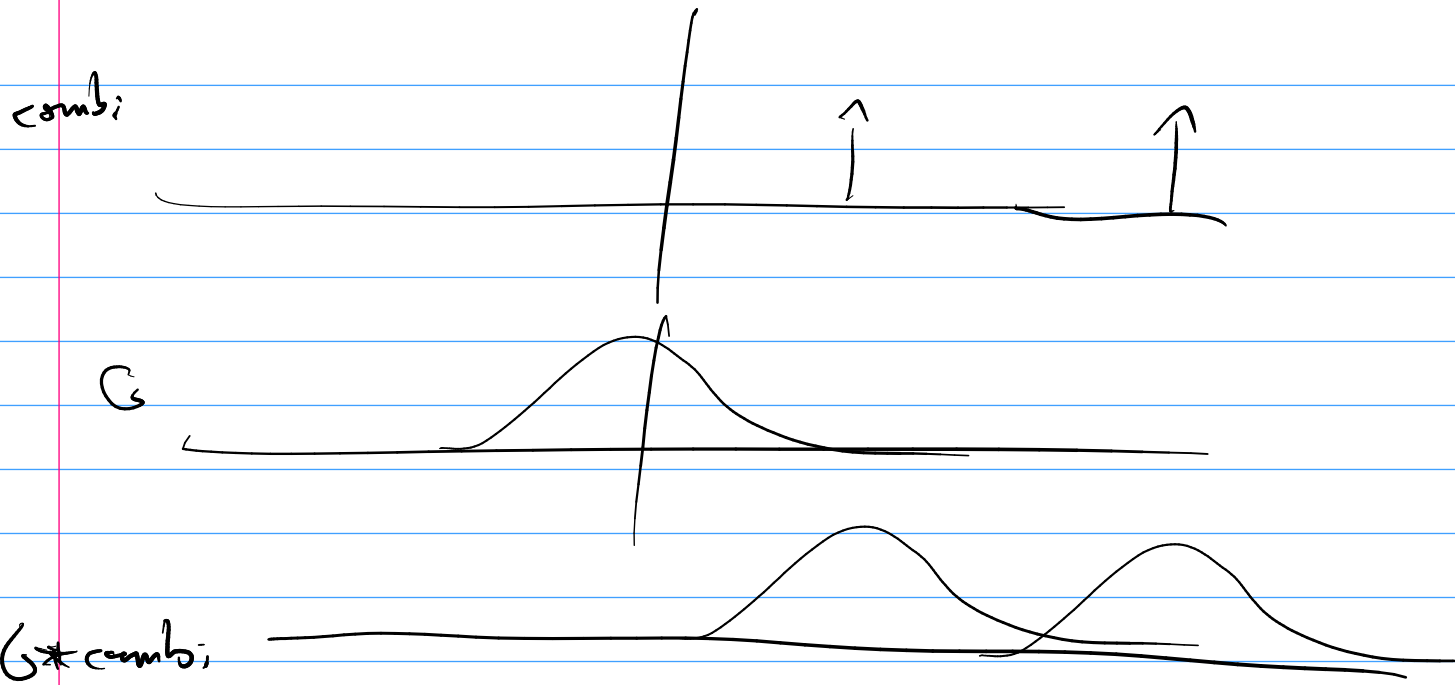
Today:

