Today

- PME
- Barnes-Hut
- Fast Multipole
- Direct solver

$Ax \to b$

HW2 due

Simple and Periodic: Ewald Summation

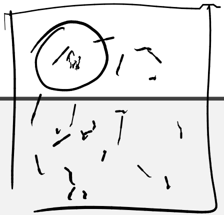
Want to evaluate potential from an infinite periodic grid of sources:

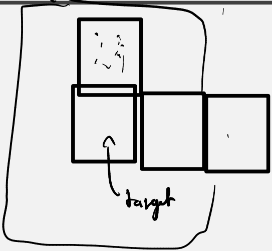
$$\psi(\mathbf{x}) = \sum_{\mathbf{i}\in\mathbb{Z}^d}\sum_{j=1}^{N_{\text{src}}} G(\mathbf{x}, \mathbf{y}_j + \mathbf{i})\varphi(\mathbf{y}_j)$$

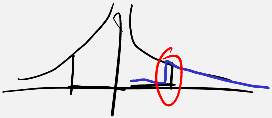
$\frac{1}{r}$

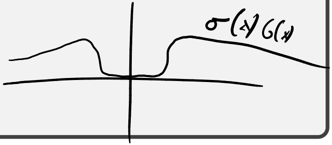
$\mathcal{F}\{\ \} = \mathcal{F}\{G\}\cdot\mathcal{F}(\dots)$

poor convergence







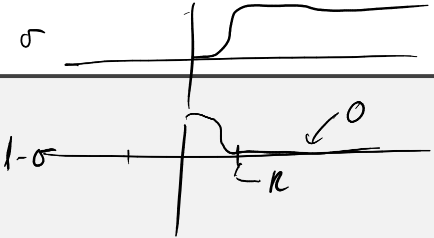


Ewald Summation: Constructing a Scheme

- 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)

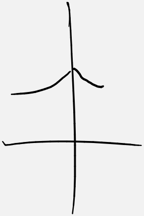
Idea: Only operate on the smooth ('far') parts of G.

Ewald Summation: Screens



- σ smooth
- $\sigma = O(\|x\|_2^4)$
- $1-\sigma$ has bounded support

$$G(x) = \underbrace{\sigma(x)\,G(x)}_{G_{LR}} + \underbrace{(1-\sigma)\,G(x)}_{G_{SR}}$$



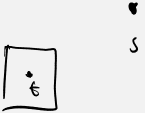
$$G(x) = \frac{1}{r^4}$$

$$= \underbrace{\sigma(x)\frac{1}{r^4}}_{= O(1)} + (1-\sigma)\frac{1}{r^4}$$

better-ish

Ewald Summation: Field Splitting

We can split the computation (from the perspective of a unit cell target) as follows:



	G_{SR}	G_{LR}
Close source	Directly*	Fourier
Far source	0	Fourier

"Close": $\|s-t\|_2 \le R$

* Hopefully, only $O(1)$ sources in $B_2(s,R)$.
If so, $< O(n^2)$ cost.

$$\big(x \mapsto \delta(x-y)\big) * \overbrace{\big(x \mapsto G(x,0)\big)}^{\hat{G}(x)} = \hat{G}(x-y)$$

$$\left(\int \hat{G}(x-y)\, \delta(y-y) \right)$$

(see later)

Ewald Summation: Convolution Recap

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

The above sum then:

$$\psi = (x \mapsto G(x,0)) * \left(x \mapsto \sum_{i\in\mathbb{Z}} \sum_{j=1}^{N_{\text{src}}} \delta(x - y_j - i) \right)$$

with the convention $f(x) = f * (\xi \mapsto \delta(\xi - x))$. Convolution is linear (in both arguments) and turns into multiplication under Fourier transforms:

$$\mathcal{F}\{f * g\} = \mathcal{F}f \cdot \mathcal{F}g,$$

possibly with a constant depending on normalization. Also:

$$\mathcal{F}\left\{ \sum_{i\in\mathbb{Z}} \delta(x-i) \right\}(\omega) = \left(\sum_{j\in\mathbb{Z}} \delta(\omega - j). \right)$$

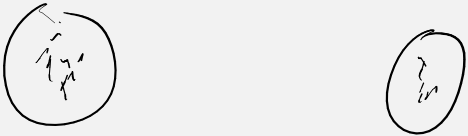
Ewald Summation: Summation (1D for simplicity)

Interesting bit: How to sum G_{LR}.

$$\mathcal{F}(f(x-y))(\omega) = e^{-2\pi i y \omega}\, \mathcal{F}(f)(\omega)$$

$$\mathcal{F}\Big\{ \sum_{i \in \mathbb{Z}} \sum_{j}^{N} G_{LR}(x - y_j - i) \Big\}$$

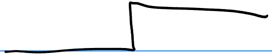
$$= \mathcal{F}\{G_{LR}\}(\omega) \sum_{i \in \mathbb{Z}} \sum_{j=1}^{N} e^{-2\pi i y_j \omega}\, \delta(\omega - i)$$



