TODAY:

- Barnes-Hut
- Fast Multipole

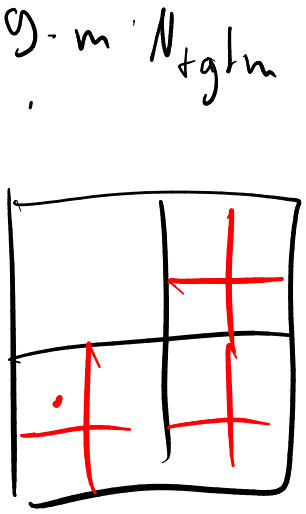
$A x \to b$

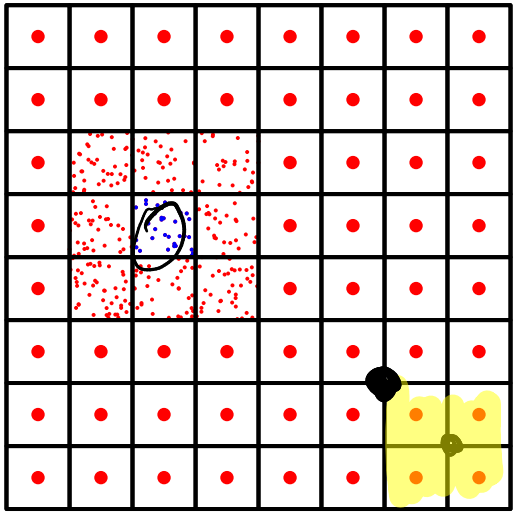
- Direct solver for interaction matrices

$b \to A^{-1} b$

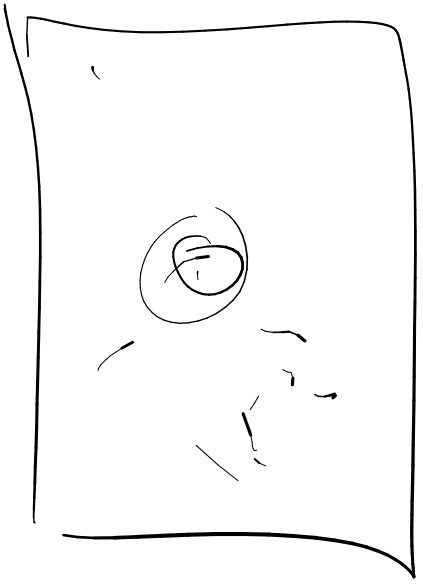
Project submission logistics

Barnes-Hut: Putting Multipole Expansions to Work





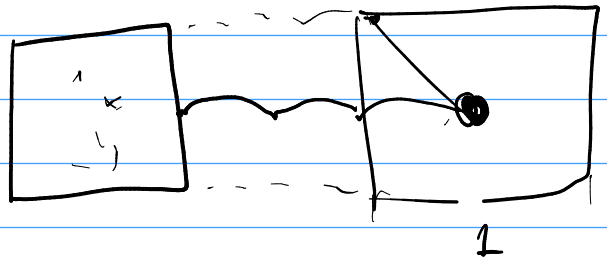
(Figure credit: G. Martinsson, Boulder)



With this computational outline, what's the accuracy?