- Ewald
-

HW2 due Monday
Office hour → Monday
3:30-4:30

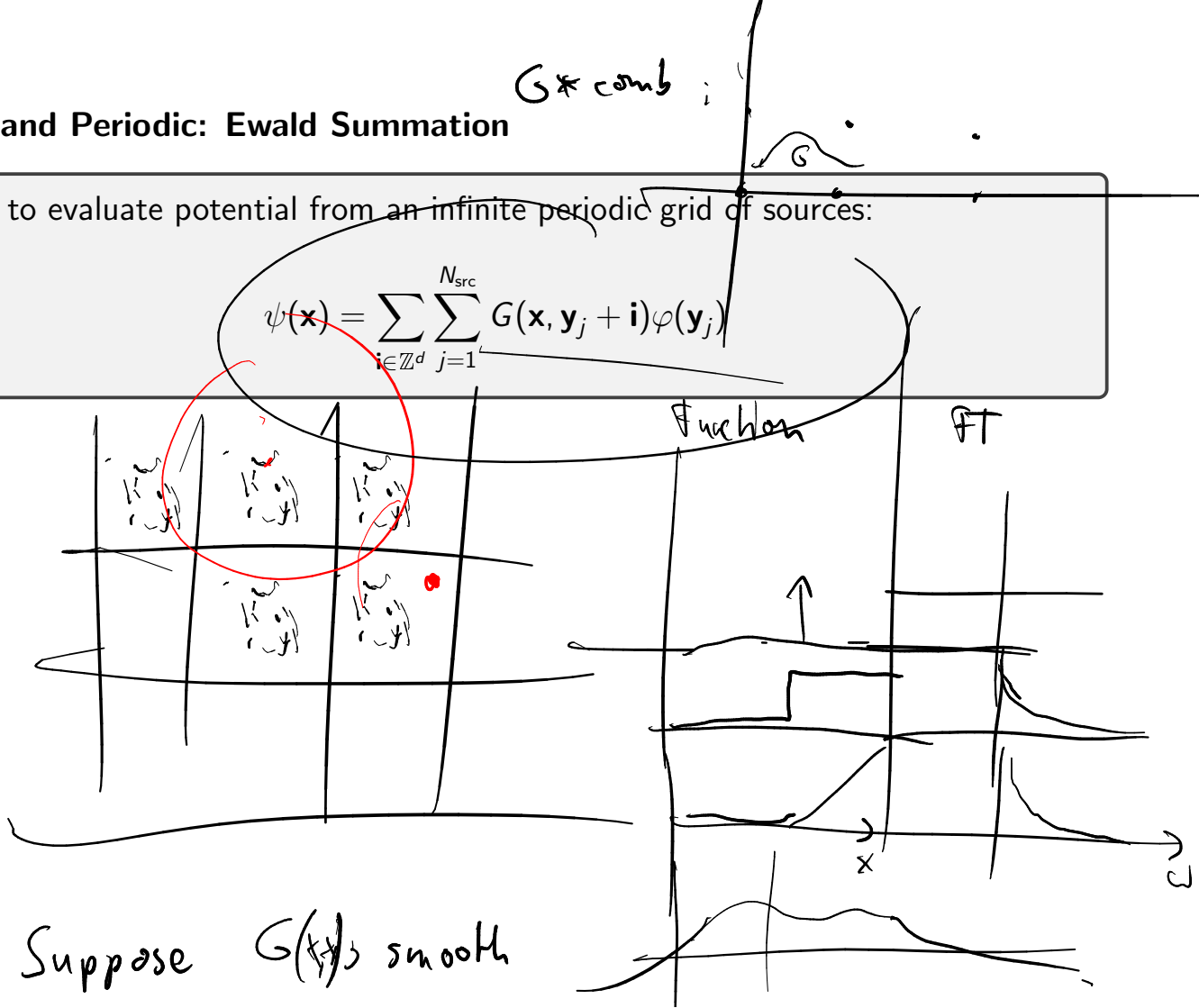
- Marhsson
- van de Geijn


comb;
G
G*comb;

