Announcements:

- hw2 due Wed night
- back in person on Thu

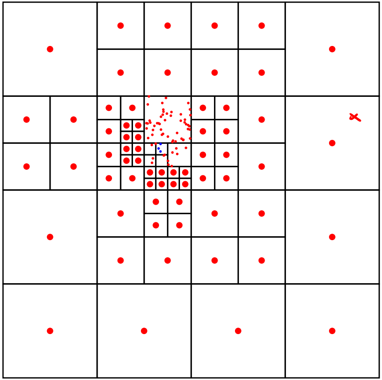
Goals:

- cost of BH
  - cost of mpole eval.
- avoid redundant mpole formation
- reduce cost mpole eval
  → FMM

Review:

BH, accuracy

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 : distance between centers
d : # dimensions

$$\left(\frac{d(c, f.s)}{d(c, c.t)}\right)^{k+1}$$

$$\in \left(\frac{r_s\sqrt{d}}{R - r_t}\right)^{k+1}$$

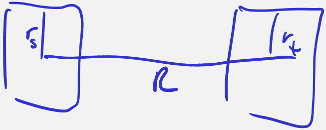
Barnes-Hut: Well-separated-ness

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

convergent iff: $\sqrt{2}\, r_s < R - r_t$ (*)

well-sep: $R \geq 3 \max(r_s, r_t)$

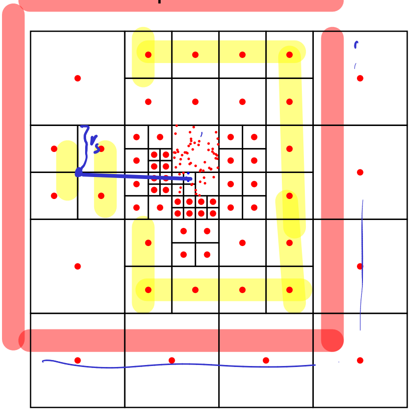
$(*) \iff (r_t + \sqrt{2}\, r_s) < R$



MAC

Barnes-Hut: Revised Cost Estimate

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



$3\max(r_s, r_t) < R$

at same level & w.-s.:

$O(1)$?

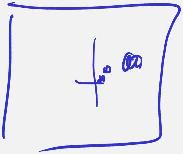
→ constant

→ yes, ∃ constant!

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

Barnes-Hut: Revised Cost Estimate

- L : # levels
- N : # particles
- K : # terms in an expansion
- m : # particles/box $= O(1)$
- " $\Rightarrow$ " $L = O(\log(N))$



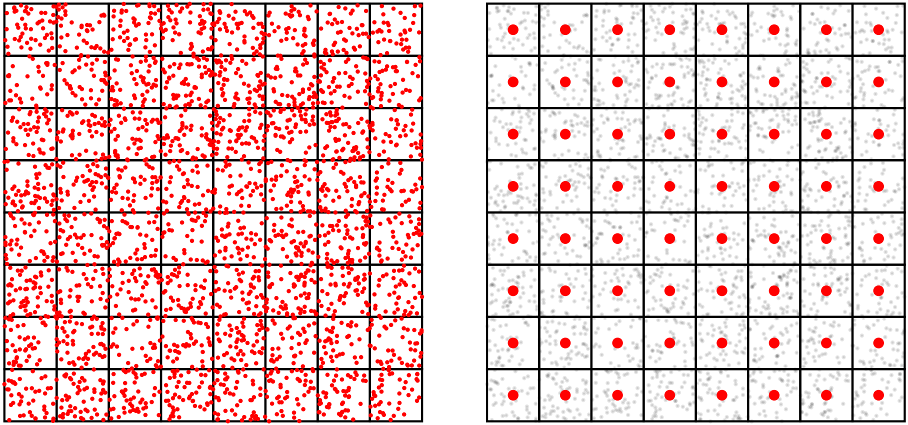
direct eval

- For near interactions: consider sum of number of near neighbors across all boxes
  That: $\le 9 \cdot \#$ boxes
  "on average" $\le 9 \cdot m = O(1)$

mpole eval

- For each level tree, there are at most a const. number of well-sep. boxes : C
  eval cost: $C \cdot L \cdot K = C \cdot K \cdot \log(N)$ per target box

Barnes-Hut: Next Revised Cost Estimate



(Figure following G. Martinsson)

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

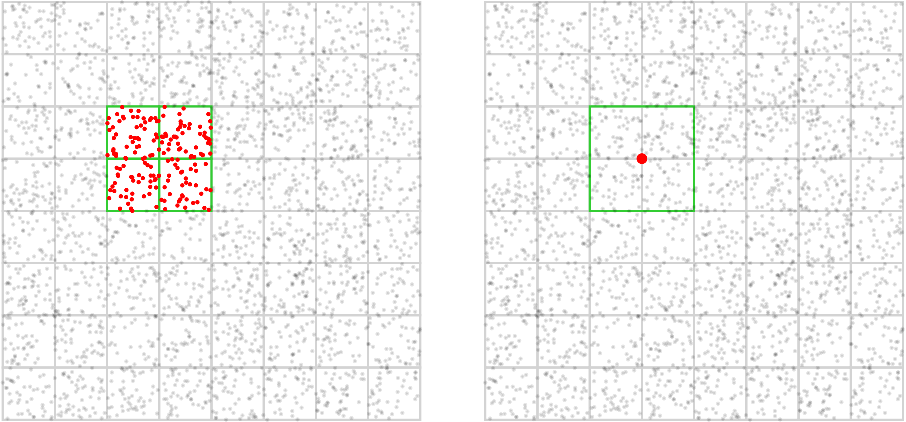
Barnes-Hut: Next Revised Cost Estimate

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

	How often	Cost	Total
Compute mpoles	$N \cdot L$	K	$KN\log(N)$
Eval mpoles	$C \cdot L \cdot (N/m)$	K	$CK\frac{N}{m}\log(N)$
Close interactions	$9(N/m)$	m^2	$9Nm$