Multipole error estimate; $\left(\frac{df_s}{d_{ct}}\right)^{p+1}$

Local error estimate; $\left(\frac{df_t}{d_{cs}}\right)^{p+1}$

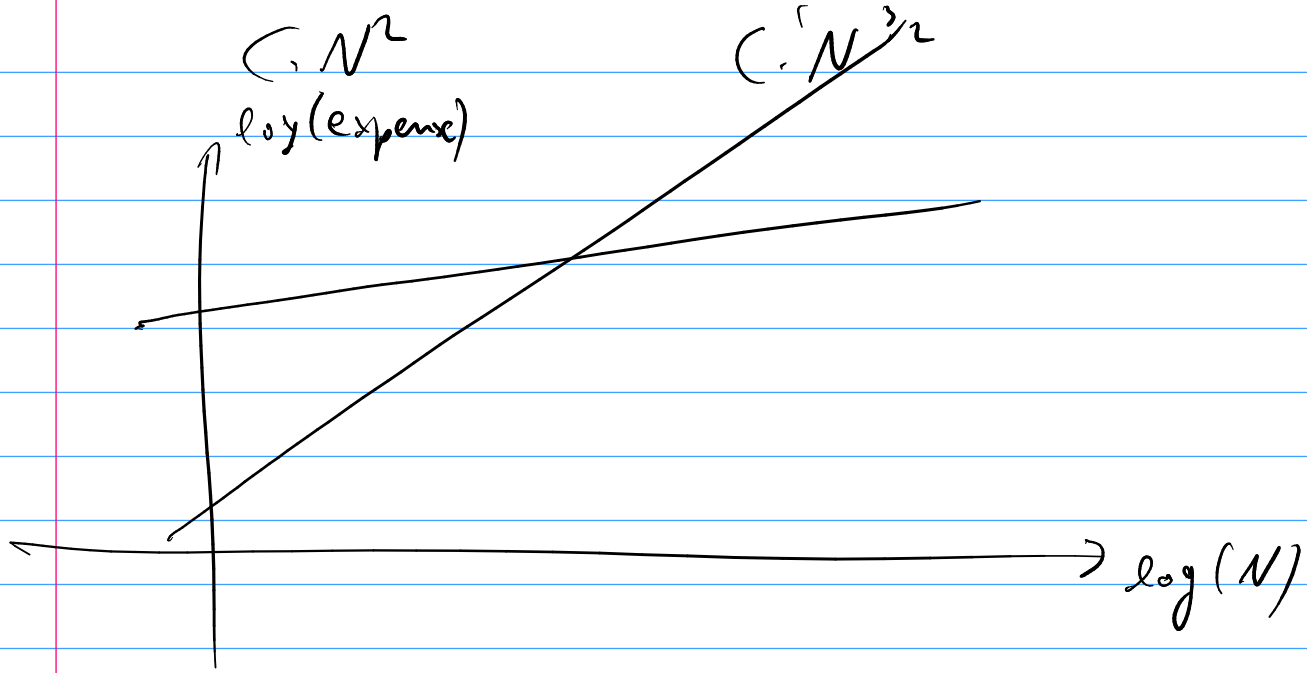


$df_s = \frac{\sqrt{2}}{2}$

$d_{ct} = \frac{3}{2}$

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

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


$C \cdot N^2$
$C \cdot N^{3/2}$
log(expense)
log(N)

$N \cdot \frac{N}{m}$	Evaluate pdle
	K

N : # particles

m : # particles per box

Barnes-Hut (single-level): Computational Cost

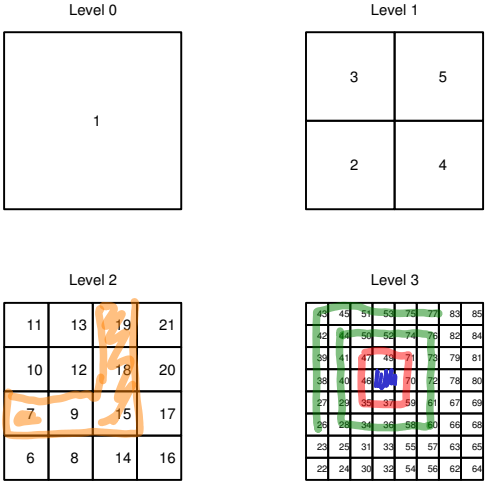
What's the cost of this algorithm?

Barnes-Hut: Putting Multipole Expansions to Work

L levels

$\Rightarrow 4^L$ boxes

$L \approx \log_4 N$



makes sense for $O(1)$ particles per box where $O(1) \approx 30$

$27 = 6^2 - 3^2$ source boxes on that level

(Figure credit: G. Martinsson, Boulder)

How many levels?

