Today

- PME Barnes Hall
- The proxy trick
- Home demo follow-up

FMN

- HW due Fri.
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Making Multipole/Local Expansions using Linear Algebra

Actual expansions cheaper than LA approaches. Can this be fixed?

Compare costs for this situation:

\[
S \quad \# \text{sources}
\]
\[
T \quad \# \text{targets}
\]

Form the full interaction matrix: \(O(st)\)
\[ A = LU \quad A = QR \]

\[ A x = b \]

\[ (LU)x = b \]

\[ L(Ux) = b \]

\[ Q(Rx) = b \]
The Proxy Trick

**Idea:** *Skeletonization using Proxies*

**Demo:** Skeletonization using Proxies

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

\[ \Delta u = 0 \]

\[ \partial_x^2 u = -\partial_y^2 u \]

Same as multipole/local

\[ \text{PDE-respecting} \]

\[ \text{rank } K \]
Why Does the Proxy Trick Work?

In particular, how general is this? Does this work for any kernel?

$$\Delta u = 0 \Rightarrow S_p(\varphi_{n+1}) - D_p(n) = u(x) \quad (x \in \mathbb{R})$$

$$S(\varphi(x)) = \int_{\mathbb{R}} G(x,y) \varphi(y) \, dy$$

$$D(\varphi)(x) = \int_{\mathbb{R}} \varphi_{y} G(x,y) \varphi(y) \, dy$$

Green's formula
Where are we now? (I)

Summarize what we know about interaction ranks.

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

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

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

(In general, it’s more source-and-target soup.)

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 few ones (which (\epsilon) constitute the bulk of...
Outline

Introduction

Dense Matrices and Computation

Tools for Low-Rank Linear Algebra

Rank and Smoothness

Near and Far: Separating out High-Rank Interactions
  Ewald Summation
  Barnes-Hut
  Fast Mutipole
  Direct Solvers

Outlook: Building a Fast PDE Solver

Going Infinite: Integral Operators and Functional Analysis

Singular Integrals and Potential Theory

Boundary Value Problems

Back from Infinity: Discretization

Computing Integrals: Approaches to Quadrature

Going General: More PDEs
Simple and Periodic: Ewald Summation

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

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

Q: When does this have a right to converge?

\[ G(x, \theta) = O \left( \| x \|_{2}^{-p} \right) \]

\[ \gamma(0) = \sum_{i=0}^{\infty} \sum_{ \text{cells disk} (0, c) \in [i, i+1) \setminus \mathbb{Z}^d \cap \mathbb{L}^d } O(i^{-p}) \]

\[ \text{#Terms in sum: } O(i^{d-1}) \]
\[ d - 1 - p < -1 \]
\[ p > d \]
Ewald Summation: Constructing a Scheme

- Use unit cells to separate near/far.
  \textit{But that's imperfect:} Sources can still get arbitrarily close to targets.

- Use Fourier transform to compute far contribution.
  \textit{But that's also imperfect:}
  - Fourier can only sum the \textit{entire} (periodic) potential
    - \textit{So:} Cannot make exception for near-field
  - \textit{G} non-smooth is the interesting case $\rightarrow$ Long Fourier series $\rightarrow$ expensive (if convergent at all)

\textbf{Idea:} Only operate on the smooth ('far') parts of \textit{G}. 