$$\rightsquigarrow O(N \log N)$$

Barnes-Hut: Putting Multipole Expansions to Work



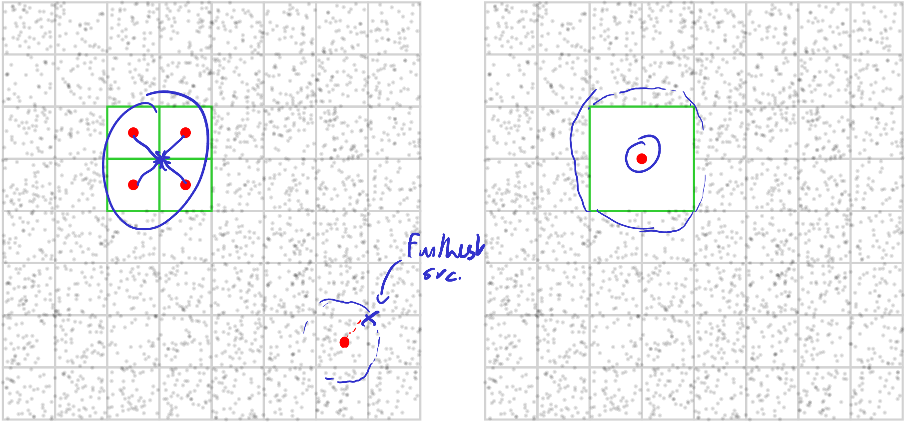
(Figure following G. Martinsson)

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.

$$\left(\frac{d(c, f.s.)}{d(c, c.t.)}\right) < 1$$

Barnes-Hut: Translations

Questions:

- How do you do it?
- What's the convergence behavior?
- What error do you introduce?
- What's the cost?

→ HW

Bounding the cost for a translation?

$$\underset{\substack{\uparrow \\ k\times k}}{A}\ \underset{\substack{\uparrow \\ k}}{\vec{\mu}_{c_1}} = \underset{\substack{\uparrow \\ k}}{\vec{\mu}_{c_2}}$$

$O(k^2)$ cost for a translation (worst-case)

Cost of Multi-Level Barnes-Hut

Compute mpoles:

Level	what	Cost	How many
L	src → mpoles	mK	(N/m)
$L-1$	mpole → mpole	K^2	$(N/m)/4$
$L-2$	mpole → mpole	K^2	$(N/m)/16$
⋮	⋮		⋮
0	mpole → mpole	K^2	

geom series

$$O(KN) + O(K^2 N)$$

$$= O(N)$$

Cost of Multi-Level Barnes-Hut: Observations

Observation: Multipole evaluation remains as the single most costly bit of this algorithm. *Fix?*

Idea: Exploit the tree structure also in performing this step.
If 'upward' translation of multipoles helped earlier, maybe 'downward' translation of *local* expansions can help now.

Outline

Introduction

Dense Matrices and Computation

Tools for Low-Rank Linear Algebra

Rank and Smoothness

Near and Far: Separating out High-Rank Interactions
- Ewald Summation
- Barnes-Hut
- Fast Mutipole
- Direct Solvers
- The Butterfly Factorization

Outlook: Building a Fast PDE Solver

Going Infinite: Integral Operators and Functional Analysis

Singular Integrals and Potential Theory

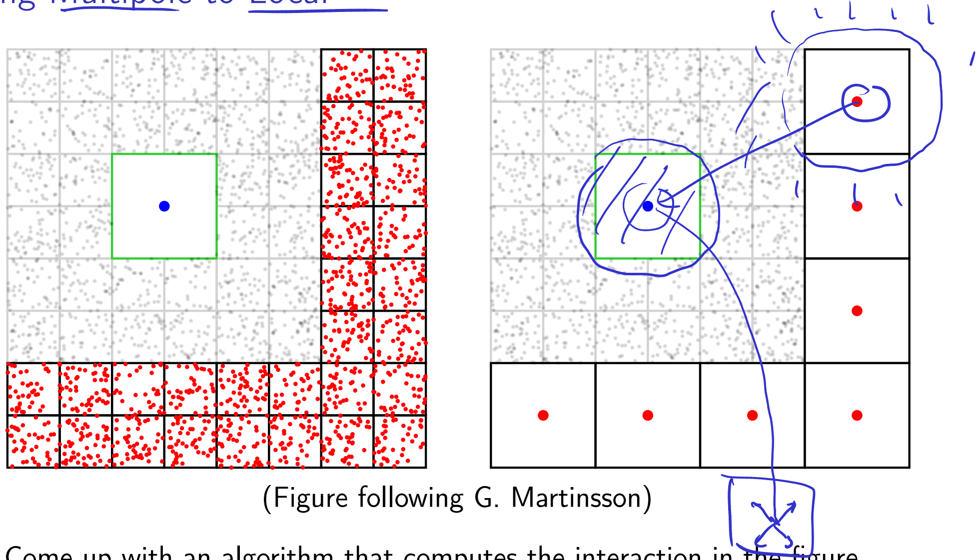
Boundary Value Problems

Back from Infinity: Discretization

Computing Integrals: Approaches to Quadrature

Going General: More PDEs

Using Multipole-to-Local



(Figure following G. Martinsson)

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

Using Multipole-to-Local

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