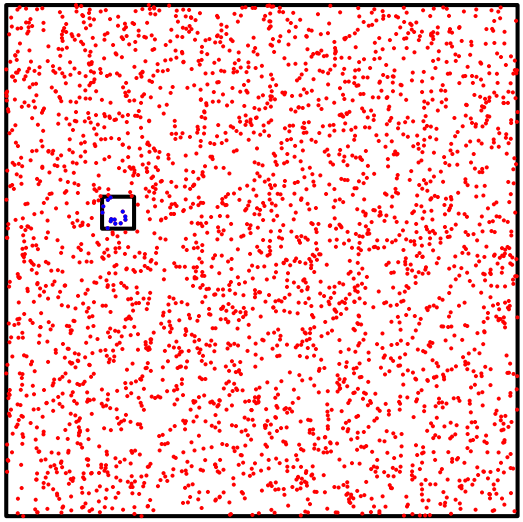
Forming multipoles

	How many	Individual cost	
Level L	N/m	mk	$\to O(N)$
Level $L-1$	$N/m \cdot \frac{1}{4}$	$4mk$	
Level $L-2$	$N/m \cdot \frac{1}{4^2}$	4^2	
Level 1			

Forming all multipoles: $O(N \log N)$

Evaluating all mpoles: $27 \cdot L \cdot \frac{N}{m}$

Barnes-Hut: Putting Multipole Expansions to Work

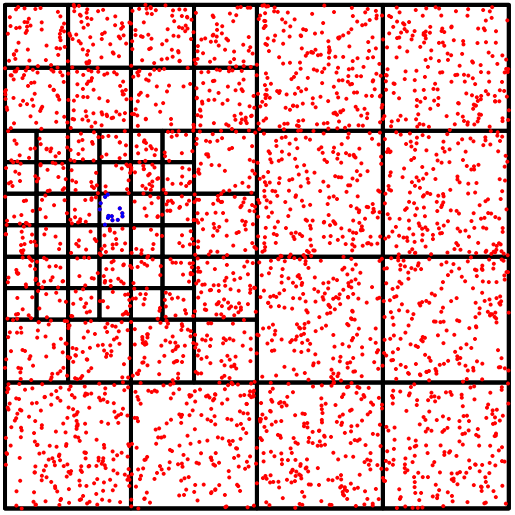


(Figure credit: G. Martinsson, Boulder)

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?

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

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)

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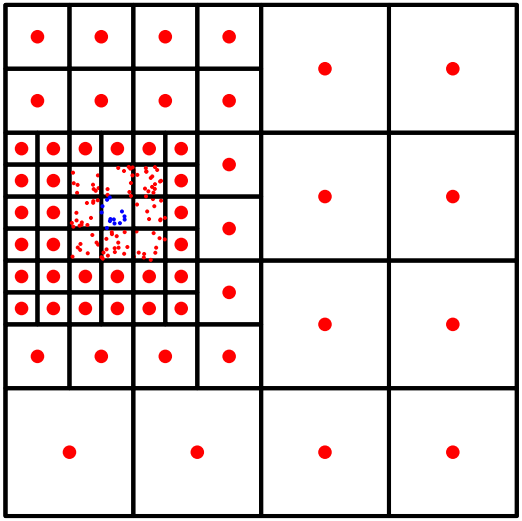

(Figure credit: G. Martinsson, Boulder)

What properties do these boxes have?

