Fast Algorithms and Integral Equation Methods

CS598APK

Andreas Kloeckner

Fall 2024

Outline

Outline

Outline

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 α 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

Class web page

https://bit.ly/fastalg-s24

contains:

- Class outline
- Notes
- Demos
- Assignments
- Discussion forum
- Grading
- Video

Why study this at all?

- Finite difference/element methods are inherently
  - ill-conditioned
  - 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!

Bonus Advertising Goodie

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

Sources

- Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions by Halko/Martinsson/Tropp
- Carrier, Greengard, Rokhlin: A Fast Adaptive Multipole Algorithm for Particle Simulations
- Rainer Kress: Linear integral equations. (second edition)
- David Colton and Rainer Kress: Inverse Acoustic and Electromagnetic Scattering Theory. (3rd edition)

Outline

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

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

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)

Point Interaction Matrices: Examples (III)

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 $\boldsymbol{u} = (u_i)$ and $\boldsymbol{v} = (v_j)$.
Can we compute $A\boldsymbol{x}$ quickly? (for a vector $\boldsymbol{x}$)

Fast Dense Matvecs (II)

$$A = \boldsymbol{u}_1 \boldsymbol{v}_1^T + \cdots + \boldsymbol{u}_K \boldsymbol{v}_K^T$$

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?

Representation (in context)

Outline

Outline

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?

Even Faster Matvecs for Range Finding

Assumptions on Ω are pretty weak–can use more or less anything we want.
$\rightarrow$ Make it so that we can apply the matvec $A\Omega$ in $O(n^2 \log \ell)$ time.
How? Pick Ω as a carefully-chosen subsampling of the Fourier transform.
(many other approaches also exist)

Outline

Errors in Random Approximations

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 $k \geqslant 2$ and an oversampling parameter $p \geqslant 2$ with $k + p \leqslant \min(m, n)$, with probability $1 - 6 \cdot p^{-p}$,

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

(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 *a-priori*. Once we're done, can we find out 'how well it turned out'?

Adaptive Range Finding: Algorithm

Outline

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?

ID Q vs ID A

What does row selection mean for the LRA?

[Martinsson, Rokhlin, Tygert '06]

ID: Remarks

Slight tradeoff here: what?

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

Demo: Interpolative Decomposition

Name a property that the ID has over other factorizations.

ID: Impact on Low-Rank Algorithms

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?

Leveraging the ID for SVD (III)

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.

Outline

Outline

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

Taylor and Error (I)

How can we estimate the error in a Taylor expansion?

Taylor and Error (II)

Now suppose that we had an estimate that $\left|\frac{f^{(p)}(c)}{p!}h^p\right| \leqslant \alpha^p$.

Connect Taylor and Low Rank

Can Taylor help us establish low rank of an interaction?

Taylor on Potentials (I)

Compute a Taylor expansion of a 2D Laplace point potential.

Taylor on Potentials (Ia)

Why is it interesting to consider Taylor expansions of Laplace point potentials?

Taylor on Potentials (II)

```
Maxima 5.42.1 http://maxima.sourceforge.net
(%i1) phi0: log(sqrt(y1**2 + y2**2));
                                        2     2
                                  log(y2  + y1 )
(%o1)                             --------------
                                        2
(%i2) diff(phi0, y1);
                                        y1
(%o2)                                ---------
                                       2     2
                                     y2  + y1
(%i3) diff(phi0, y1, 5);
                                           3              5
                   120 y1        480 y1         384 y1
(%o3)           ------------ - ------------ + ------------
                   2     2 3      2     2 4      2     2 5
                (y2  + y1 )    (y2  + y1 )    (y2  + y1 )
(%i4)
```

Taylor on Potentials (III)

Which of these is the most dangerous (largest) term?

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

'Generalize' this bound:

Taylor on Potentials (IV)

What does this mean for the convergence of the Taylor series as a whole?

Taylor on Potentials (V)

Lesson?

Taylor on Potentials (VI)

Generalize this to multiple source points:

Local expansions as a Computational Tool

Low rank makes evaluating interactions cheap(er). Do local expansions help with that goal?

Outline

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?

Multipole Expansions (II)

The abstract idea of a *multipole expansion* is that:

Multipole Expansions (III)

If our particle distribution is like in the figure: is a multipole expansion is a computationally useful thing?
Set

- $S = \#$sources,
- $T = \#$targets,
- $K = \#$terms in expansion.

Demo: Multipole/local expansions

Outline

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 ε?

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':

$$H_0^{(1)}(\kappa \|x - y\|_2) =$$

$$\sum_{\ell=-\infty}^{\infty} \underbrace{H_\ell^{(1)}(\kappa \|y - c\|_2)\, e^{i\ell\theta'}}_{\text{singular}} \underbrace{J_\ell(\kappa \|x - c\|_2)\, e^{-i\ell\theta}}_{\text{nonsingular}}$$

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

Can apply same family of tricks as with Taylor to derive multipole/local expansions.

Outline

Making Multipole/Local Expansions using Linear Algebra

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?

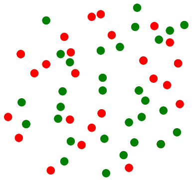
Where are we now? (I)

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
$$\psi(\boldsymbol{x}) = \sum_j G(\boldsymbol{x}, \boldsymbol{y}_j)\varphi(\boldsymbol{y}_j)$$
satisfies a PDE (e.g. Laplace), i.e. if $G(\boldsymbol{x}, \boldsymbol{y}_j)$ 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.
($\Leftrightarrow$ 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.)

Outline

Outline

Preliminaries: Convolution

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

- Convolution with shifted δ is the same as shifting the function;

$$[f * (\xi \mapsto \delta(\xi - a))](x) = f(x - a)$$

- 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: $\mathcal{F}\{f * g\} = \mathcal{F}f \cdot \mathcal{F}g$,
- A single δ turns into: $\mathcal{F}\{\delta(x-a)\}(\omega) = e^{-ia\omega}$
- And a "train" of δs turns into (see e.g. [Décoret '04]):

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

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

Simple and Periodic: Ewald Summation

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

$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{m}\in\mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(\boldsymbol{x}, \boldsymbol{y}_j + \boldsymbol{m})\varphi(\boldsymbol{y}_j)$$

Lattice Sums: Convergence

Q: When does this have a right to converge?

Ewald Summation: Dealing with Smoothness

$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{i} \in \mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(\boldsymbol{x}, \boldsymbol{y}_j + \boldsymbol{i}) \varphi(\boldsymbol{y}_j)$$

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}.

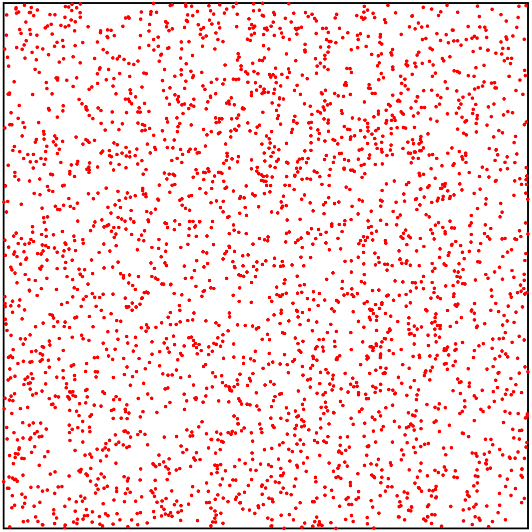
Ewald Summation: Remarks

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')

Outline

Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

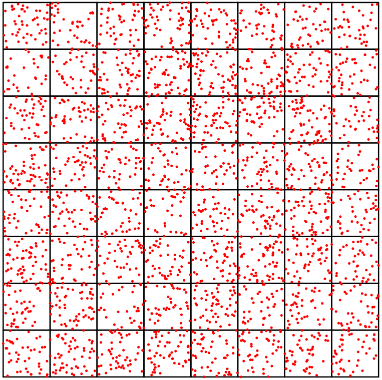
Barnes-Hut: The Task At Hand

Want: All-pairs interaction.

Caution:

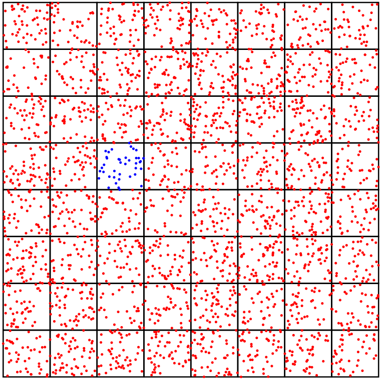
- In these figures: targets sources
- Here: targets and sources

Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

Barnes-Hut: Putting Multipole Expansions to Work



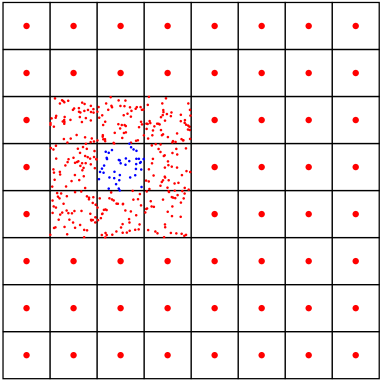
(Figure following G. Martinsson)

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



(Figure following G. Martinsson)

Barnes-Hut: Accuracy

With this computational outline, what's the accuracy?

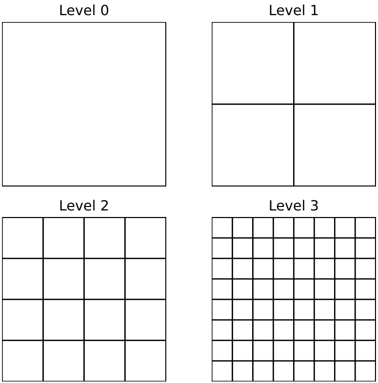
Q: Does this get better or worse as dimension increases?

Barnes-Hut (Single-Level): Computational Cost

What's the cost of this algorithm?

Barnes-Hut Single Level Cost: Observations

Box Splitting

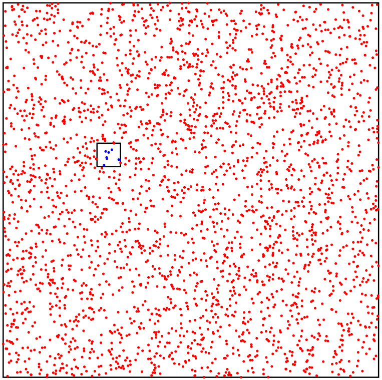


(Figure following G. Martinsson)

Level Count

How many levels?

Box Sizes

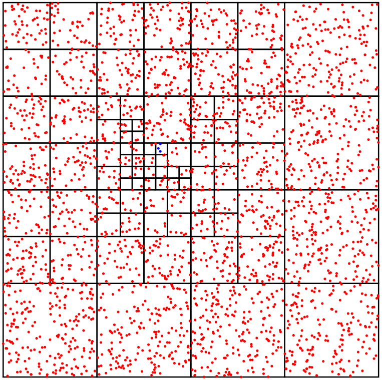


(Figure following G. Martinsson)

Want to evaluate all the source interactions with the targets in the box.

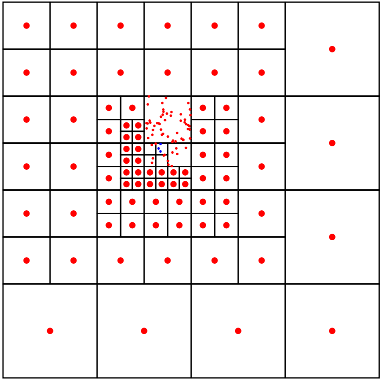
Q: What would be good sizes for source boxes? What's the requirement?

