

September 22<sup>4</sup>, 2026  
Announcements

HW2

→ HW3

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Goals

Fast algorithms  
Barnes-Hut  
FMM

Review

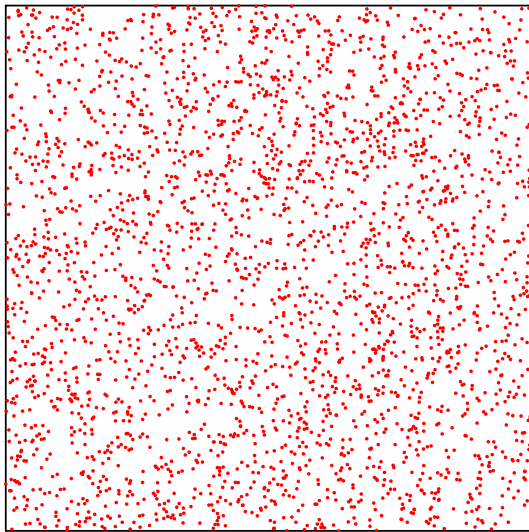
tail estimates:

local  $\left( \frac{d(\vec{c}, \text{furthest tgt})}{d(\vec{c}, \text{closest src})} \right)^{prl}$

mpole  $\left( \frac{d(\vec{c}, \text{furthest src})}{d(\vec{c}, \text{closest tgt})} \right)^{prl}$



## Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

## Barnes-Hut: The Task At Hand

Want: All-pairs interaction.

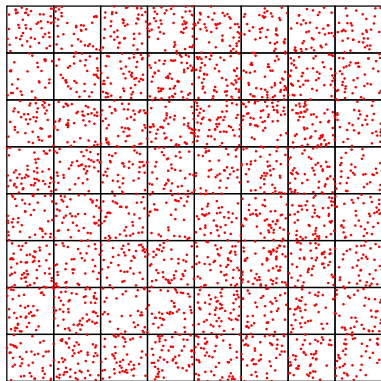
Caution:

- ▶ In these figures: **targets** **sources**
- ▶ Here: **targets and sources** (ignore self interactions)

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

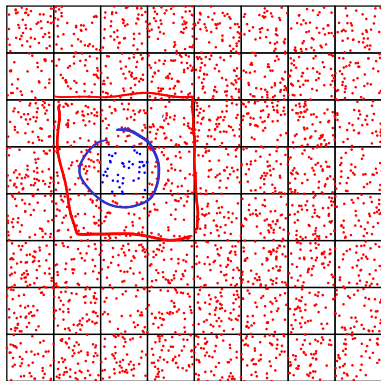
$$A_{ij} = \log(\|x_i - y_j\|_2)$$

## Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

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## Barnes-Hut: Box Targets

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

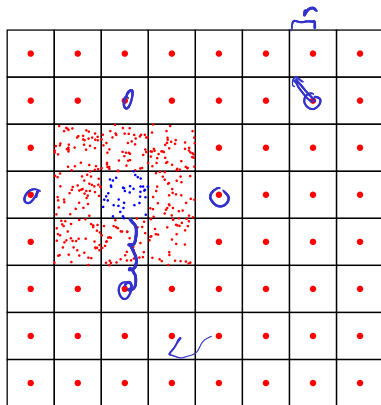
Q: For which boxes can we then use multipole expansions?



# Barnes-Hut: Putting Multipole Expansions to Work

$$2D: \sqrt{l^2 + l^2}$$

$$3D: \sqrt{l^2 + l^2 + 1}$$



$$\left( \frac{d(c, \text{farthest src})}{d(c, \text{closest tgt})} \right)^{p+1}$$

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

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

(Figure following G. Martinsson)

## Barnes-Hut: Accuracy

With this computational outline, what's the accuracy?



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

# Barnes-Hut (Single-Level): Computational Cost

What's the cost of this algorithm?

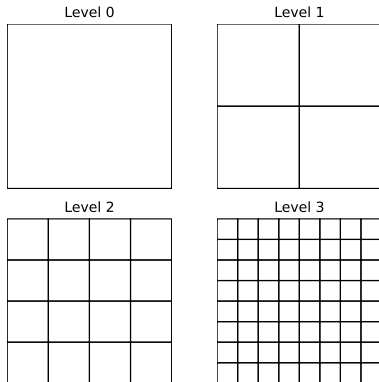
|   | $N$ # particles | $K$ # terms in an expansion $\neq p$ | $m$ # particles in a box        |             |
|---|-----------------|--------------------------------------|---------------------------------|-------------|
|   |                 | Cost                                 | How often                       | Total       |
| ① | Form inputs     | $Km$                                 | $N/m$ boxes                     | $KN$        |
| ② | Evaluate        | $K$                                  | $N$ tpts. $\frac{N}{m}$ sectors | $N^2 K / m$ |
| ③ | Close boxes     | $m^2$                                | $g(N/m)$ boxes                  | $g N m$     |