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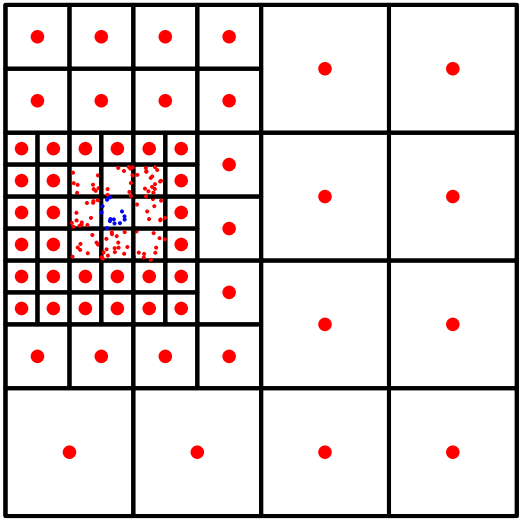

(Figure credit: G. Martinsson, Boulder)

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

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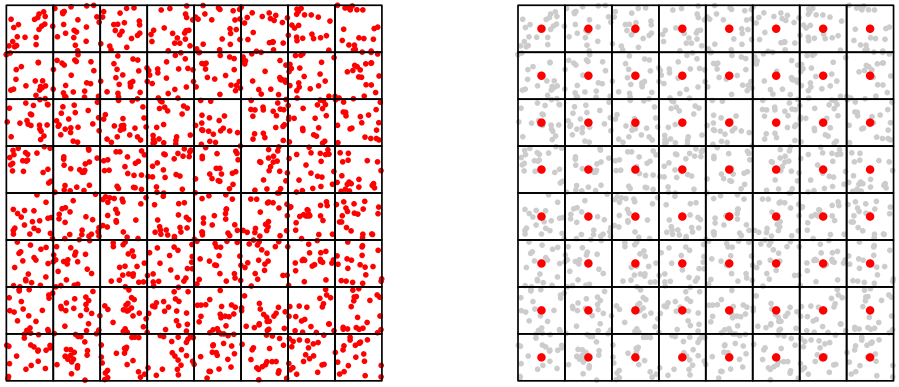
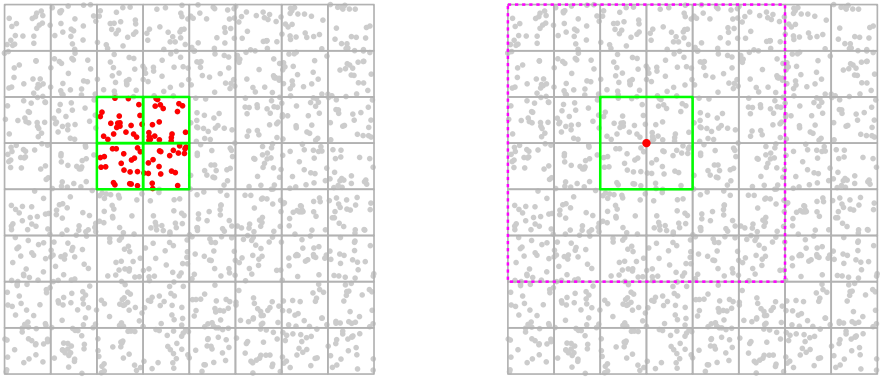


(Figure credit: G. Martinsson, Boulder)

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

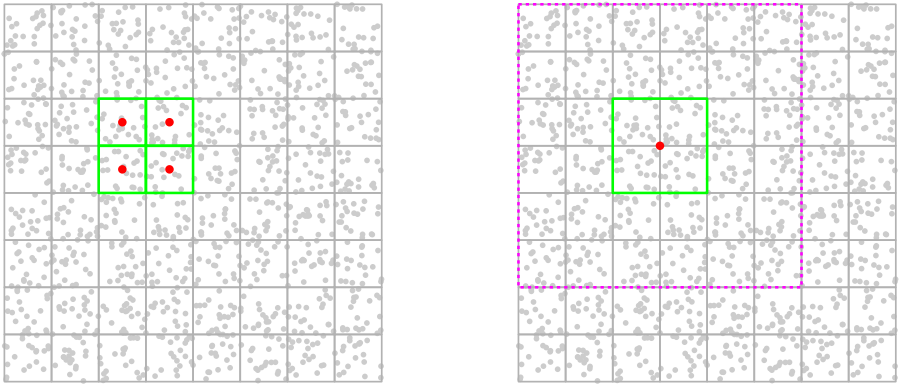
Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

How could this process be sped up?