Multipole Sources



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)

Barnes-Hut: Box Properties



What properties do these boxes have?

Simple observation: The further, the bigger.

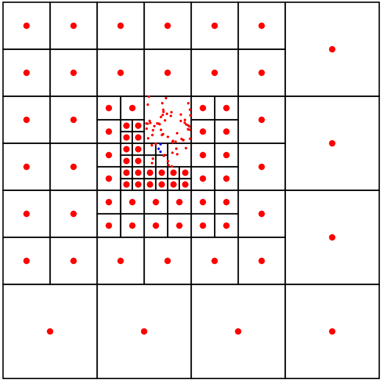
Barnes-Hut: Box Properties

Barnes-Hut: Well-separated-ness

Which boxes in the tree should be allowed to contribute via multipole?

Barnes-Hut: Revised Cost Estimate

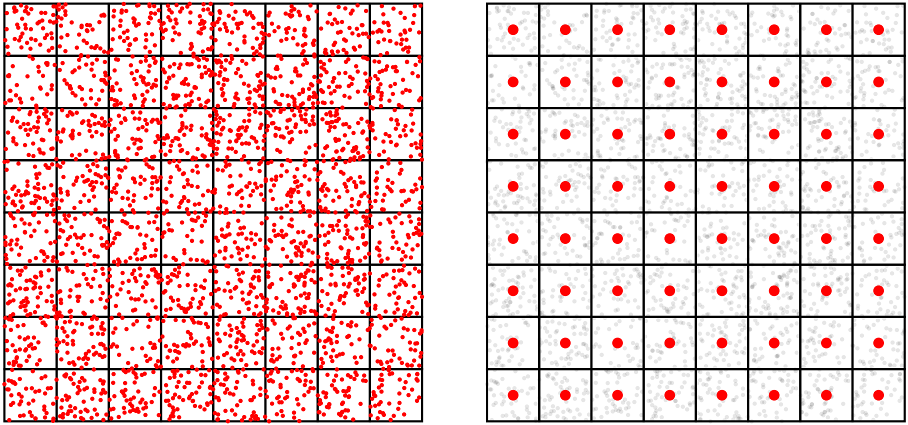
Which of these boxes are well-separated from the target?



What is the cost of evaluating the target potentials, assuming that we know the multipole expansions already?

Barnes-Hut: Revised Cost Estimate

Barnes-Hut: Next Revised Cost Estimate



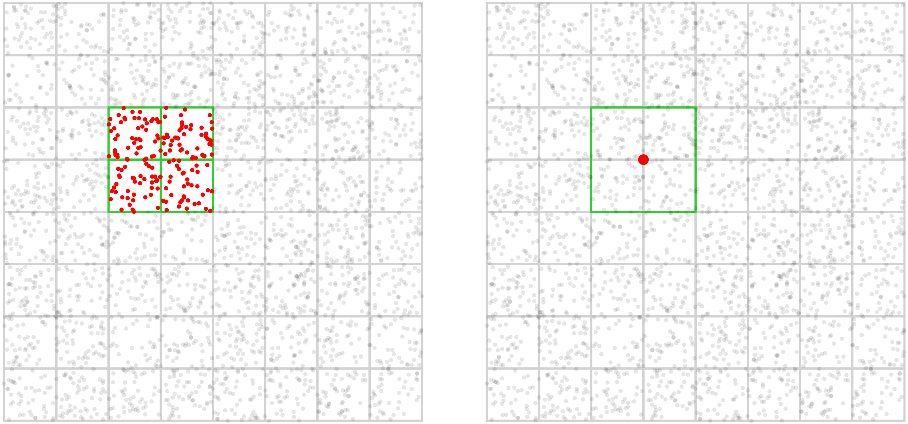
(Figure following G. Martinsson)

Summarize the algorithm (so far) and the associated cost.

Barnes-Hut: Next Revised Cost Estimate

Summarize the algorithm (so far) and the associated cost.

Barnes-Hut: Putting Multipole Expansions to Work



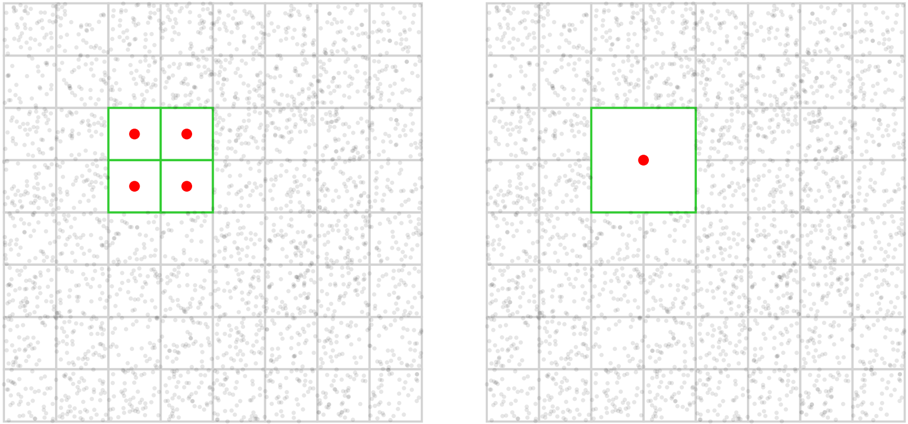
(Figure following G. Martinsson)

How could this process be sped up?

Barnes-Hut: Clumps of Boxes?

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. . .

Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

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

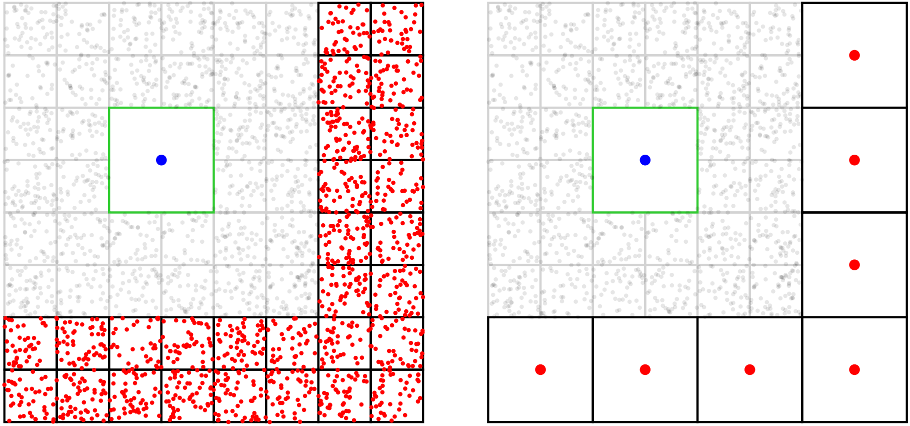
Cost of Multi-Level Barnes-Hut: Observations

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.

Outline

Using Multipole-to-Local



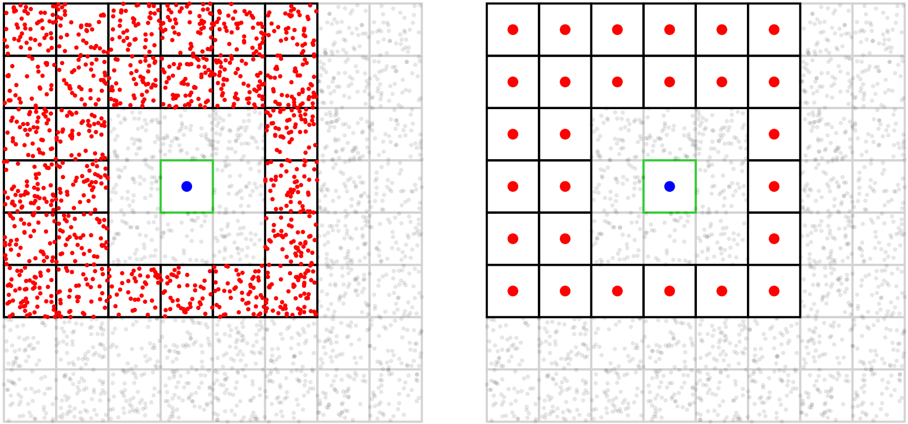
(Figure following G. Martinsson)

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



(Figure following G. Martinsson)

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

Provide an upper bound on the number of elements of I_b.

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 ℓ by mp $\to$ mp

Downward pass

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

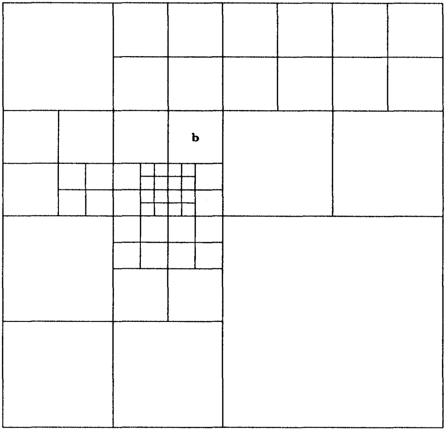


Figure credit: Carrier et al. ('88)

Recall target convergence factor of $\sqrt{2}/3$!

Adaptivity: Solution

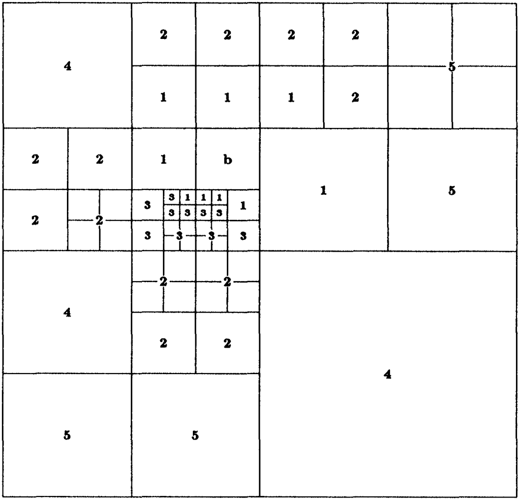


Figure credit: Carrier et al. ('88)

Adaptivity: what changes?

FMM: List of Interaction Lists

Make a list of cases:

Outline

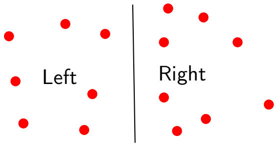
What about solving?

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?

Proxy Recap

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
- Π_i shared for entire column

Block-Separable Matrix: Questions

Q: Why is it called that?

Q: How expensive is a matvec?

Q: How about a solve?

BSS Solve (I)

Separate out 'coarse' unknowns. Use the following notation:

$$B = \begin{bmatrix} 0 & P_1\tilde{A}_{12} & P_1\tilde{A}_{13} & P_1\tilde{A}_{14} \\ P_2\tilde{A}_{21} & 0 & P_2\tilde{A}_{23} & P_2\tilde{A}_{24} \\ P_3\tilde{A}_{31} & P_3\tilde{A}_{32} & 0 & P_3\tilde{A}_{34} \\ P_4\tilde{A}_{41} & P_4\tilde{A}_{42} & P_4\tilde{A}_{43} & 0 \end{bmatrix}$$

and

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

BSS Solve (II)

Q: What are the matrix sizes? The vector lengths of $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$?

Now work towards doing *just* a 'coarse' solve on $\tilde{\boldsymbol{x}}$, using the Schur complement:

BSS Solve (III)

Focus in on the second row:

$$(\mathrm{Id} + \Pi D^{-1} B)\widetilde{\boldsymbol{x}} = \Pi D^{-1} \boldsymbol{b}$$

Every non-zero (i.e. off-diagonal) entry in $\Pi D^{-1} B$ looks like

Define a diagonal entry:

BSS Solve (IV)

Next, left-multiply $(\mathrm{Id} + \Pi D^{-1} B)$ by block-diag$_i(\tilde{A}_{ii})$:

BSS Solve: Summary

What have we achieved?

