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

Goals:
- BH / FMM

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

\[ G = \sigma G + (1 - \sigma) G \]
\[
\frac{\sigma}{CR} \quad \frac{SR}{SR}
\]

\[ \sigma = O(1/x^4) \quad (x \to 0) \]
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

\[ \ddot{u} = A \dot{q} \]

\[ A_{ij} = \log(||x_i - x_j||_{2}) \]

\[ A_{ii} = 0 \]
Barnes-Hut: Putting Multipole Expansions to Work

(Figure following G. Martinsson)
Barnes-Hut: Putting Multipole Expansions to Work

(Figure following G. Martinsson)
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, f.s.) = \sqrt{2}r

d(c, c.t.) = 3r
Barnes-Hut: Accuracy

With this computational outline, what’s the accuracy?

\[
\varepsilon \leq \left( \frac{d(c, f.s.)}{d(c, c.f.)} \right)^{k+1}
\leq \left( \frac{\sqrt{2} \, k}{3 \, k} \right)^{k+1}
\]

**Obs 1:** Expn order gives accuracy

**Obs 2:** \( n \Omega : \left( \frac{\sqrt{d}}{3} \right)^{k+1} \)

Q: Does this get better or worse as dimension increases?
Barnes-Hut (Single-Level): Computational Cost

What's the cost of this algorithm?

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
<th>How often</th>
<th>Cost (K)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Compute impole</td>
<td>$N/m$</td>
<td>$Km$</td>
<td>$NK$</td>
</tr>
<tr>
<td>2</td>
<td>Eval. impoles</td>
<td>$N_{tqfs} \cdot N/m$</td>
<td>$K$</td>
<td>$N^K/m$</td>
</tr>
<tr>
<td>3</td>
<td>9 close boxes</td>
<td>$9(N/m \text{ boxes})$</td>
<td>$m^2$</td>
<td>$9Nm$</td>
</tr>
</tbody>
</table>

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)
How many levels?

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

$Q = d(\text{source box center, target box center})$

$$\left( \frac{d(\text{source, f.s.})}{d(\text{source, c.t.})} \right)^{4/3} \leq \left( \frac{r_s \sqrt{2}}{Q - r_t} \right)^{4/3}$$

Towards MAC ("multipole acceptance criterion")
Barnes-Hut: Well-separated-ness

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

Convergent iff \( r_5 \sqrt{2} < R - r_c \) \((*)\)

Convergent if \( R \geq 3 \max (r_t, r_s) \) \((***)\)

\((*) \iff \ (r_c + \sqrt{2} r_5) < R\)

\((***) \implies (*)\)

\((***) \) as MAC: “well-separated”
Barnes-Hut: Revised Cost Estimate

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?