Barnes-Hut: Putting Multipole Expansions to Work

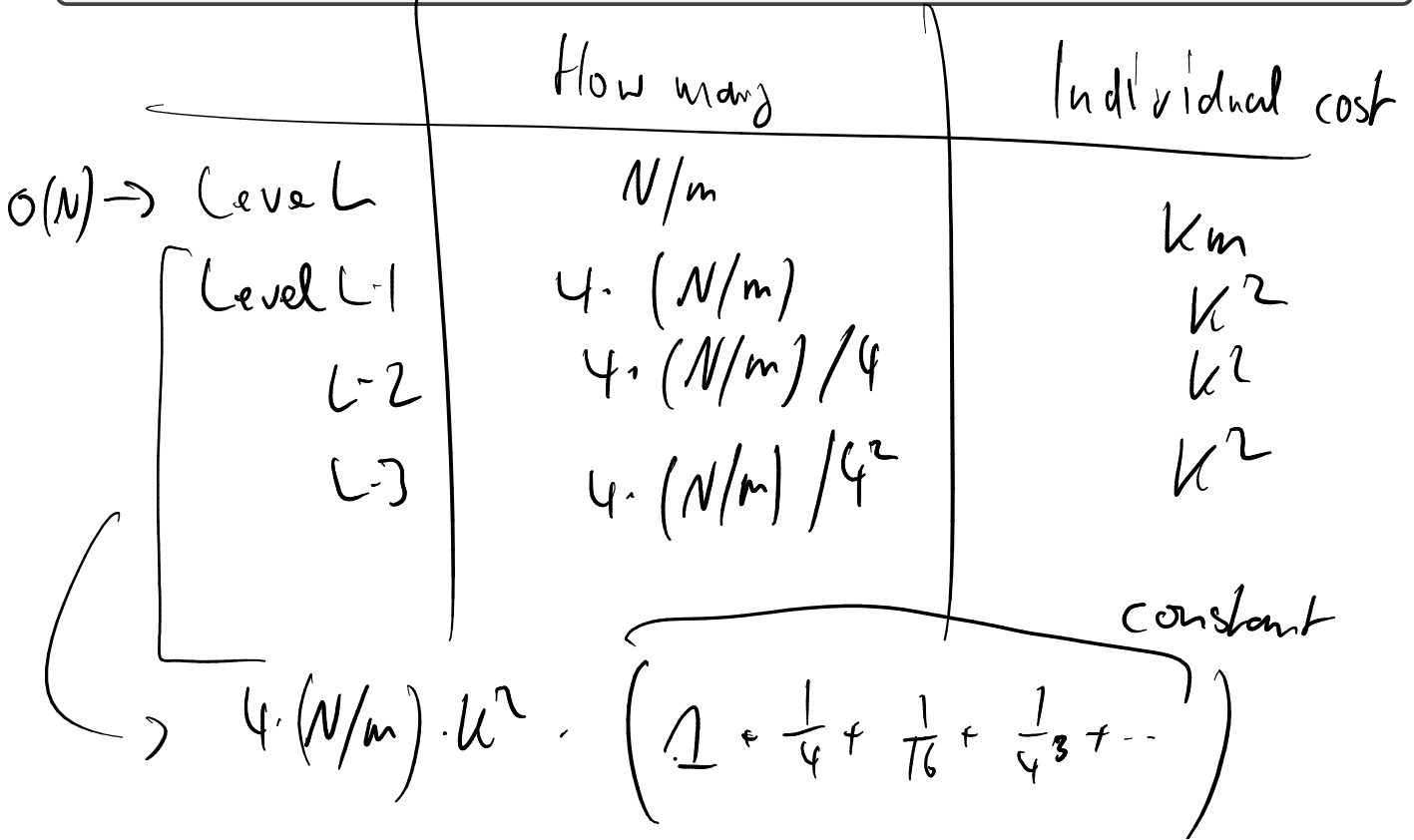


(Figure credit: G. Martinsson, Boulder)