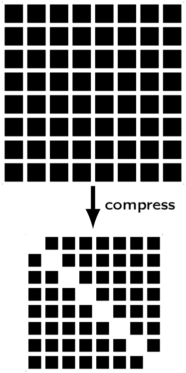
- Instead of solving a linear system of size

$$(N_{L0\,\text{boxes}} \cdot m) \times (N_{L0\,\text{boxes}} \cdot m)$$

  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 following G. Martinsson, drawn by A. Fikl)

Hierarchically Block-Separable

To get to $O(N)$, realize we can *recursively*

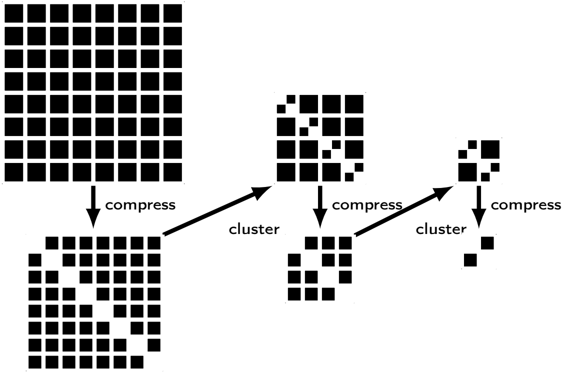
- group skeletons
- eliminate more variables.

Where does this process start?

Demo: Skeletonization using Proxies (Hierarchical)

Hierarchically Block-Separable

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



(Figure following G. Martinsson, drawn by A. Fikl)

Hierarchically Block-Separable

- Using this hierarchical grouping gives us *Hierarchically Block-Separable* (*HBS*) matrices.
- If you have heard the word $\mathcal{H}$*-matrix* and $\mathcal{H}^2$*-matrix*, the ideas are very similar. Differences:
  - $\mathcal{H}$-family matrices don't typically use the ID (instead often use *Adaptive Cross Approximation* or *ACA*)
  - $\mathcal{H}^2$ does target clustering (like FMM), $\mathcal{H}$ does not (like Barnes-Hut)

Outline

Recap: Fast Fourier Transform

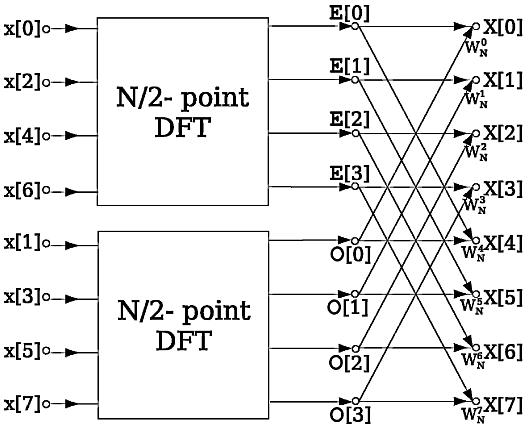
The *Discrete Fourier Transform (DFT)* is given by:

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

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

$$X_k = \underbrace{\sum_{m=0}^{N/2-1} x_{2m} e^{-\frac{2\pi i}{N/2} mk}}_{\text{DFT of even}-\text{indexed part of } x_n} + e^{-\frac{2\pi i}{N} k} \underbrace{\sum_{m=0}^{N/2-1} x_{2m+1} e^{-\frac{2\pi i}{N/2} mk}}_{\text{DFT of odd}-\text{indexed part of } x_n} .$$

FFT: Data Flow



(Figure credit: Wikipedia)
Perhaps a little bit like a butterfly?

Fourier Transforms: A Different View

Claim:

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

(i.e. rank is proportional to 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?

Cost

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

Comments?

Outline

PDEs: Simple Ones First, More Complicated Ones Later

Laplace

$\triangle u = 0$

Applications:

- Steady-state $\partial_t u = 0$ of wave propagation, heat conduction
- Electric potential u for applied voltage
- Minimal surfaces/"soap films"
- ∇u as velocity of incompressible/potential 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:

$$\partial_t^2 \tilde{u} = \triangle \tilde{u}$$

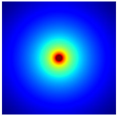
Applications:

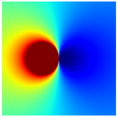
- Propagation of sound
- Electromagnetic waves

Fundamental Solutions

Laplace

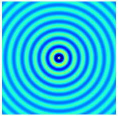
$-\triangle u = \delta$

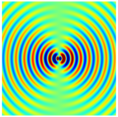


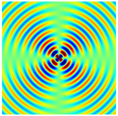


Helmholtz

$\triangle u + k^2 u = \delta$







aka. *Free space Green's Functions*

How do you assign a precise meaning to the statement with the δ-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

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

$$\frac{\partial}{\partial_x} G(x)$$

Helmholtz

$$G(x) = \begin{cases} \frac{i}{4} H_0^1(k|x|) & \text{2D} \\ \frac{1}{4\pi}\frac{e^{ik|x|}}{|x|} & \text{3D} \end{cases}$$

$$\frac{\partial}{\partial_x} G(x)$$

Layer Potentials (I)

Let G_k be the Helmholtz kernel ($k = 0 \to$ Laplace).

These operators map function σ on Γ to...

Layer Potentials (II)

Called *layer potentials*:

- S is called the *single-layer potential*
- D is called the *double-layer potential*
- S'' (and higher) analogously

(Show pictures using `pytential/examples/layerpot.py`, observe continuity properties.)

Alternate ("standard") nomenclature:

How does this actually solve a PDE?

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

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

IE BVP Solve: Observations (I)

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?

IE BVP Solve: Observations (II)

- 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?

$\rightarrow$ Need some theory

Outline

Outline

Norms

Definition

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

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

Can create norm from *inner product*: $\|x\| = \sqrt{\langle x, x\rangle}$

Function Spaces

Name some function spaces with their norms.

Convergence

Name some ways in which a sequence can 'converge'.

Operators

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

Definition (Operator norm)

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

Theorem

$\|A\|$ bounded $\Leftrightarrow$ A continuous

- 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

Volterra	Fredholm
$\int_a^x k(x,y)f(y)dy = g(x)$	$\int_G k(x,y)f(y)dy = g(x)$

First kind	Second Kind
$\int_G k(x,y)f(y)dy = g(x)$	$f(x) + \int_G k(x,y)f(y)dy = g(x)$

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?

Connections to Complex Variables

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:

$$f^{(n)}(a) = \frac{n!}{2\pi i} \oint_{\gamma} \frac{1}{(z-a)^{n+1}} f(z)\, dz$$

Integral Operators: Boundedness (=Continuity)

Theorem (Continuous kernel $\Rightarrow$ 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 '$\leqslant$'.

Solving Integral Equations

Given

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

are we allowed to ask for a solution of

$$(\mathrm{Id} - A)\varphi = g?$$

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?

Attempt 1: The Neumann series (II)

Theorem

$A : X \to X$ Banach, $\|A\| < 1$ $(I - A)^{-1} = \sum_{k=0}^{\infty} A^k$ with $\|(I - A)^{-1}\| \le 1/(1 - \|A\|)$.

- 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?

Outline

Compact Sets

Definition (Precompact/Relatively compact/Sequentially compact)

$M \subseteq X$ precompact:$\Leftrightarrow$ all sequences $(x_k) \subset M$ contain a subsequence converging in X

Definition (Compact/'Sequentially complete')

$M \subseteq X$ compact:$\Leftrightarrow$ all sequences $(x_k) \subset M$ contain a subsequence converging in M

- Precompact $\Rightarrow$ bounded
- Precompact $\Leftrightarrow$ bounded (finite dim. only!)
- Question: Is a set consisting of two elements precompact?

Theorem (Finite subcover)

$M \subseteq X$ compact $\Leftrightarrow$ For all covers C with $M = \bigcup_{S \in C} S$ consisting of open sets $S \subseteq X$, there exists a finite subcover $F \subseteq C$ so that $M = \bigcup_{S \in F} S$.

Compact Sets (II)

Counterexample to 'precompact $\Leftrightarrow$ bounded'? (∞ dim)

Compact Operators

X, Y: Banach spaces

Definition (Compact operator)

$T : X \to Y$ is *compact* $:\Leftrightarrow$ T(bounded set) 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?

Arzelà-Ascoli

Let $G \subset \mathbb{R}^n$ be compact.

Theorem (Arzelà-Ascoli [Kress LIE 3rd ed. Thm. 1.18])

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

Equicontinuous means

Continuous means:

Arzelà-Ascoli: Proof Sketch for b $\wedge$ e $\Rightarrow$ precompact

Arzelà-Ascoli (II)

Intuition?

“Uniformly continuous”?

When does *uniform continuity* happen?

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

Outline

Integral Operators are Compact

Theorem (Continuous kernel $\Rightarrow$ compact [Kress LIE 3rd ed. Thm. 2.28])

$G \subset \mathbb{R}^m$ 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?

Integral Operators are Compact (II)

Show that $A(U)$ is 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

$$|K(x,y)| \leq C|x-y|^{\alpha-n} \qquad (x \neq y)$$

Theorem (Weakly singular kernel $\Rightarrow$ compact [Kress LIE 3rd ed. Thm. 2.29])

K weakly singular. Then

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

is compact on $C(G)$, where $\mathrm{cl}(G^\circ) = G$.

Weakly singular: Proof Outline

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

$$|K(x,y)| \le C|x-y|^{\alpha-n+1} \qquad (x, y \in \partial\Omega,\ x \ne y)$$

Theorem (Weakly singular kernel $\Rightarrow$ compact [Kress LIE 3rd ed. Thm. 2.30])

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?

Outline

Riesz Theory (I)

Still trying to solve

$$L\phi := (I - A)\phi = \phi - A\phi = f$$

with A compact.

Theorem (First Riesz Theorem [Kress LIE 3rd ed., Thm. 3.1])

$N(L)$ is finite-dimensional.

Questions:

- What is $N(L)$ again?
- Why is this good news?

Riesz First Theorem: Proof Outline

Show it.

Riesz Theory (II)

Theorem (Riesz theory [Kress LIE 3rd ed., Thm. 3.4]**)**

A compact. Then:

- *$(I - A)$ injective $\Leftrightarrow$ $(I - A)$ 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.

(Quite a bit more to the proof: Riesz' second, third theorems, Riesz numbers, . . .)

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

$$(A\phi, \psi) = (\phi, B\psi) \qquad (\phi \in U, \psi \in Y).$$

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

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

Adjoint Operators

Definition (Adjoint oeprator)

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 3rd ed. Thm. 4.17])

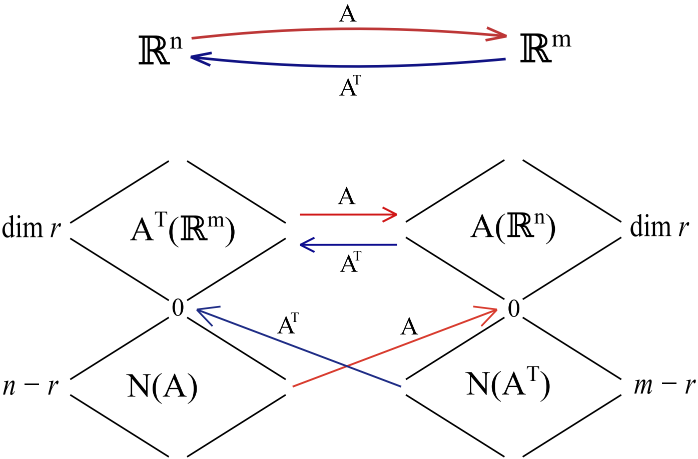
$A : X \to X$ compact. Then either:

- *$I - A$ 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



[Credit: Wikipedia]

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?

