-4 \\
\hline
\end{array} \]

\[ \ell^\infty \text{ error in Green's formula } S(\partial_n u) - D(u) = u/2, \text{ scaled by } 1/\|u\|_{\infty}, \text{ for the 65-armed starfish } \gamma_{65}, \text{ using the conventional QBX FMM algorithm.} \]

3250 Gauss-Legendre panels, with 33 nodes per panel.
Layer Potentials: Accuracy in 3D

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<td>9.18e-3</td>
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<tr>
<td>1.78e-1</td>
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<td>1.41e-6</td>
<td>2.51e-7</td>
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\(\ell^\infty\) error in Green’s formula \(S(\partial_n u) - D(u) = u/2\), scaled by \(1/\|u\|_\infty\), for the 8-armed ‘urchin’ geometry \(\gamma_8\).

Stage 1: 48500 triangles, stage 2: 277712 triangles, with 295 nodes per triangle.
Layer Potentials: Accuracy in 3D

<table>
<thead>
<tr>
<th>((3/4)^{p_{\text{FMM}}+1})</th>
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<td>1.43e−3</td>
</tr>
<tr>
<td>4.22e−2</td>
<td>10</td>
<td>6.08e−5</td>
</tr>
<tr>
<td>1.00e−2</td>
<td>15</td>
<td>6.08e−5</td>
</tr>
<tr>
<td>2.38e−3</td>
<td>20</td>
<td>6.08e−5</td>
</tr>
</tbody>
</table>

\(\ell^\infty\) error in Green’s formula \(S(\partial_n u)\) for the 8-armed ‘urchin’ geometry \(\gamma_8\). Stage 1: 48500 triangles, stage 2: 277712 triangles. With 295 nodes per triangle.

‘Urchin’ geometry \(\gamma_8\), based on 8th order spherical harmonics.
Layer Potentials: (Somewhat) Complex Geometry
Cost Scaling: 3D GIGAQBX FMM

Modeled operation counts for the GIGAQBX FMM for $S_{\mu}$.

$n_{\text{max}} = 512$ and $t_f = 0.9$. Geometries: $\gamma_2, \gamma_4, \ldots, \gamma_{10}$. 

$p_{\text{QBX}} = 9, p_{\text{FMM}} = 20$

$U_b, V_b, W_{\text{close}}, W_{\text{far}}, X_{\text{close}}, X_{\text{far}}, \text{all}$
“Balancing” an FMM

Impact of $n_{\text{max}}$ on Modeled Process Time

Modeled Process Time (s)

$n_{\text{max}}$

$10^2$  $10^3$  $10^4$

$U_b$  $V_b$  $W_b^{\text{close}}$  $W_b^{\text{far}}$  $X_b^{\text{close}}$  $X_b^{\text{far}}$  all
Line/Target-Specific Expansions: Cost Impact

- Operator: Single layer
- Orders: QBX: 9, FMM: 20 (9~digits)
- Points: 19M → 2.1M

![Diagram showing percentage of baseline speedup]

- $W_b^{\text{close}}$ (other)
- $W_b^{\text{far}}$
- $U_b$
- $V_b$
- $n_{\text{max}}$
- $n_{\text{mpole}}$
Line/Target-Specific Expansions: Cost Impact

- Operator: Single layer
- Orders: QBX: 9, FMM: 20 (9~digits)
- Points: 19M → 2.1M

$\text{\textbf{\textit{base}}}$

$\text{\textbf{\textit{ts}}}$

$n_{\text{\textbf{\textit{max}}}}$

$n_{\text{\textbf{\textit{mpole}}}}$

\[ n_{\text{\textbf{\textit{max}}}}: 96 \rightarrow 928, \quad n_{\text{\textbf{\textit{mpole}}}}: 40 \rightarrow 380 \]

Speedup: $3.3 \times$ [Wala-K ‘19]
Outline

Introduction

Dense Matrices and Computation

Tools for Low-Rank Linear Algebra

Rank and Smoothness

Near and Far: Separating out High-Rank Interactions

Outlook: Building a Fast PDE Solver

Going Infinite: Integral Operators and Functional Analysis

Singular Integrals and Potential Theory

Boundary Value Problems

Back from Infinity: Discretization

Computing Integrals: Approaches to Quadrature
  A Bag of Quadrature Tricks
  Quadrature by expansion (‘QBX’)  
  QBX Acceleration
  Reducing Complexity through better Expansions
  Results: Layer Potentials
    Results: Poisson

Going General: More PDEs
Poisson: 3D, CAD Geometry

Volume degree: 7 · Boundary degree: 6 · QBX order: 3
Outline

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Going General: More PDEs
Inhomogeneous Problems

Example: Poisson

\[ \triangle u = f, \quad u = g \text{ on } \partial \Omega. \]

Steps:

1. Solve the PDE (without the boundary condition) using the free-space Green’s function \( G \):

\[ \tilde{u} = G \ast f, \]

where ‘\( \ast \)’ represents convolution.

2. Solve

\[ \triangle \hat{u} = 0, \quad \hat{u} = g - \tilde{u} \text{ on } \partial \Omega \]

using a boundary integral equation.

3. Add

\[ u = \tilde{u} + \hat{u}, \]

which solves the Poisson problem.
Example: Solve

\[ \triangle u = \lambda u. \]

Two options:

▶ Volume linear eigenvalue problem with Laplace kernel
▶ Surface nonlinear eigenvalue problem with Helmholtz kernel
Maxwell’s equations

Example: Solve a scattering problem from a perfect electric conductor. Use Vector Potential \( \vec{A} \) to represent magnetic field:

\[
\vec{H} = \nabla \times \vec{A},
\]

where

\[
\triangle \vec{A} + k^2 \vec{A} = \vec{0}.
\]

Since \( \vec{A} \) solves vector Helmholtz, simply represent as

\[
\vec{A}(x) = S_k \vec{J}_s,
\]

where \( \vec{J}_s \) (physically) amounts to a surface current density.
Maxwell’s: Towards the MFIE

Then use

- the *continuity condition*

\[ \vec{n} \times [\vec{H}_{\text{tot}}] = \vec{J}_s, \]

- the *extinction theorem* for perfect electrical conductors:

\[ \vec{H}_{\text{tot}}^- = \vec{0} \]

inside the scatterer.

- the jump conditions
together to obtain the *Magnetic Field Integral Equation (MFIE):*

\[ \vec{n} \times \vec{H}_{\text{inc}}^+ = \frac{\vec{J}_s}{2} - \vec{n} \times (\text{PV}) \nabla \times S_k \vec{J}_s. \]
Stokes flow

(see project presentation)