S

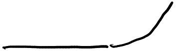
T

$$\mathcal{F}\{\ \delta\ \}(\omega) = O(1)$$

$\mathcal{F}\{$  $\}(\omega) = O\left(\frac{1}{\omega}\right)$

Heaviside

$\mathcal{F}\{$  $\}(\omega) = O\left(\frac{1}{\omega^2}\right)$

$\mathcal{F}\{$  $\}(\omega) = O\left(\frac{1}{\omega^3}\right)$

$$\mathcal{F}\{f'(x)\} = (i\omega)\,\mathcal{F}(f)(\omega)$$

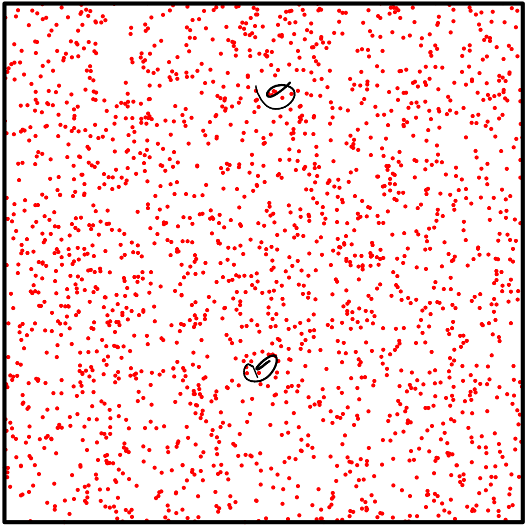
$$\mathcal{F}\left(\int f\right)(\omega) = \frac{1}{(i\omega)}$$

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')

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson)

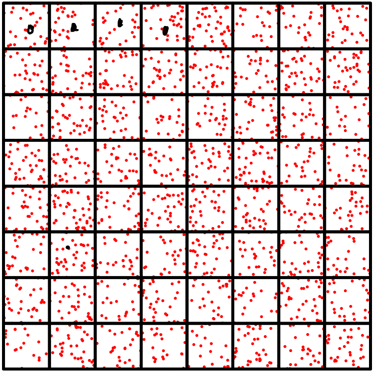
Barnes-Hut: The Task At Hand

Want: All-pairs interaction.

Caution:

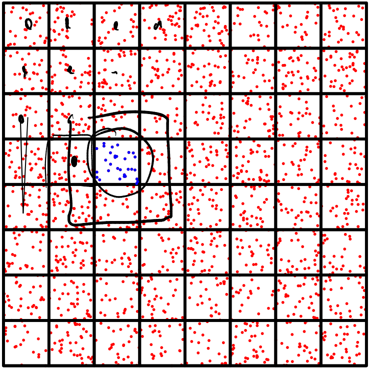
- In these (stolen) figures: targets sources
- Here: targets and sources

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson)

Barnes-Hut: Putting Multipole Expansions to Work



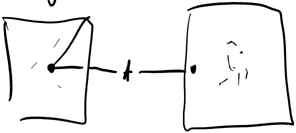
(Figure credit: G. Martinsson)

mpole error

$$= \left(\frac{d(\text{furthest src})}{d(\text{closest tgt})}\right)^{p+1}$$

$$\le \left(\frac{\sqrt{2}}{3}\right)^{p+1}$$

$\sqrt{2}$

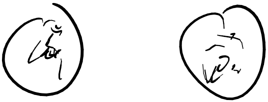


Barnes-Hut: Box Targets

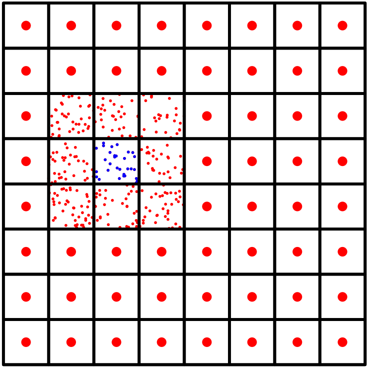
For sake of discussion, choose one 'box' as targets.

Q: For which boxes can we then use multipole expansions?

Barnes-Hut: Putting Multipole Expansions to Work



KS + KT



(Figure credit: G. Martinsson)

Barnes-Hut: Accuracy

With this computational outline, what's the accuracy?

$$\left(\frac{\sqrt{2}}{3}\right)^{p+1}$$

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

Barnes-Hut (Single-Level): Computational Cost

What's the cost of this algorithm?

$m = \sqrt{N}$

N = # particles

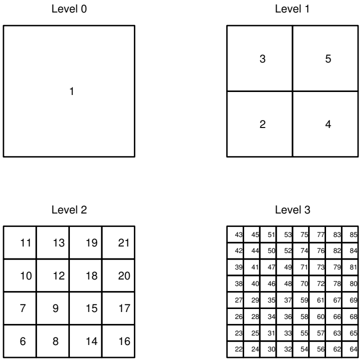
K = # terms in mpole exp.

m = # particles in a box

Step	How often	Cost	
Compute mpoles	N/m	Km	NK
Evaluate mpoles	$N/m \cdot N$	K	N^2K/m
9 close boxes	9 (N/m boxes)	m^2	Nm

Barnes-Hut Single Level Cost: Observations

Box Splitting



(Figure credit: G. Martinsson)