Outline

Spectral Theory: Terminology

$A : X \to X$ 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 ∞-dim here?

Resolvent Set and Spectrum

Definition (Resolvent set)

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

Definition (Spectrum)

$\sigma(A) := \mathbb{C} \setminus \rho(A)$

Spectral Theory of Compact Operators

Theorem

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

- $0 \in \sigma(A)$
- $\sigma(A) \setminus \{0\}$ *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!

Outline

Outline

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)

$\triangle u = 0$

Where are layer potentials harmonic?

On the double layer again

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

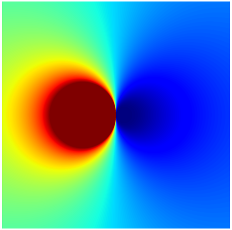
Definition (Weakly singular kernel)

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

$$|K(x,y)| \le C|x-y|^{\alpha-n+1} \qquad (x, y \in \partial\Omega,\ x \neq y)$$

Actual Singularity in the Double Layer (2D)

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



- Singularity with approach on $y = 0$?
- Singularity with approach on $x = 0$?

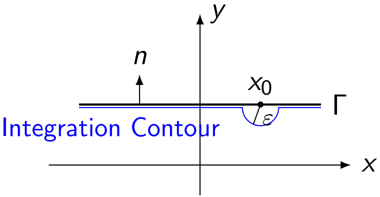
Cauchy Principal Value

But I don't want to integrate across a singularity! $\rightarrow$ 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



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.

Outline

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)

Ω bounded

Theorem (Green's Formula [Kress LIE 2nd 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 Ω 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 $\Delta u = 0,\ u(x) = \overline{\int}_{B(x,r)} u(y)dy = \overline{\int}_{\partial B(x,r)} u(y)dy$

Define $\overline{\int}$?

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. . .

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])

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

for some constant u_∞. *Only for* $n = 2$,

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

Realize the power of this statement:

Green's Formula at Infinity: Proof (1/4)

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 $x \geq R_0$.

Green's Formula at Infinity: Proof (2/4)

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 figure out 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?

Green's Formula at Infinity: Proof (4/4)

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_∞.

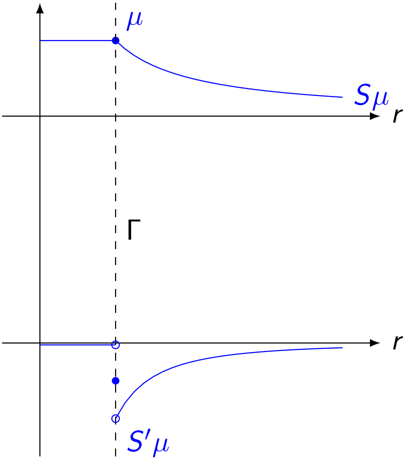
Green's Formula at Infinity: Impact

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?

Outline

Jump relations:



Jump Relations: Mathematical Statement

Let $[X] = X_+ - X_-$. (Normal points towards "+"="exterior".) Let $x_0 \in \Gamma$.

Theorem (Jump Relations [Kress LIE 3rd ed. Thm. 6.15, 6.18,6.19]**)**

$$[S\sigma] = 0$$

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

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

$$[D'\sigma] = 0$$

Truth in advertising: Assumptions on Γ?

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.

Outline

Outline

Boundary Value Problems: Overview

	Dirichlet	**Neumann**
Int.	$\lim_{x\to\partial\Omega-} u(x) = g$ ⊕ unique	$\lim_{x\to\partial\Omega-} \hat{n}\cdot\nabla u(x) = g$ Ⓞ may differ by constant
Ext.	$\lim_{x\to\partial\Omega+} u(x) = g$ $u(x) = \begin{cases} O(1) & 2D \\ o(1) & 3D \end{cases}$ as $\lvert x\rvert \to \infty$ ⊕ unique	$\lim_{x\to\partial\Omega+} \hat{n}\cdot\nabla u(x) = g$ $u(x) = o(1)$ as $\lvert x\rvert \to \infty$ ⊕ unique

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 Ω?

What's a DtN map?

Finding IE representations

Find integral representations that lead to second-kind IEs for each of the BVPs:

	Dirichlet	**Neumann**
Int.		
Ext.		

Uniqueness of Integral Equation Solutions

Theorem (Nullspaces [Kress LIE 3rd ed. Thm 6.21])

- $N(I/2 - D) = N(I/2 - S') = \{0\}$
- $N(I/2 + D) = \mathrm{span}\{1\}$, $N(I/2 + S') = \mathrm{span}\{\psi\}$, *where* $\int \psi \neq 0$.

Disclaimer: $\int \psi \neq 0$ not shown here, takes a little extra work.

IE Uniqueness: Proofs (1/3)

Show $N(I/2 - D) = \{0\}$.

IE Uniqueness: Proofs (2/3)

Show $N(I/2 - S') = \{0\}$.

IE Uniqueness: Proofs (3/3)

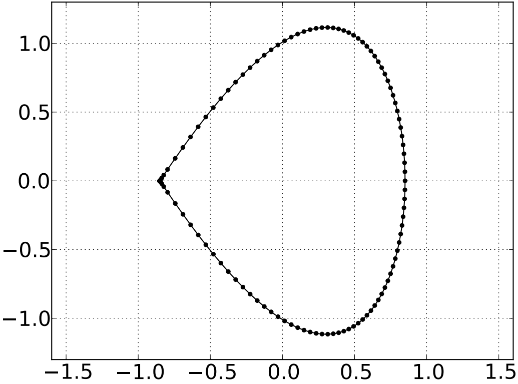
Show $N(I/2 + D) = \text{span}\{1\}$.

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

Patching up Exterior Dirichlet

Problem: $N(I/2 + S') = \{\psi\} \ldots$ do not know ψ. Assume $0 \in \Omega$.

Domains with Corners



What's the problem?

Domains with Corners (II)

At corner x_0: (2D)

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

Name some problems.

Workarounds?

Numerically: Needs consideration, can drive up cost through refinement.

Outline

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

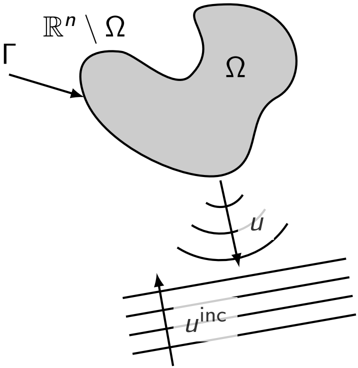
Helmholtz Equation

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

Yukawa Equation

- $-\triangle u + k^2 u(x) = 0$
- 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: $v = (1/\rho_0)\nabla U$
- Pressure: $p = -\partial_t U = i\omega u e^{-i\omega t}$
  - Equation of state: $p = f(\rho)$

What's ρ_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
  - $u = f \to$ Dirichlet
- Sound-hard: Scatterer "does not give"
  - Pressure varies, same on both sides of interface
  - $\hat{n} \cdot \nabla u = 0 \to$ Neumann
- Impedance: Some pressure translates into motion
  - Scatterer "resists"
  - $\hat{n} \cdot \nabla u + ik\lambda u = 0 \to$ Robin ($\lambda > 0$)
- Sommerfeld radiation condition: allow only outgoing waves (n-dim)

$$r^{\frac{n-1}{2}} \left(\frac{\partial}{\partial r} - ik \right) u(x) \to 0 \qquad (r \to \infty)$$

Many interesting BCs $\to$ many IEs! :)

Unchanged from Laplace

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

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

$$(S(\hat{n} \cdot \nabla u) - Du)(x) = \begin{cases} u(x) & x \in D \\ \frac{u(x)}{2} & x \in \partial D \\ 0 & x \notin D \end{cases}$$

$$[Su] = 0$$

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

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

$$[D'u] = 0$$

Unchanged from Laplace

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

Why does Green's formula survive?

Resonances

$-\triangle$ 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 $\triangle u + k^2 = 0$ such that

	Dirichlet	**Neumann**
Int.	$\lim_{x \to \partial D-} u(x) = g$ unique ($-$resonances)	$\lim_{x \to \partial D-} \hat{n} \cdot \nabla u(x) = g$ unique ($-$resonances)
Ext.	$\lim_{x \to \partial D+} u(x) = g$ Sommerfeld unique	$\lim_{x \to \partial D+} \hat{n} \cdot \nabla u(x) = g$ Sommerfeld unique

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

Find layer potential representations for each.

Patching up spurious resonances inherited from adjoint

Issue: Exterior IE inherits non-uniqueness from 'adjoint' interior BVP.

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:

Outline

D' is Self-Adjoint

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

Towards Calderón

Show that $(S\varphi, D'\psi) = ((S' + I/2)\varphi, (D - I/2)\psi)$. [Kress LIE 3rd ed. Sec 7.6]

$(\varphi, SD'\psi)$?

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?

Outline

Outline

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*) $\leftrightarrow$ 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 $|u_h - u| \leq Ch^p$

Thought experiment:

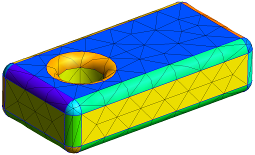
First order	Fifth order
1,000 DoFs $\approx$ 1,000 triangles	1,000 DoFs $\approx$ 66 triangles
Error: 0.1	Error: 0.1
Error: 0.01 $\to$?	Error: 0.01 $\to$?

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

Fixed-order	Spectral
Number of DoFs n	Number of DoFs n
$\sim$	$\sim$
Number of 'elements'	Number of modes resolved
$$\text{Error} \sim \frac{1}{n^p}$$	$$\text{Error} \sim \frac{1}{C^n}$$
Examples?	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

$$\begin{bmatrix} \phi_0(x_0) & \phi_1(x_0) & \cdots & \phi_n(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_n(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_n) & \phi_1(x_n) & \cdots & \phi_n(x_n) \end{bmatrix} \text{MODAL COEFFS} = \text{NODAL COEFFS}$$

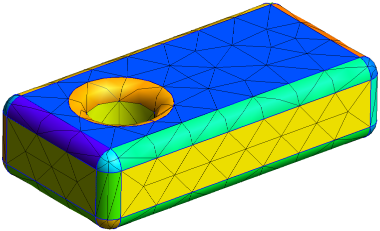
- Node placement? **Demo:** Interpolation node placement
- Vandermonde conditioning? **Demo:** Vandermonde conditioning
- What about multiple dimensions?
  - **Demo:** Visualizing the 2D PKDO Basis
  - **Demo:** 2D Interpolation Nodes

Common Operations

(Generalized) Vandermonde matrices simplify common operations:

- Modal $\leftrightarrow$ 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

Outline

Integral Equation Discretizations: Overview

$$\phi(x) - \int_\Gamma K(x,y)\phi(y)dy = f(y)$$

Nyström	Projection
▶ Approximate integral by quadrature: $\int_\Gamma f(y)dy \to \sum_{k=1}^n \omega_k f(y_k)$ ▶ Evaluate quadrature'd IE at quadrature nodes, solve	▶ Consider residual: $R := \phi - A\phi - f$ ▶ Pick projection P_n onto finite-dimensional subspace $P_n\phi := \sum_{k=1}^n \langle \phi, v_k\rangle w_k \quad \to$ DOFs $\langle \phi, v_k\rangle$ ▶ Solve $P_n R = 0$

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?

Outline

Nyström Discretizations (1/4)

Nyström consists of two distinct steps:

1. Approximate integral by quadrature:

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

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

$$\varphi_j^{(n)} - \sum_{k=1}^{n} \omega_k K(x_j, y_k)\varphi_k^{(n)} = f(x_j) \tag{2}$$

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) $\Rightarrow$ (2) hold?