$\rightarrow p \ll K \quad m \approx \sqrt{N}$

## Barnes-Hut Single Level Cost: Observations

$$N^{3/2}$$

# Box Splitting



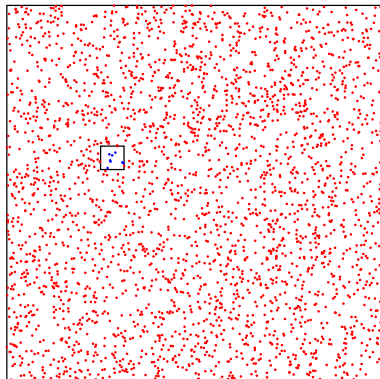
(Figure following G. Martinsson)

## Level Count

How many levels?

$$\begin{aligned} \text{Insist. } m &= O(1) \text{ items as } N \rightarrow \infty \\ \Rightarrow \# \text{ levels} &= O(\log N) \end{aligned}$$

## Box Sizes

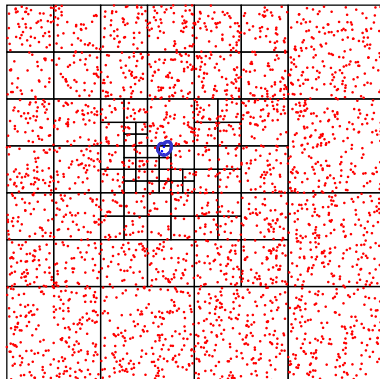


(Figure following G. Martinsson)

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

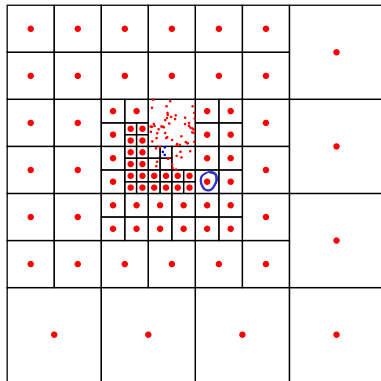
**Q:** What would be good sizes for source boxes? What's the requirement?

## 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



$$\left( \frac{d(c, \text{farthest src})}{d(c, \text{closest tgt})} \right)^{p+1} \approx \left( \frac{\sqrt{2} r_s}{R - r_t} \right)^{p+1}$$

$$\text{conv.} \Leftrightarrow \sqrt{2} r_s \leq R - r_t$$

$$\text{conv. with } \beta_3 \Leftrightarrow \frac{\sqrt{2} r_s}{R - r_t} \leq \frac{\sqrt{2}}{3}$$

$\Leftarrow$  "Multipole acceptance  
criterion"

## Barnes-Hut: Well-separated-ness

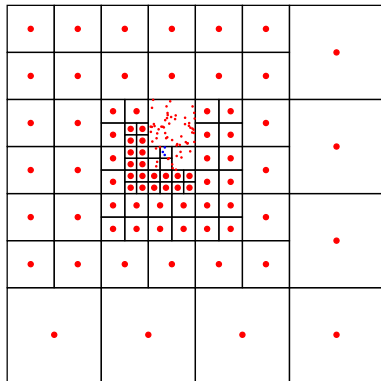
Which boxes in the tree should be allowed to contribute via multipole?

$$3r_s + r_e \leq R_\infty$$

$$\|c_1 - c_2\|_\infty$$

## Barnes-Hut: Revised Cost Estimate

Which of these boxes are well-separated from the target?



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

# Barnes-Hut: Revised Cost Estimate



$L$  #level,  $\sim \log(N)$

$N$

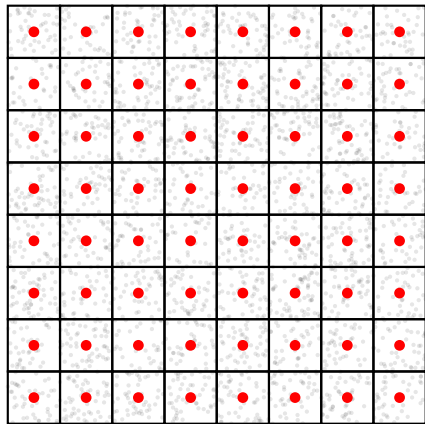
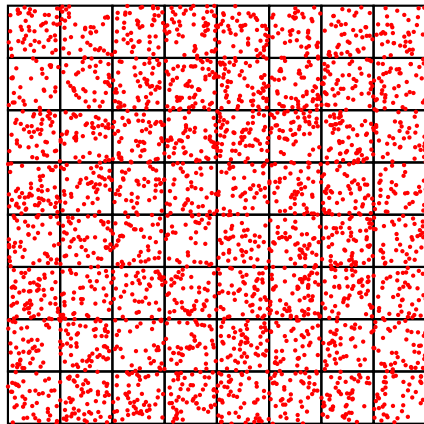
$K$