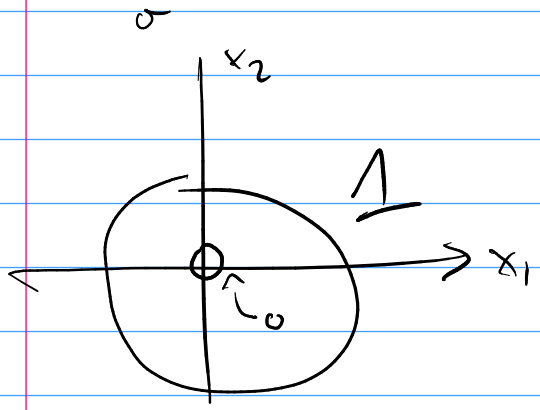
Simple and Periodic: Ewald Summation

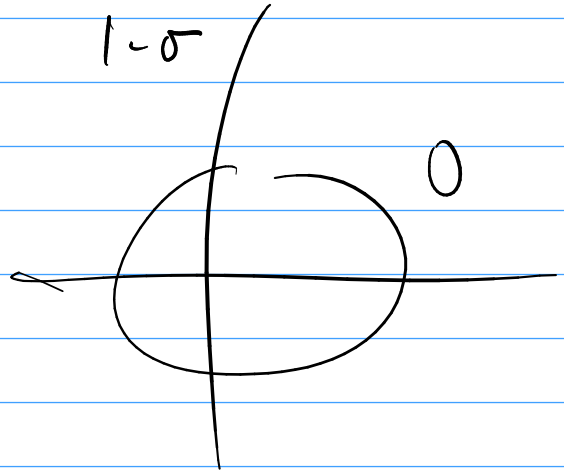
Want to evaluate potential from ~~an infinite~~ periodic grid of sources:

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



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



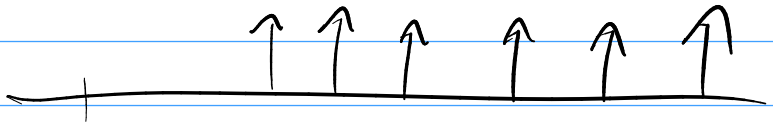


Convolution: $(f * g)(x) = \int f(\xi)\, g(x-\xi)\, d\xi$

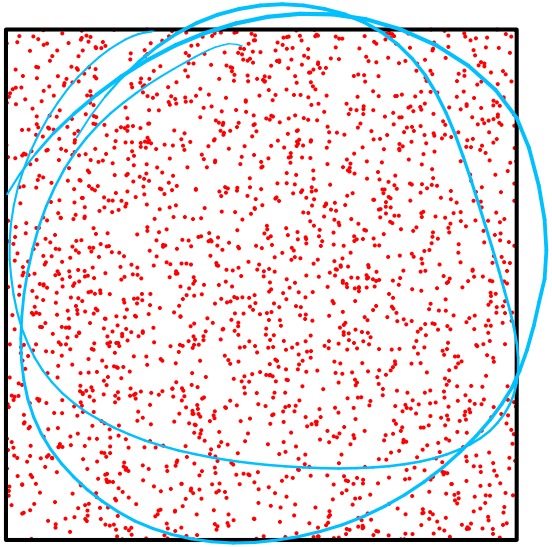
$$\mathcal{F}(f * g) = \mathcal{F}\{f\} \cdot \mathcal{F}(g)$$

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

$$\mathcal{F}\left(\sum_{j=-\infty}^{\infty} \delta(x - aj)\right) = C \sum_{j=-\infty}^{\infty} \delta\left(\omega - C\tfrac{1}{a} j\right)$$