Does (2) $\Rightarrow$ (1) hold?

Nyström Discretizations (4/4)

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? [Kress LIE 3rd 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 3rd ed. Cor. 10.7])

$A_n : X \to X$ bounded linear operators,
functionwise convergent to $A : X \to X$
Then convergence is uniform on compact subsets $U \subset X$, i.e.

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

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)?

Collective Compactness: Questions (1/2)

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

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

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

$I + (I - A)^{-1} A = ?$

Anselone's Theorem: Proof (I)

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

How good of an inverse is it?

$$
\begin{aligned}
\mathrm{Id} &\approx^? B_n(I - A_n) \\
&= (I + (I - A)^{-1} A_n)(I - A_n) \\
&= [I + (I - A)^{-1} A_n] - [A_n + (I - A)^{-1} A_n A_n] \\
&= [I + (I - A)^{-1} A_n] - [(I - A)^{-1}(I - A) A_n + (I - A)^{-1} A_n A_n] \\
&= [I + (I - A)^{-1} A_n] - [(I - A)^{-1} I A_n - (I - A)^{-1} A A_n + (I - A)^{-1} A_n A_n] \\
&= I + (I - A)^{-1}\, \mathrm{AA}_n - (I - A)^{-1} A_n A_n \\
&= I + \underbrace{(I - A)^{-1}(A - A_n) A_n}_{-S_n} = I - S_n
\end{aligned}
$$

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)

Anselone: A Question

Nyström: *specific to* $I +$ *compact.* Why?

Nyström: Collective Compactness

We *assumed* collective compactness. Do we have that? Assume

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

Nyström: Collective Compactness

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

Outline

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 $\Leftrightarrow P|_U = \mathrm{Id} \Leftrightarrow P^2 = P$
- $\|P\| \geq 1$
- 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, $A : X \to Y$ 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

$$\|A_n^{-1}\| \leqslant \frac{\|A^{-1}\|}{1 - \|A^{-1}(A_n - A)\|}.$$

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

$$\|\varphi_n - \varphi\| \leqslant \frac{\|A^{-1}\|}{1 - \|A^{-1}(A_n - A)\|} \left[\|(A_n - A)\varphi\| + \|f_n - f\|\right].$$

Norm Convergence of Inverses: Proof

Prove the result:

Projection Methods for Second Kind

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

Error Estimate for Second Kind Projection

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

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

Assume $\|P_n A - A\| \to 0$ $(n \to \infty)$. *Then for sufficiently large* n,

$$\varphi_n - P_n A \varphi_n = P_n f$$

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

Error Estimate for Second Kind Projection: Proof

Prove the result:

Perturbations of Projection Methods for Second Kind

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

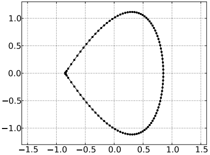
X Banach, $A : X \to X$ compact, $I - A$ injective

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

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

$$\|\tilde{\varphi}_n - \varphi\| \leqslant M\left(\|P_n\varphi - \varphi\| + \|(P_nA_n - P_nA)\varphi_n\| + \|P_n(f_n - f)\|\right).$$

Iterative Methods and Corners [Bremer et al. '11]



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:

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

So $\overline{\boldsymbol{\sigma}}_h \cdot \overline{\boldsymbol{\sigma}}_h = ?$
Also fixes system conditioning! Why?

Outline

Outline

'Off-the-shelf' ways to compute integrals

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

Why not Gaussian?

Singular and Near-Singular Quadrature

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

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

Give a typical application.

Drawbacks?

High-Order Corrected Trapezoidal Quadrature

- Conditions for new nodes, weights
  ($\to$ 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

$$\int\int_{\partial\Omega} K(\boldsymbol{x},\boldsymbol{y})\phi(y)ds_y$$

$$=$$

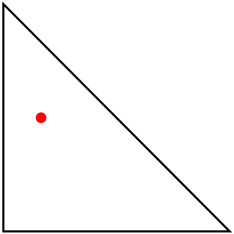
$$\int_0^R \int_{\boldsymbol{x}+\boldsymbol{r}\in\partial\Omega\cap\partial B(\mathrm{x},r)} K(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{r})\phi(\mathrm{x}+\mathrm{r})d\langle\text{angles}\rangle\, r\, dr$$

$$=$$

$$\int_0^R \int_{\boldsymbol{x}+\boldsymbol{r}\in\partial\Omega\cap\partial B(\mathrm{x},r)} \frac{K_{\text{less singular}}(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{r})}{r}\phi(\boldsymbol{x}+\boldsymbol{r})d\langle\text{angles}\rangle\, r\, dr$$

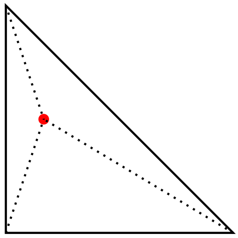
where $K_{\text{less singular}} = K \cdot r$.

Quadrature on Triangles



Problem: Singularity can sit *anywhere* in triangle
$\rightarrow$ need *lots* of quadrature rules (one per target)

Quadrature on Triangles



Problem: Singularity can sit *anywhere* in triangle
$\rightarrow$ need *lots* of quadrature rules (one per target)

Kernel regularization

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

$$\frac{\cdots}{\sqrt{(x-y)^2}} \quad \to \quad \frac{\cdots}{\sqrt{(x-y)^2+\epsilon^2}}$$

Use Richardson extrapolation to recover limit as $\epsilon \to 0$.

(May also use geometric motivation: limit along line towards singular point.)

Primary drawbacks:

- Low-order accurate
- Need to make ϵ smaller (i.e. kernel more singular) to get better accuracy

Can take many forms–for example:

- Convolve integrand to smooth it ($\to$ 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

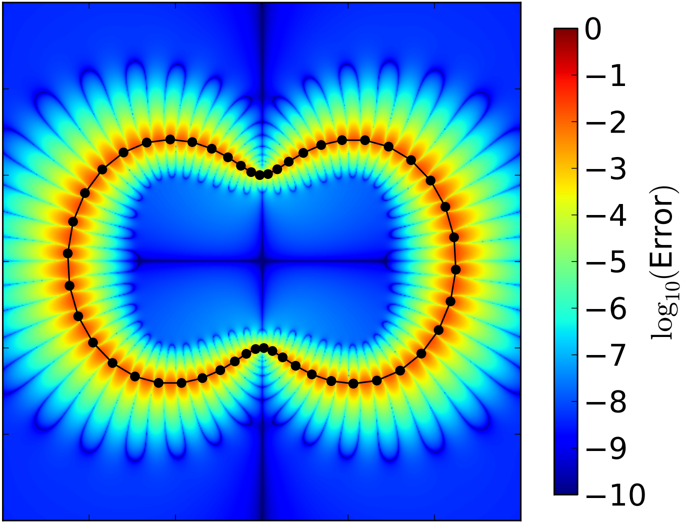
How does an FMM evaluate a double layer?

How does an FMM evaluate S'?

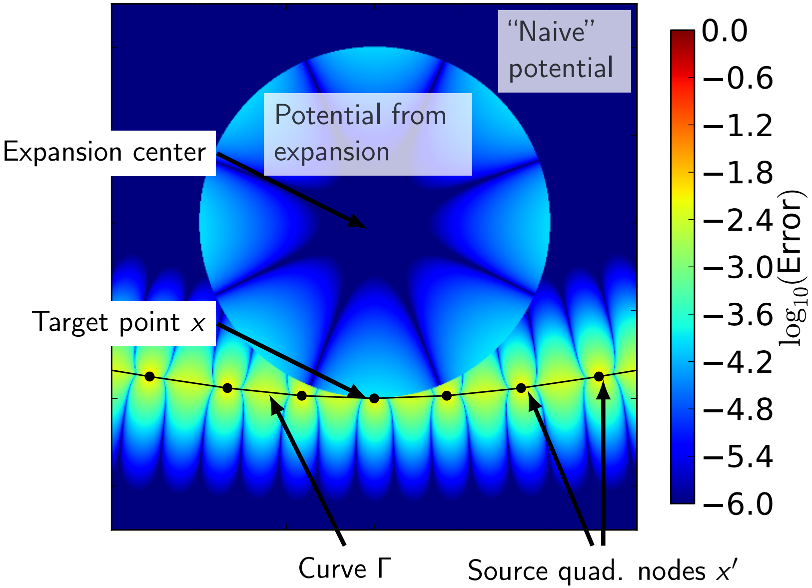
What effect does this have on accuracy?

Outline

Layer Potential Evaluation: Some Intuition

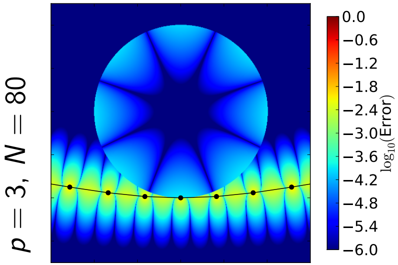


QBX: Idea

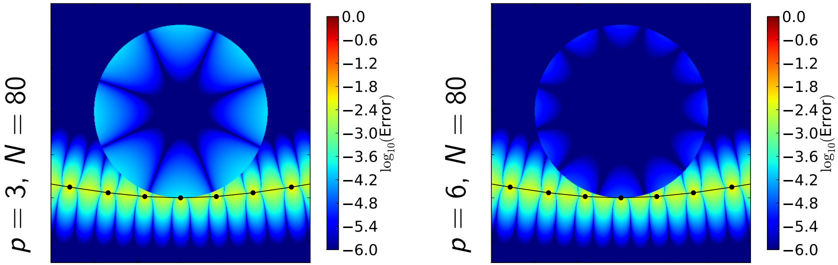


"Naive" potential
Potential from expansion
Expansion center
Target point x
Curve Γ
Source quad. nodes x'
0.0
−0.6
−1.2
−1.8
−2.4
−3.0
−3.6
−4.2
−4.8
−5.4
−6.0
$\log_{10}$(Error)

