Ann:

- ~~no video~~ of the class (sorry)
- filled-out demos available (expand, "run interactively")

Goals:

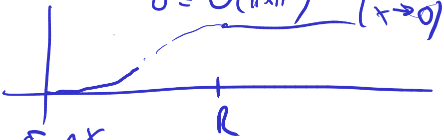
- BH / FMM

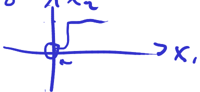
Review:

- Ewald summation
- "Tree codes" / "Barnes-Hut"

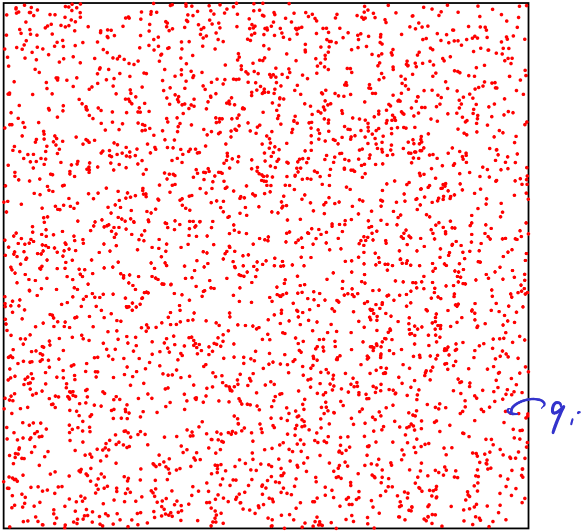
$$G = \underbrace{\sigma G}_{LR} + \underbrace{(1-\sigma) G}_{SR}$$

$\sigma = O(\|x\|^4)$ $(x \to 0)$





Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

Barnes-Hut: The Task At Hand

Want: All-pairs interaction.

Caution:

- In these figures: targets sources
- Here: targets and sources

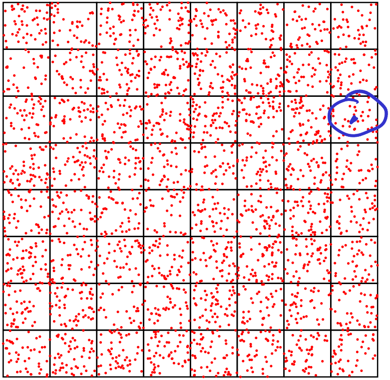
$$\vec{u} = A\vec{q}$$

$$\uparrow$$

$$A_{ij} = \log(\|x_i - x_j\|_2)$$

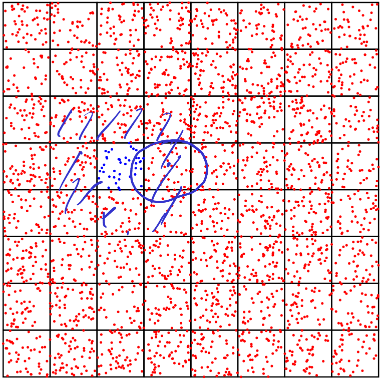
$$A_{ii} = 0$$

Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

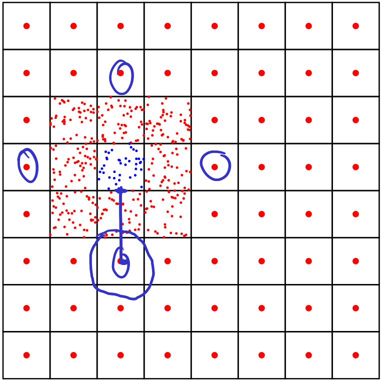
Barnes-Hut: Box Targets

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

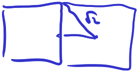
Q: For which boxes can we then use multipole expansions?

dep. on accuracy

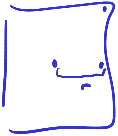
Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)



box radius



$d(c, \text{f.s.}) = \sqrt{2}\, r$

$d(c, \text{c.t.}) = 3r$

Barnes-Hut: Accuracy

$$\frac{d(c, \text{p.s.})}{d(c, \text{c.f.})}$$

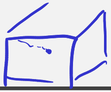
With this computational outline, what's the accuracy?

$$\varepsilon \le \left(\frac{d(c, \text{p.s.})}{d(c, \text{c.f.})}\right)^{k+1}$$

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

Obs 1: expn order gives accuracy

Obs 2: nD: $\left(\frac{\sqrt{d}}{3}\right)^{k+1}$



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

Barnes-Hut (Single-Level): Computational Cost

What's the cost of this algorithm?