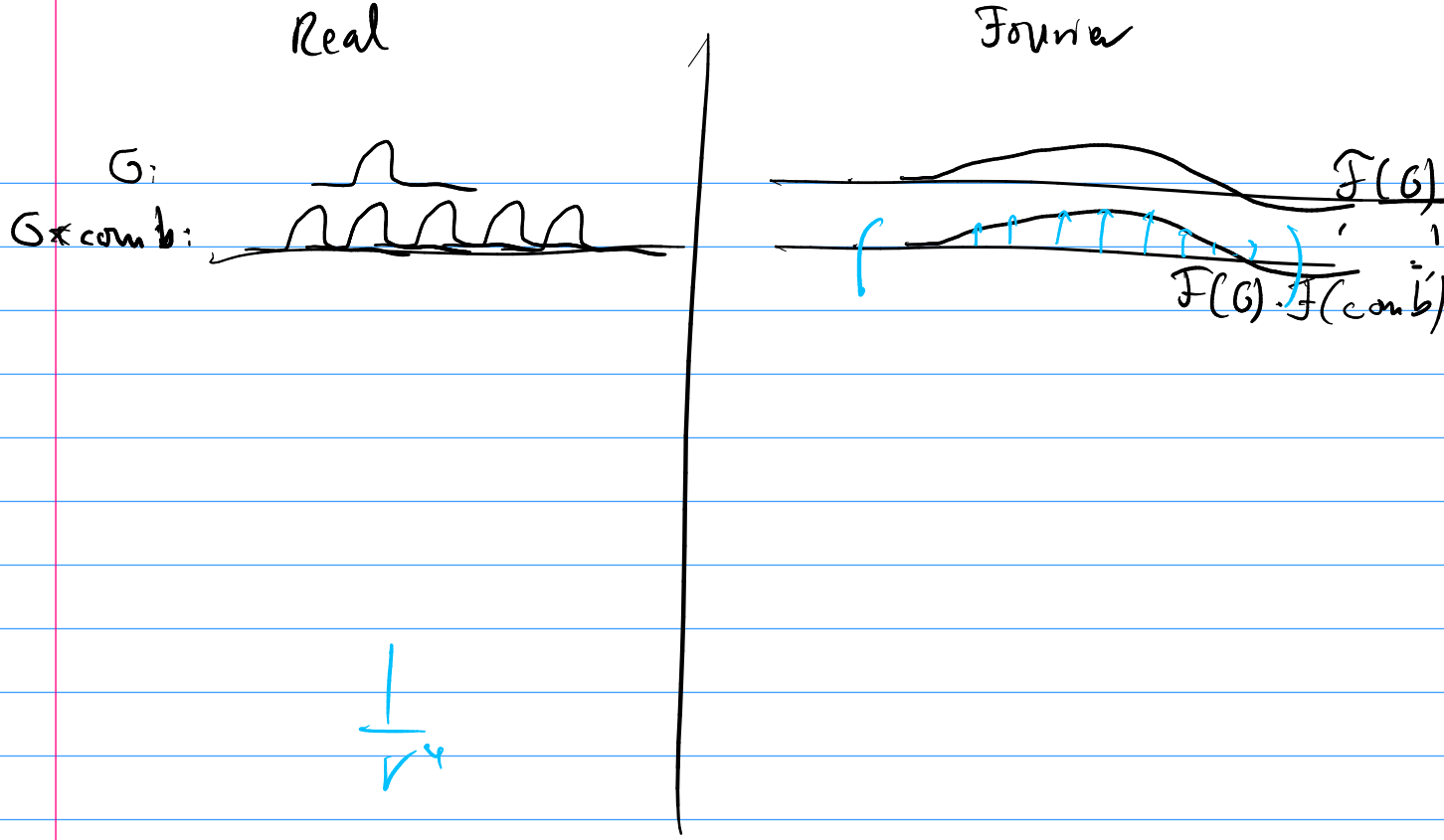


Barnes-Hut: Putting Multipole Expansions to Work

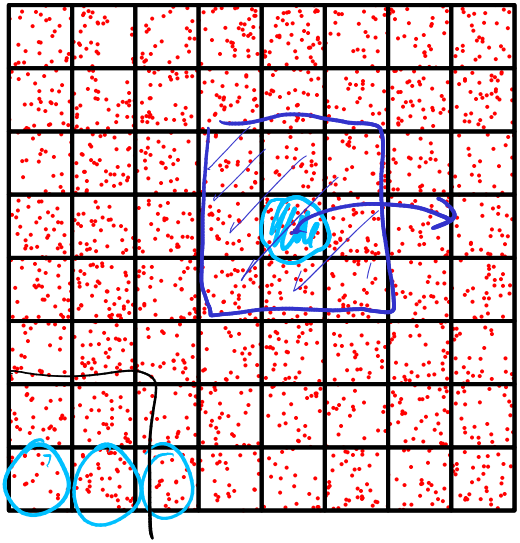


(Figure credit: G. Martinsson, Boulder)