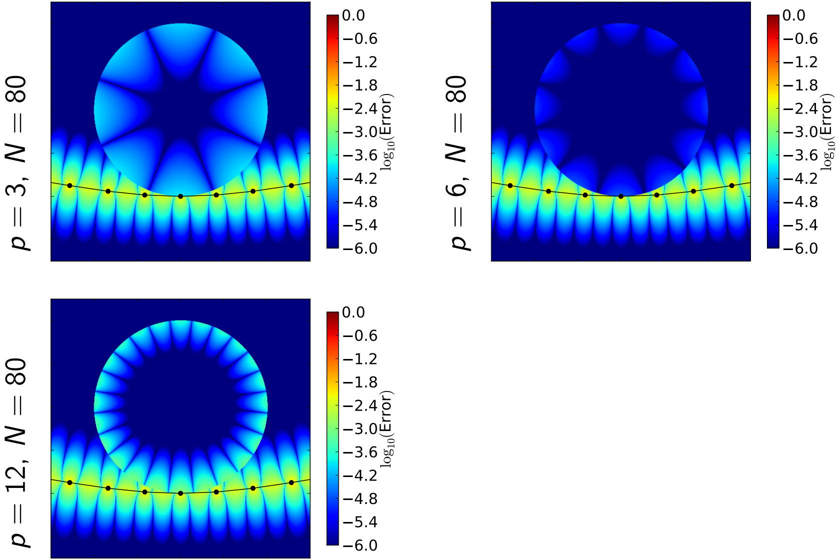
QBX: An Experiment



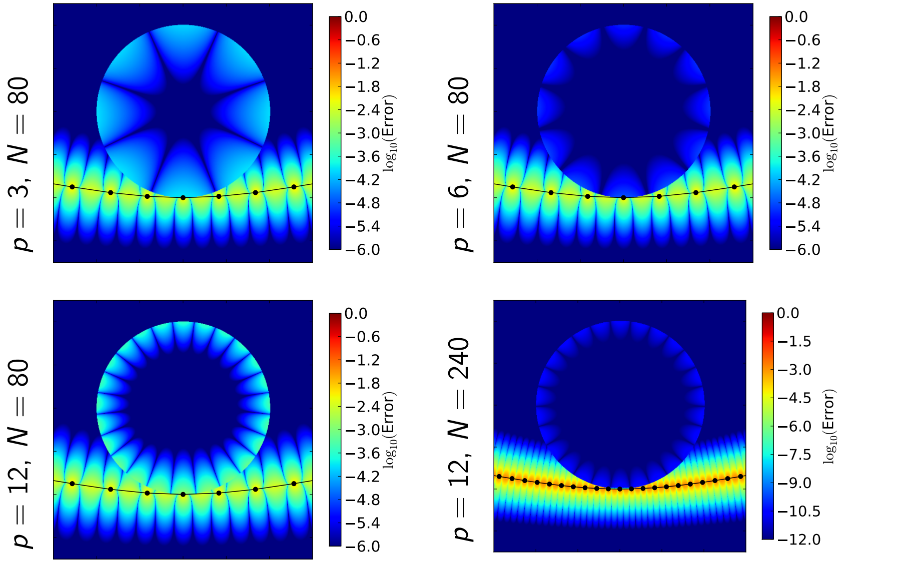
QBX: An Experiment



QBX: An Experiment

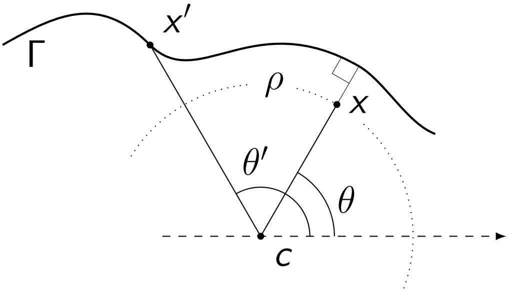


QBX: An Experiment



QBX: Notation, Basics

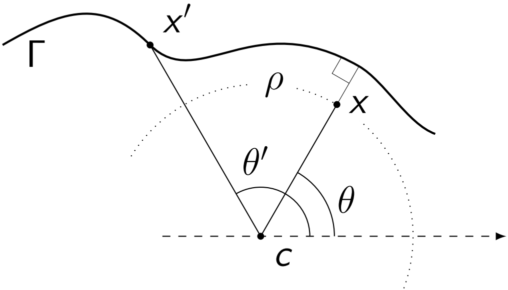
Graf's addition theorem



QBX: Notati

Graf's ad

Requires: $|x - c| < |x' - c|$ ("local expansion")



$$H_0^{(1)}(k|x - x'|) = \sum_{l=-\infty}^{\infty} H_l^{(1)}(k|x' - c|)e^{il\theta'} J_l(k|x - c|)e^{-il\theta}$$

QBX: Formulation, Discretization

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

$$\alpha_l = \frac{i}{4} \int_\Gamma H_l^{(1)}(k|x' - c|) e^{il\theta'} \sigma(x') \, \mathrm{d}x' \quad (l = -\infty, \dots, \infty)$$

$S\sigma$ is a smooth function *up to* Γ.

QBX: Formulation, Discretization

Compute layer potential on the disk as

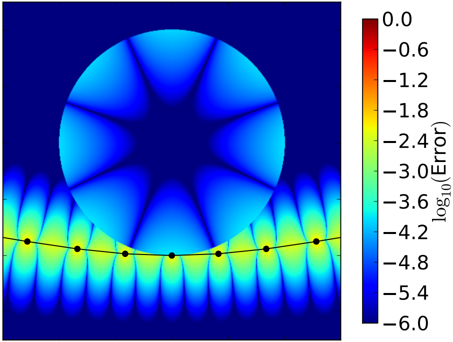
$$S_k\sigma(x) = \sum_{l=-p}^{p} \alpha_l J_l(k\rho) e^{-il\theta}$$

with

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

$S\sigma$ is a smooth function *up to* Γ.

Quadrature by Expansion (QBX)



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

[K, Barnett, Greengard, O'Neil JCP '13]

Achieving high order

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

Two approaches:

- *Asymptotically convergent*: $r = \sqrt{h}$
  - ⊕ Error $\to 0$ as $h \to 0$
  - ⊖ Low order: $h^{(p+1)/2}$
- *Convergent with controlled precision*: $r = 5h$
  - ⊖ Error $\not\to 0$ as $h \to 0$
  - ⊕ High order: h^{p+1} to controlled precision $\epsilon := (1/5)^q$

Other layer potentials

Can't just do single-layer potentials:

$$\alpha_l^D = \frac{i}{4}\int_\Gamma \frac{\partial}{\partial \hat{n}_{x'}} H_l^{(1)}(k|x'-c|)e^{il\theta'}\mu(x')\,\mathrm{d}x'.$$

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 Ψ be the exterior Riemann map that maps the exterior Ω^+ 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 φ 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 λ_k, μ_k, where $\theta(w) = \arg \Psi(w)$ is the boundary correspondence.

[Wala, K '18]

QBX and Conformal Mapping

Require: A smooth Jordan boundary Γ, with 0 in the interior.
Require: A boundary sign s: $+1$ for exterior, -1 for interior.
Ensure: Computes the boundary correspondence θ.

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

$$\begin{cases} \zeta = \left(\mathcal{D} - \frac{1}{2}\right)\sigma(\zeta) & \text{if } s = +1 \\ \overline{\zeta^{-1}} = \left(\mathcal{D} + \int + \frac{1}{2}\right)\sigma(\zeta) & \text{if } s = -1. \end{cases}$$

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

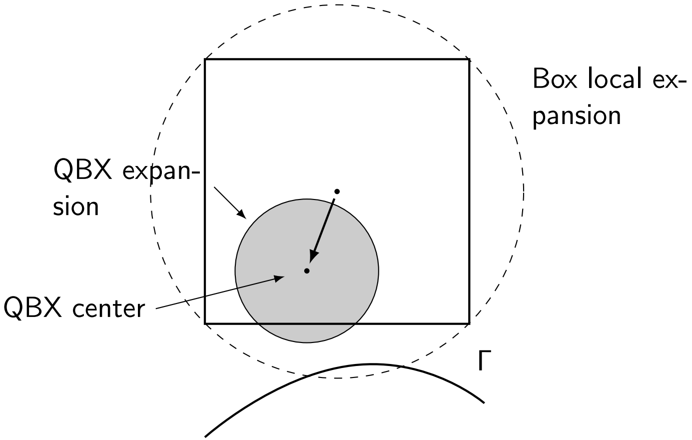
Stage 3
Let $\theta(\zeta) = \arg\left(-s\frac{\tilde{\sigma}(\zeta)}{|\tilde{\sigma}(\zeta)|}\right)$ $(\zeta \in \Gamma)$.

Outline

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

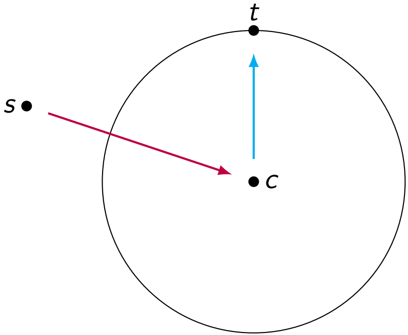


Accuracy vs FMM/QBX orders: Straightforward (2D)

$(1/2)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}}=3$	$p_{\text{QBX}}=5$	$p_{\text{QBX}}=7$	$p_{\text{QBX}}=9$
0	(direct)	4.35e−6	6.21e−7	1.05e−7	5.71e−8
6e−2	3	2.55e−2	2.96e−2	4.07e−2	5.77e−2
2e−2	5	6.94e−3	1.61e−2	2.29e−2	3.10e−2
5e−4	10	4.95e−4	1.75e−3	5.80e−3	9.48e−3
2e−5	15	1.58e−5	1.85e−4	6.40e−4	3.17e−3
5e−7	20	4.35e−6	1.31e−5	8.99e−5	5.01e−4

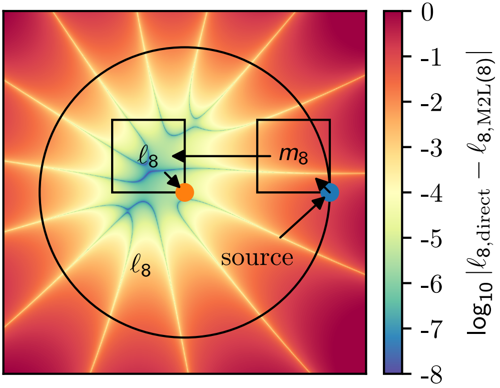
ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish γ_{65}, using the conventional QBX FMM algorithm. 3250 Gauss-Legendre panels, with 33 nodes per panel.

Recap: Local Expansions of Potentials



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

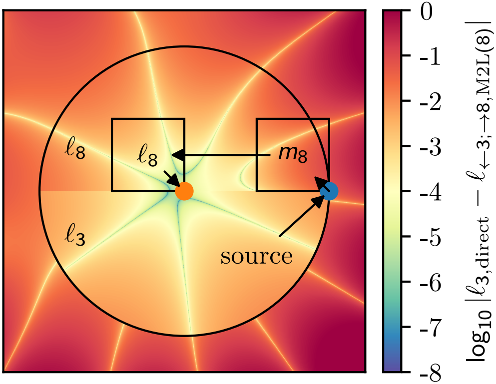
QBX + FMM: Sources of Inaccuracy



Possible Expansion Sequences

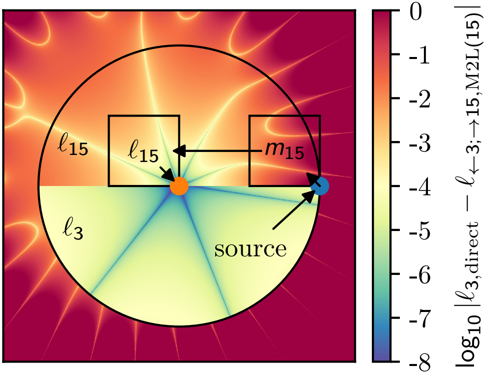
- Source $\to$ Multipole(p) $\to$ QBX-Local(q)
- Source $\to$ Local(p) $\to$ QBX-Local(q)
- Source $\to$ Multipole(p) $\to$ Local(p) $\to$ QBX-Local(q)

Translation chains for QBX



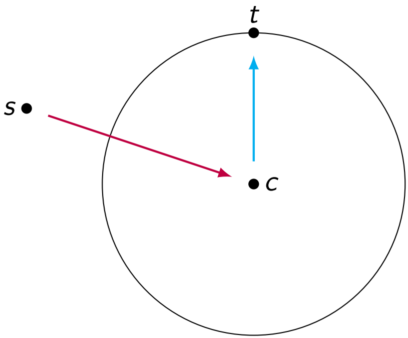
%

Translation chains for QBX



%

Expansions of Expansions?



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

This holds for point evaluations of a single expansion.

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

Example: Local(p) $\to$ 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 ϕ due to the charge is described by a power series $\phi(y) = \sum_{l=0}^{\infty} \beta_l (y - z)^l$. 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) $\to$ Local(q) Truncation Error (2D Lap.)