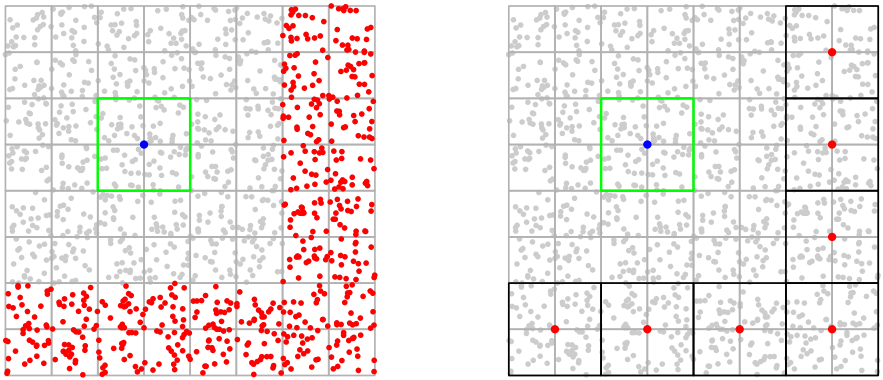
To get a new 'big' multipole from a 'small' multipole, we need a new mathematical tool.

Cost of Multi-Level Barnes-Hut

Summarize the cost of the final algorithm (with upward translation)



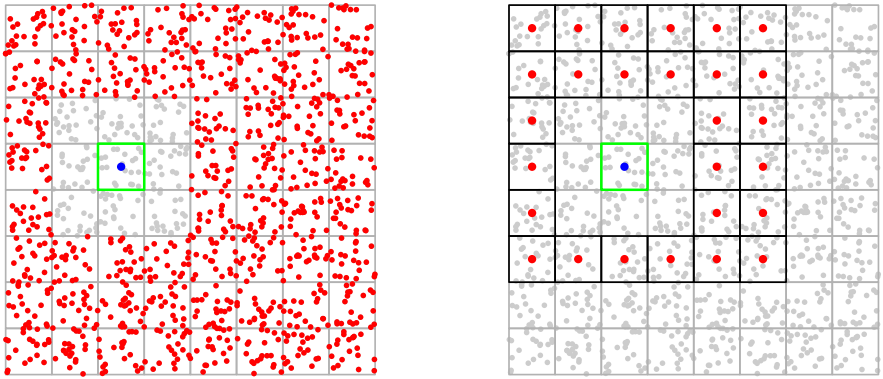
Using Multipole-to-Local



(Figure credit: G. Martinsson, Boulder)

Come up with an algorithm that computes the interaction in the figure.

Using Multipole-to-Local



(Figure credit: G. Martinsson, Boulder)

Assuming we retain information from the previous level, how can we obtain a valid local expansion on the target box?

Define 'Interaction List'

For a box b, the interaction list I_b consists of all boxes b' so that

The Fast Multipole Method ('FMM')

Upward pass

1. Build tree
2. Compute interaction lists
3. Compute lowest-level multipoles from sources
4. Loop over levels $\ell = L - 1, \ldots, 2$:
   (a) Compute multipoles at level ℓ by mp $\rightarrow$ mp

Downward pass

1. Loop over levels $\ell = 2, 3, \ldots, L - 1$:
   (a) Loop over boxes b on level ℓ :
      i. Add contrib from I_b to local expansion by mp $\rightarrow$ loc
      ii. Add contrib from parent to local exp by loc $\rightarrow$ loc
2. Evaluate local expansion and direct contrib from 9 neighbors.

Overall algorithm: Now $O(N)$ complexity.