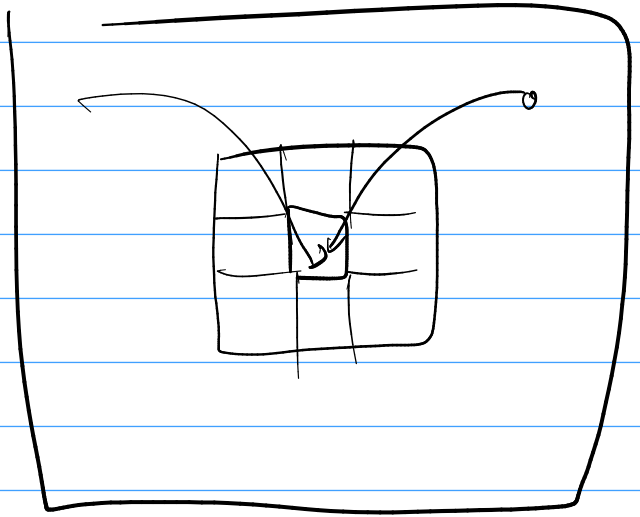
Want: All-pairs interaction.
Caution: In these (stolen) figures: targets sources.
Here: targets and sources.


Real
Fourier
G:
G*comb:
F(G)
F(G)·F(comb)
1/Δ

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)



	How often	individuals
Compute mpoles	N/m	Km
→ Evaluate mpoles	$N_{tgt\ pnts} \cdot \underbrace{N/m}_{\text{source boxes}}$	K
9 close boxes	$9(N/m)$	$\cdot m^2$

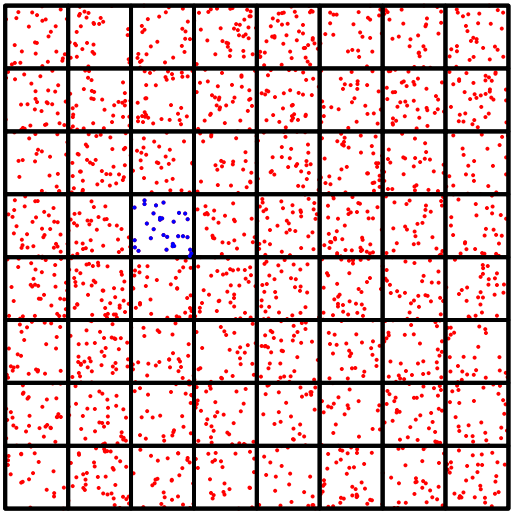
N: # particles

K: # terms in expansion

m # particles in box

boxes: $\frac{N}{m}$

Barnes-Hut: Putting Multipole Expansions to Work

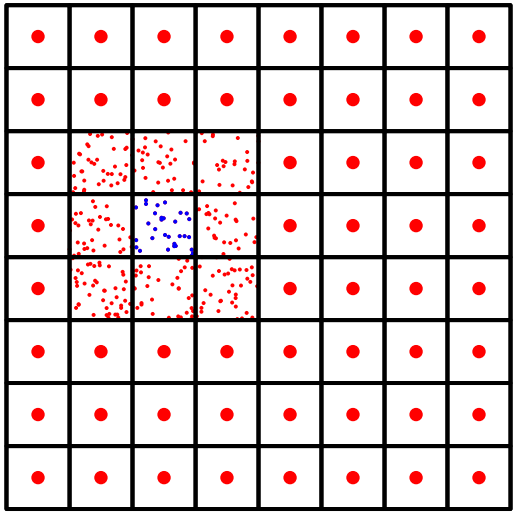


(Figure credit: G. Martinsson, Boulder)

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



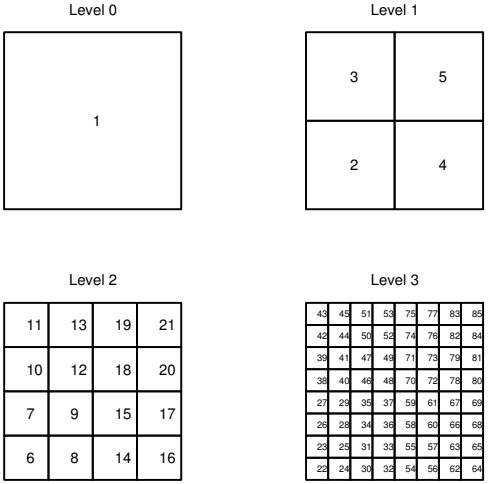
(Figure credit: G. Martinsson, Boulder)

With this computational outline, what's the accuracy?

Barnes-Hut (single-level): Computational Cost

What's the cost of this algorithm?

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

How many levels?