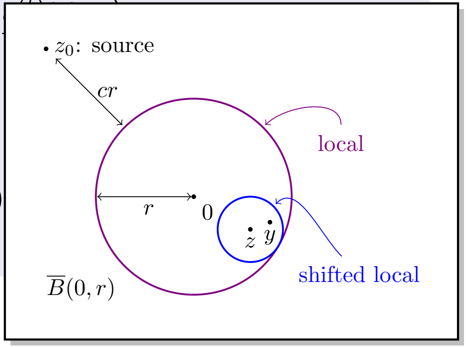
Lemma

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 ϕ due to the charge is described by a power series $\phi(y) = \sum_{l=0}^{\infty} \beta_l (y-z)^l$. Fix the intermediate local order $p \geq 0$. For $n \geq 0$, let

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

Fix the local expansion order $q \geq 0$. Define

$$\left| \sum_{k=0}^{q} \beta_k (y-z)^k - \sum_{k=0}^{q} \tilde{\beta}_k (y-z) \right.$$



[Wala, K '18a – arxiv:1801.04070]

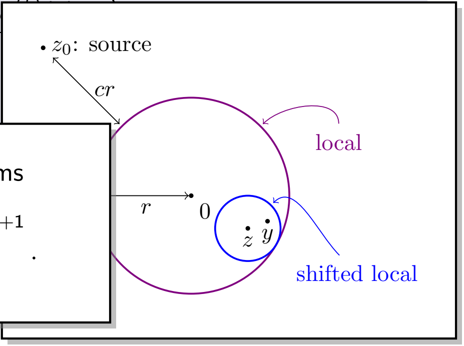
Example: Local(p) $\to$ Local(q) Truncation Error (2D Lap.)

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 ϕ due to the charge is described by a power series $\phi(y) = \sum_{l=0}^{\infty} \beta_l (y-z)^l$. Fix the intermediate local order $p \geq 0$. For $n \geq 0$, let

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

Fix the local expansion order $q \geq 0$. Define

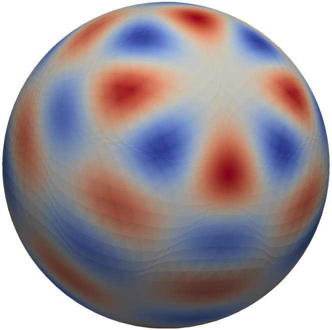


Slightly more subtle, but essentially confirms

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

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 $d = 2, 3$)
  $\mathbb{S}^{d-1} = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x}\| = 1\}$
- A polynomial $p : \mathbb{R}^d \to \mathbb{C}$ is *homogeneous* of degree k if p if p satisfies $p(r\boldsymbol{x}) = r^k p(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^d$.
- Space of spherical harmonics $\mathbb{Y}_n^d$: restrictions to the unit sphere $\mathbb{S}^{d-1}$ of the harmonic ($\triangle p = 0$), homogeneous polynomials of degree n.
- Fourier-Laplace series:

$$\mathcal{F}_p f(\boldsymbol{\xi}) = \sum_{n=0}^{p} \mathcal{P}_n f(\boldsymbol{\xi}), \quad \boldsymbol{\xi} \in \mathbb{S}^{d-1},$$

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

Convergence of Fourier-Laplace Series

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

$$\|\mathcal{F}_p f\|_\infty \leq \Lambda_{p,d} \|f\|_\infty ,$$

where, in dimensions $d = 2$ and $d = 3$,

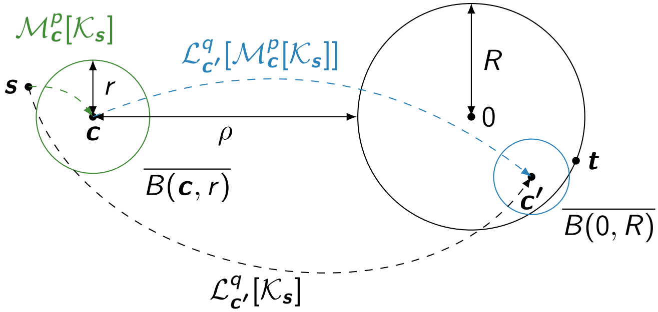
$$\Lambda_{p,2} = \frac{4}{\pi^2} \log p + O(1),$$

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

asymptotically as $p \to \infty$.

[Rivlin '69], [Gronwall 1911]

Expansions of Expansions: M2QBXL



Analyzing M2QBXL

Lemma (Source $\to$ Multipole(p) $\to$ Local(q))

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

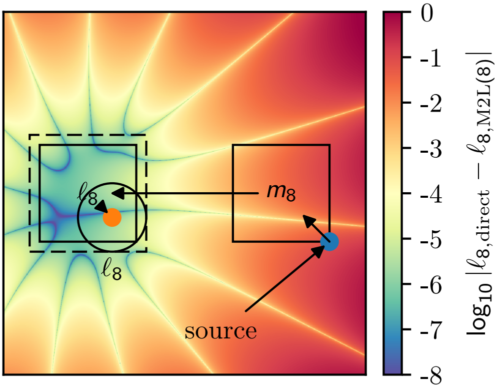
Then, in the situation of the previous slide:

$$\left|\mathcal{L}^q_{\boldsymbol{c'}}[\mathcal{K}_{\boldsymbol{s}}](\boldsymbol{t}) - \mathcal{L}^q_{\boldsymbol{c'}}[\mathcal{M}^p_{\boldsymbol{c}}[\mathcal{K}_{\boldsymbol{s}}]](\boldsymbol{t})\right| \leq \Lambda_{q,d} \left\| (\mathcal{K}_{\boldsymbol{s}} - \mathcal{M}^p_{\boldsymbol{c}}[\mathcal{K}_{\boldsymbol{s}}])|_{\overline{B(0,R)}} \right\|_\infty .$$

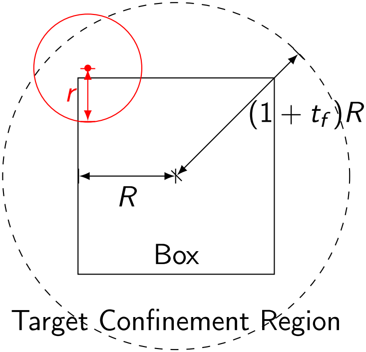
[Wala-K ‘19—in prep.]

Translation Chains for QBX

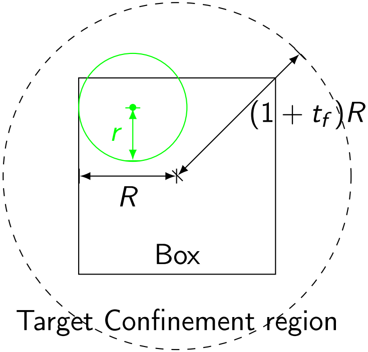
Rigorous truncation error bounds for local expansions for scenarios QBX locals *near* box locals:



Targets with Extent: Target Confinement Regions

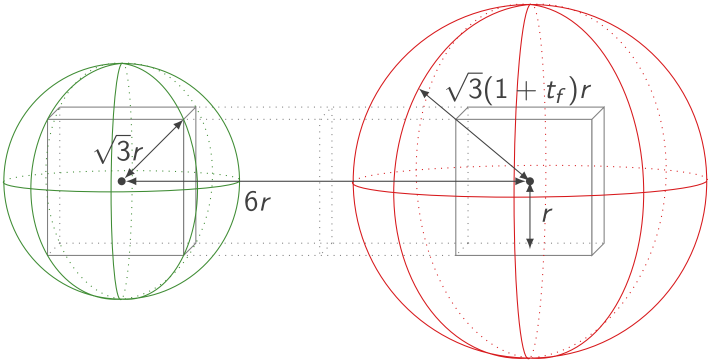


QBX center '*not in*' box



QBX center '*in*' box

M2L Convergence Factor with 2-Away, TCF (3D)



3D, $t_f = 0.9$: Conv. factor ≈ 0.77

GIGAQBX Fast Algorithm: End-to-End Accuracy (2D/3D)

Theorem (GIGAQBX FMM for Laplace (2D/3D))

Let the center $\boldsymbol{c}$ be owned by the box b and let $\boldsymbol{t}$ be a target associated with the center $\boldsymbol{c}$. 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:

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

[Wala-K '19—in prep.]

GIGAQBX Fast Algorithm: End-to-End Accuracy (2D/3D)

Theorem (GIGAQBX FMM for Laplace (2D/3D))

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

$$\omega = \frac{\sqrt{d}(1 + \ldots}{6 - \sqrt{\ldots}}$$

and letting D *be the minimum bo… acceleration error in the GIGAQBX…*

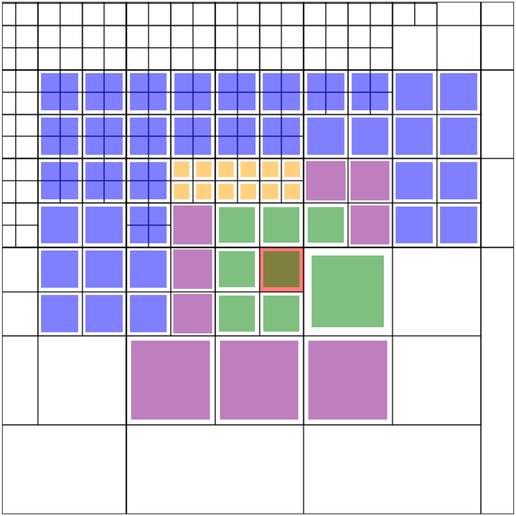
$$\|\mathcal{L}_{\boldsymbol{c}}^{q}[\phi](\boldsymbol{t}) - G_{\boldsymbol{c}}^{p,q}[\phi](\boldsymbol{t})\| \leq \begin{cases} A\Lambda_{q,\mathbf{2}} \max \ldots \\ \frac{A\Lambda_{q,\mathbf{3}}}{D} \max \ldots \end{cases}$$

[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)

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

Complexity (3D)

Theorem

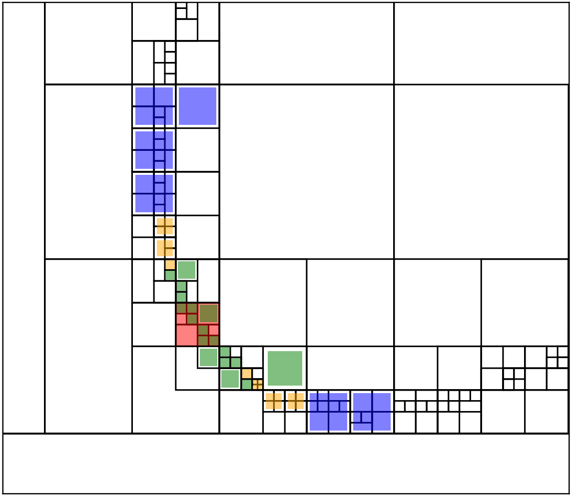
Assume that $p_{FMM} = O(|\log \epsilon|)$, and that $p_{QBX} \leq p_{FMM}$. For a fixed value of n_{max}, using a level-restricted octree and with $t_f < \sqrt{3} - 1$, the cost in modeled flops of the evaluation stage of the GIGAQBX FMM is

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

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]

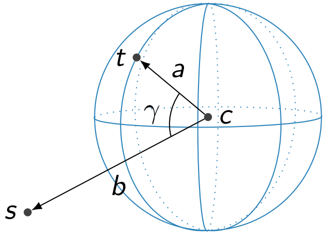
Curve Interaction Lists



Outline

Spherical Harmonic Expansions: Notation

- s: source point
- t: target point
- c: expansion center
- $a = t - c$
- $b = s - c$
- γ: angle between a and b
- p: expansion order



Spherical Harmonic Expansions: Notation

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'):

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

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]: ℓ^2 TC, improved geom. proc.
- GIGAQBX-TS [Wala, K '19]: Reduce accel. cost
- Fourier-Laplace bounds [Wala, K '19–in prep.]:
  2D/3D analysis

Outline

Layer Potentials: Accuracy (2D GIGAQBX)

$(1/2)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$	$p_{\text{QBX}} = 5$	$p_{\text{QBX}} = 7$	$p_{\text{QBX}} = 9$
0	(direct)	4.35e−6	6.21e−7	1.05e−7	5.71e−8
6e−2	3	5.16e−3	6.35e−3	6.33e−3	6.34e−3
2e−2	5	3.83e−4	5.95e−4	5.95e−4	5.93e−4
5e−4	10	4.35e−6	4.82e−6	6.94e−6	9.30e−6
2e−5	15	4.35e−6	6.21e−7	1.05e−7	1.76e−7
5e−7	20	4.35e−6	6.21e−7	1.05e−7	5.71e−8

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish γ_{65}, using the GIGAQBX FMM algorithm.
3250 Gauss-Legendre panels, with 33 nodes per panel.

