

Today

- Mpole demo follow-up
- The proxy trick
- PME, Barnes-Hut,  
FMM

- HW1 graded

- HW2 due Fri

## Making Multipole/Local Expansions using Linear Algebra

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

Compare costs for this situation:

$S$  #sources

$T$  #targets

Form the full interaction matrix:  $O(ST)$

100



$$A = LU$$

$$A = QR$$

$$Ax = b$$

$$(LU)x = b$$

$$L(\underbrace{Ux}_y) = b$$

$$QRx = b$$

$$Q(\underbrace{Rx}_s) = b$$

# The Proxy Trick

Handwritten scribble

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 mpole / local



PDE-respecting



## Why Does the Proxy Trick Work?

Green's formula

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

$$\Delta u = 0: \int_{\Gamma} (\partial_n u) - D_{\Gamma}(u) = u(x) \quad (x \in \Omega)$$



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

$$D(\varphi)(x) = \int_{\Gamma} \partial_{n_y} G(x,y) \varphi(y) dy$$

## 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

$$\psi(\mathbf{x}) = \sum_j G(\mathbf{x}, \mathbf{y}_j) \varphi(\mathbf{y}_j)$$

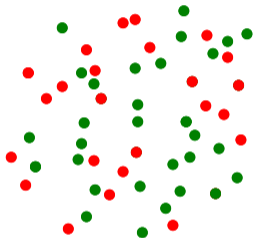
satisfies a PDE (e.g. Laplace), i.e. if  $G(\mathbf{x}, \mathbf{y}_j)$  satisfies a PDE, then that low rank is *even* lower.

- ▶ 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 ball of the form  $(\text{ball}(s)) \times \text{ball}(t)$  to get a ball 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 Multipole

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

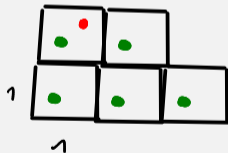
## Simple and Periodic: Ewald Summation

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

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



$$\begin{pmatrix} \sin(kx) & \cos(kx) \\ \sin(ky) & \cos(ky) \end{pmatrix}$$



## Lattice Sums: Convergence

Q: When does this have a right to converge?

$$\sum_i \frac{1}{i}$$

$$G(x, \theta) = O(\|x\|_2^{-p})$$

$$\psi(0) = \sum_{i=0}^{\infty} \sum_{\substack{\text{cells @ disk}(0, c) \\ \in [i, i+1) \setminus \text{disk}}} O(i^{-p})$$

# terms in sum:  $O(i^{d-1})$

$$= \sum_{i=0}^{\infty} O(i^{d-1-p})$$

$$d-1-p < -1$$

$$p > d$$

## Ewald Summation: Constructing a Scheme

- ▶ Use unit cells to separate near/far.  
*But that's imperfect: Sources can still get arbitrarily close to targets.*
  - ▶ Use Fourier transform to compute far contribution.  
*But that's also imperfect:*
    - ▶ Fourier can only sum the *entire* (periodic) potential  
So: Cannot make exception for near-field
    - ▶  $G$  non-smooth is the interesting case  $\rightarrow$  Long Fourier series  $\rightarrow$  expensive (if convergent at all)
- Idea:** Only operate on the smooth ('far') parts of  $G$ .