N = # particles

K = # terms in an expansion

m = # particles in a box

		How often	Cost	Total
1	Compute mpole	N/m	Km	NK
2	Eval. mpoles	N tgts $\cdot$ N/m src boxes	K	N^2K/m
3	9 close boxes	$9(N/m$ boxes$)$	m^2	$9Nm$

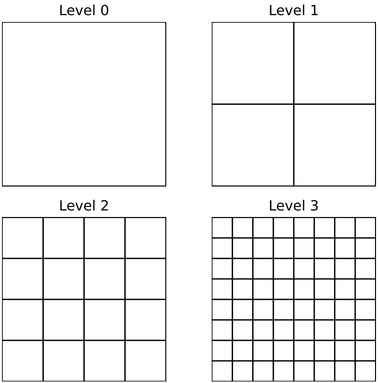
Pick $m = \sqrt{N}$

Barnes-Hut Single Level Cost: Observations

cost $\sim O(N^{3/2})$ better than $O(N^2)$

To reduce cost of Step 2: tree of boxes

Box Splitting



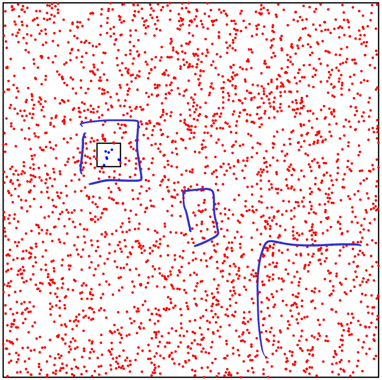
(Figure following G. Martinsson)

Level Count

How many levels?

Until # particles in leaf box
is $\mathcal{O}(1)$

Box Sizes

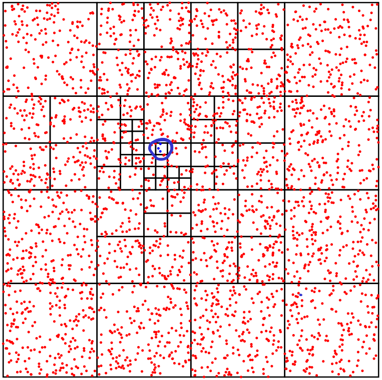


(Figure following G. Martinsson)

Want to evaluate all the source interactions with the targets in the box.

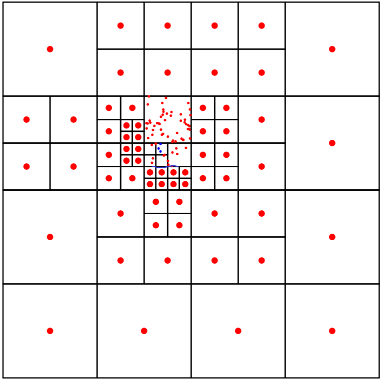
Q: What would be good sizes for source boxes? What's the requirement?

Multipole Sources



Data from which of these boxes could we bring in using multipole expansions? Does that depend on the type of expansion? (Taylor/special function vs skeletons)

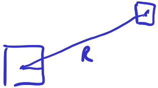
Barnes-Hut: Box Properties



What properties do these boxes have?

Simple observation: The further, the bigger.

Barnes-Hut: Box Properties



r_s : source box radius

r_t : target box radius

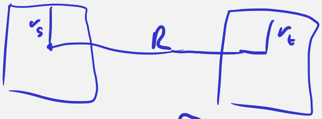
R : d(source box center, target box center)

$$\left(\frac{d(\text{source c, f.s.})}{d(\text{source c, c.t})}\right)^{k+1} \le \left(\frac{r_s\sqrt{2}}{R - r_t}\right)^{k+1}$$

Towards: MAC ("multipole acceptance criterion")

Barnes-Hut: Well-separated-ness

Which boxes in the tree should be allowed to contribute via multipole?



Convergent iff $\quad r_s\sqrt{2} < R - r_t \quad (*)$

Convergent <u>if</u> $\quad R \geq 3\max(r_t, r_s) \quad (**)$

$(*) \iff (r_t + \sqrt{2}\, r_s) < R$

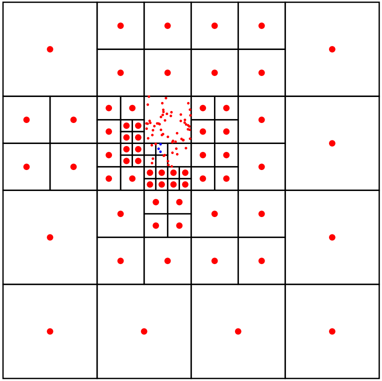
$(**) \Rightarrow (*)$

$(**)$ as MAC : "well-separated"

Barnes-Hut: Revised Cost Estimate

don't care

Which of these boxes are well-separated from one another?



What is the cost of evaluating the target potentials, assuming that we know the multipole expansions already?

Barnes-Hut: Revised Cost Estimate