Layer Potentials: Accuracy (2D Straightforward)

$(1/2)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$	$p_{\text{QBX}} = 5$	$p_{\text{QBX}} = 7$	$p_{\text{QBX}} = 9$
0	(direct)	4.35e−6	6.21e−7	1.05e−7	5.71e−8
6e−2	3	2.55e−2	2.96e−2	4.07e−2	5.77e−2
2e−2	5	6.94e−3	1.61e−2	2.29e−2	3.10e−2
5e−4	10	4.95e−4	1.75e−3	5.80e−3	9.48e−3
2e−5	15	1.58e−5	1.85e−4	6.40e−4	3.17e−3
5e−7	20	4.35e−6	1.31e−5	8.99e−5	5.01e−4

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish γ_{65}, using the conventional QBX FMM algorithm. 3250 Gauss-Legendre panels, with 33 nodes per panel.

Layer Potentials: Accuracy in 3D

$(3/4)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$	$p_{\text{QBX}} = 5$	$p_{\text{QBX}} = 7$	$p_{\text{QBX}} = 9$
3.16e−1	3	8.29e−3	9.68e−3	9.15e−3	9.18e−3
1.78e−1	5	1.43e−3	2.67e−3	2.85e−3	2.78e−3
4.22e−2	10	6.08e−5	6.44e−5	1.27e−4	1.47e−4
1.00e−2	15	6.08e−5	6.38e−6	3.24e−6	7.07e−6
2.38e−3	20	6.08e−5	6.38e−6	1.41e−6	2.51e−7

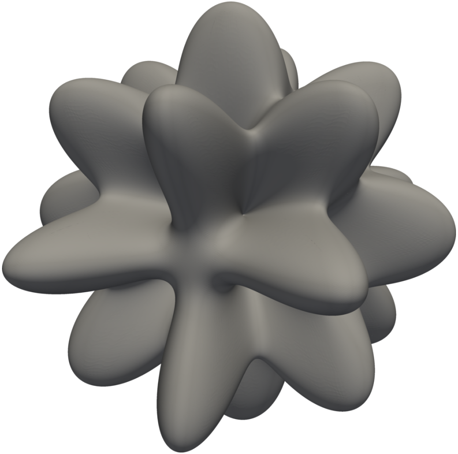
ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 8-armed 'urchin' geometry γ_8.

Stage 1: 48500 triangles, stage 2: 277712 triangles, with 295 nodes per triangle.

Layer Potentials: Accuracy in 3D

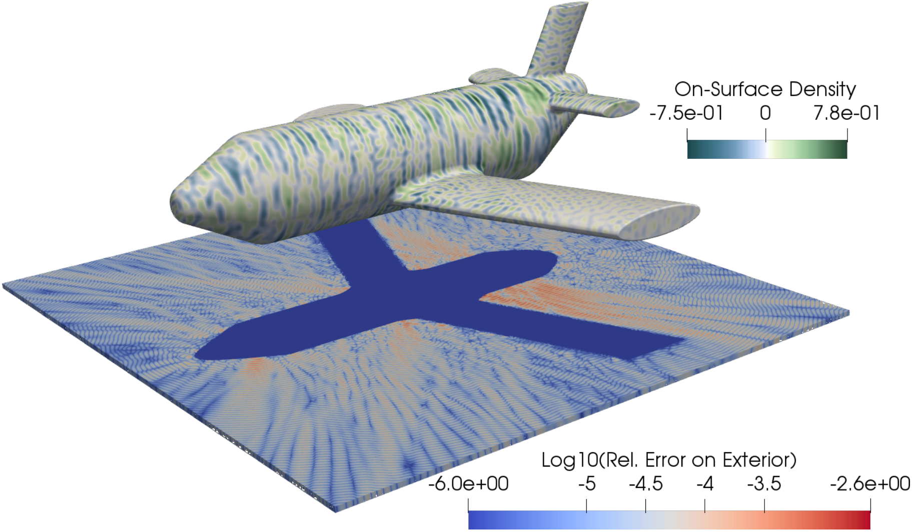
$(3/4)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$
3.16e−1	3	8.29e−3
1.78e−1	5	1.43e−3
4.22e−2	10	6.08e−5
1.00e−2	15	6.08e−5
2.38e−3	20	6.08e−5

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u)$
8-armed 'ur
Stage 1: 48500 triangles, stage 2: 27

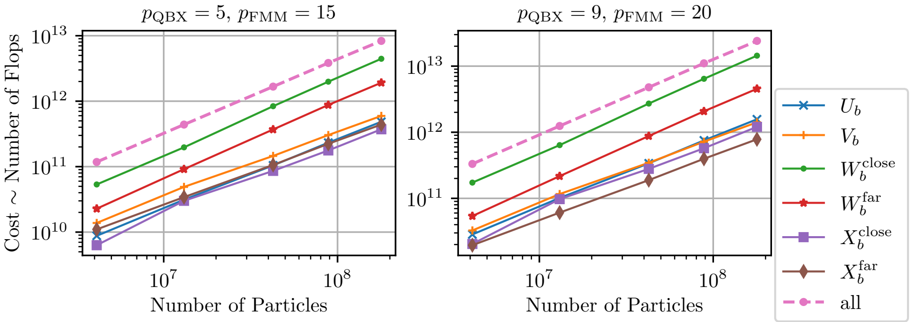


'Urchin' geometry γ_8, based on 8th order spherical harmonics

Layer Potentials: (Somewhat) Complex Geometry

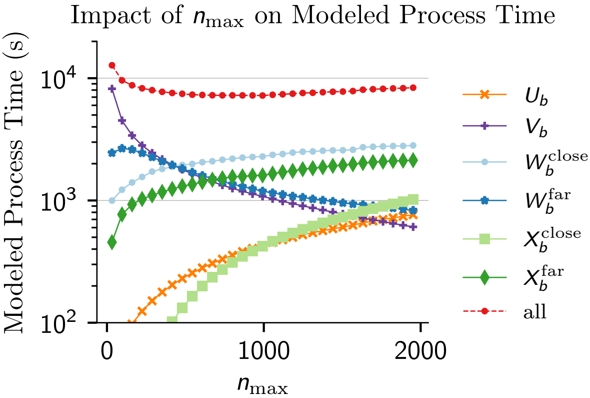


Cost Scaling: 3D GIGAQBX FMM



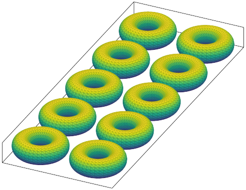
Modeled operation counts for the GIGAQBX FMM for $S\mu$.
$n_{\mathsf{max}} = 512$ and $t_f = 0.9$. Geometries: $\gamma_2, \gamma_4, \ldots, \gamma_{10}$.

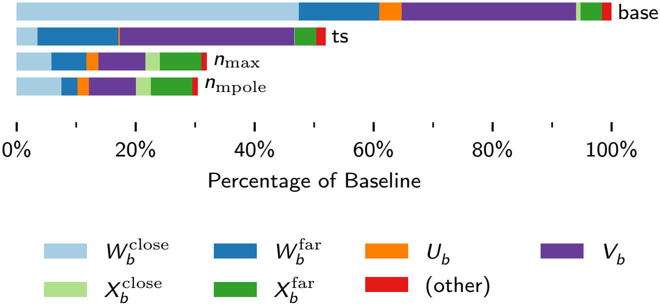
"Balancing" an FMM



Line/Target-Specific Expansions: Cost Impact

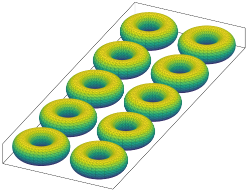
- Operator: Single layer
- Orders: QBX: 9, FMM: 20 (9~digits)
- Points: 19M → 2.1M

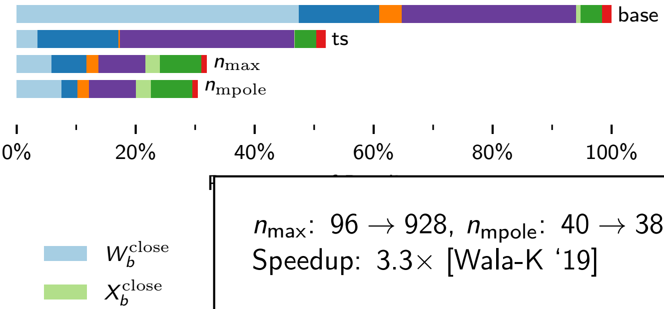




Line/Target-Specific Expansions: Cost Impact

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



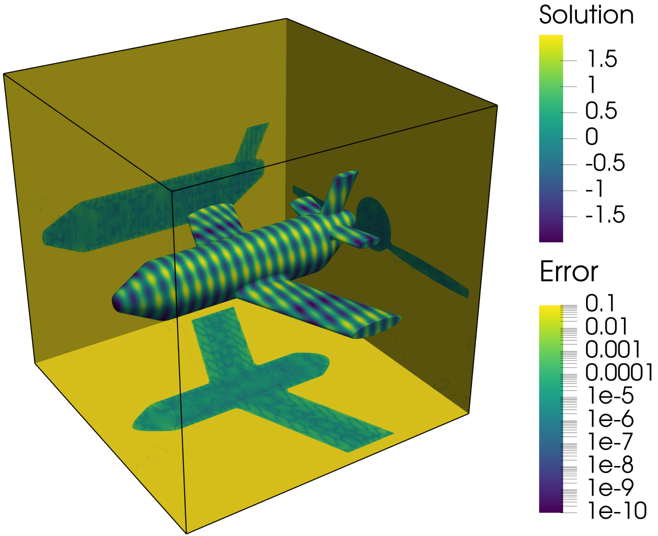


n_{max}: 96 $\rightarrow$ 928, n_{mpole}: 40 $\rightarrow$ 380

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

Outline

Poisson: 3D, CAD Geometry



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

Outline

Inhomogeneous Problems

Example: Poisson

$$\triangle u = f, \qquad u = g \text{ on } \partial\Omega.$$

Steps:

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

$$\tilde{u} = G * f,$$

   where '$*$' represents convolution.

2. Solve

$$\triangle \hat{u} = 0, \qquad \hat{u} = g - \tilde{u} \text{ on } \partial\Omega$$

   using a boundary integral equation.

3. Add

$$u = \tilde{u} + \hat{u},$$

   which solves the Poisson problem.

Eigenvalue Problems

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:

$$\vec{H} = \vec{\nabla} \times \vec{A},$$

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 $\overrightarrow{J}_s$ (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*):

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

Stokes flow

(see project presentation)