$m$

|                    | How often                           | Cost  | Total         |
|--------------------|-------------------------------------|-------|---------------|
| ① Compute mpdos    | $N \cdot L$                         | $K$   | $K N \log(N)$ |
| ② Eval mpdos       | $N \text{ tgl } 2^L$                | $K$   | $K N \log(N)$ |
| ③ Self + neighbors | $C \cdot \frac{N}{m} \text{ boxes}$ | $m^2$ | $C \cdot N m$ |

mpds coeffs       $(y-c)^m$

## Barnes-Hut: Next Revised Cost Estimate



(Figure following G. Martinsson)

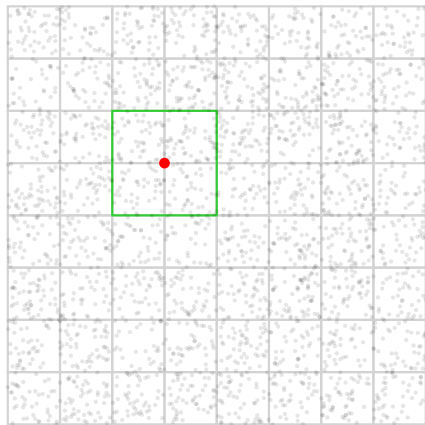
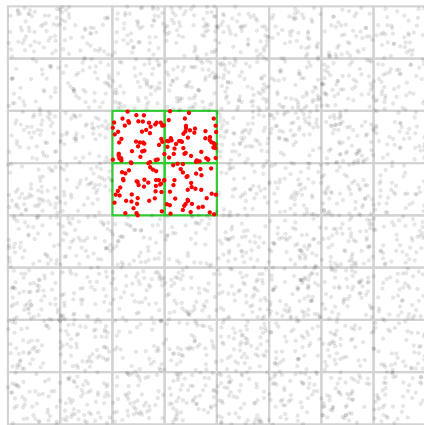
Summarize the algorithm (so far) and the associated cost.

## Barnes-Hut: Next Revised Cost Estimate

Summarize the algorithm (so far) and the associated cost.



## Barnes-Hut: Putting Multipole Expansions to Work



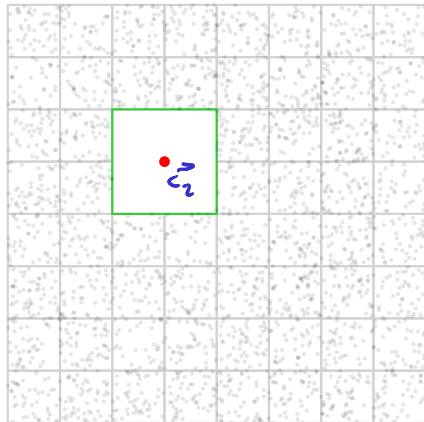
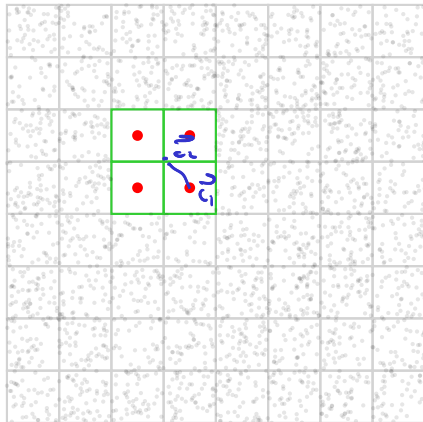
(Figure following G. Martinsson)

How could this process be sped up?

## Barnes-Hut: Clumps of Boxes?

**Observation:** The amount of work does not really decrease as we go up the tree: Fewer boxes, but more particles in each of them.  
But we already compute multipoles to summarize lower-level boxes. . .

## Barnes-Hut: Putting Multipole Expansions to Work



(Figure following G. Martinsson)

To get a new 'big' multipole from a 'small' multipole, we need a new mathematical tool.

$$(y - c_1)^{\frac{3}{2}}$$

$$(y - c_2)^{\frac{3}{2}}$$