Today

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

- HW1 graded
- HW2 due Fri

Making Multipole/Local Expansions using Linear Algebra

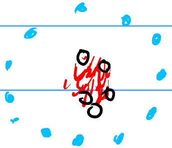
Actual expansions cheaper than LA approaches. Can this be fixed?

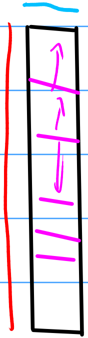
Compare costs for this situation:

S #sources

T # targets

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





$$A = LU \qquad A = QR$$

$$Ax = b$$

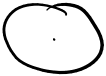
$$(LU)x = b \qquad QRx = b$$

$$L(\underbrace{Ux}_{y}) = b \qquad Q(\underbrace{Rx}_{b}) = b$$

The Proxy Trick

Idea: *Skeletonization using Proxies*

Demo: Skeletonization using Proxies



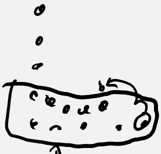
Q: What error do we expect from the proxy-based multipole/local 'expansions'?

$\Delta u = 0$

$\partial_x^2 u = -\partial_y^2 u$

Same as mpole / local

PDE-respecting

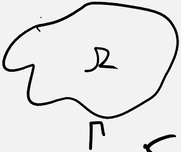


Why Does the Proxy Trick Work?

Green's formula

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

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



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

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

Where are we now? (I)

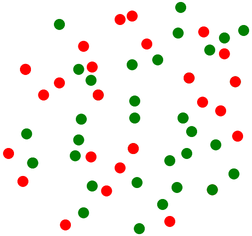
Summarize what we know about interaction ranks.

- 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.)

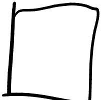
So maybe we can do business yet–we just need to split out the near

Outline

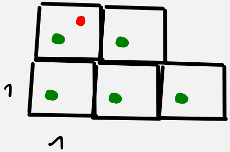
Simple and Periodic: Ewald Summation

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

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



$(\sin(nx) \quad \cos(nx)) \cdot (\sin(ny) \cdot \cos(ny))$



Lattice Sums: Convergence

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

Q: When does this have a right to converge?

$$G(x,0) = O\left(\|x\|_2^{-p}\right)$$

$$\psi(0) = \sum_{i=0}^{\infty} \underbrace{\sum_{\substack{\text{cells @ dist}(0,c) \\ \in [i,i+1)}}}_{\text{\# terms in sum: } O(i^{d-1})} O(i^{-p})$$

ℓ^∞ dist

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

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

$$p > d$$

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 $\to$ Long Fourier series $\to$ expensive (if convergent at all)

Idea: Only operate on the smooth ('far') parts of G.