

# Parallel Multipole Methods

Paul Beckman, Mariya Savinov

NYU Courant

May 2, 2022

# Motivating Problem

# Motivating Problem

- Consider a collection of interacting particles with a potential

## Motivating Problem

- Consider a collection of interacting particles with a potential
- **Total potential** at a point  $x$  due to **particles**  $x_j$  with **charges**  $q_j$  is

$$u(x) = \sum_{j=1}^n \frac{q_j}{|x - x_j|} = \sum_{j=1}^n q_j \phi(x - x_j)$$

## Motivating Problem

- Consider a collection of interacting particles with a potential
- **Total potential** at a point  $x$  due to **particles**  $x_j$  with **charges**  $q_j$  is

$$u(x) = \sum_{j=1}^n \frac{q_j}{|x - x_j|} = \sum_{j=1}^n q_j \phi(x - x_j)$$

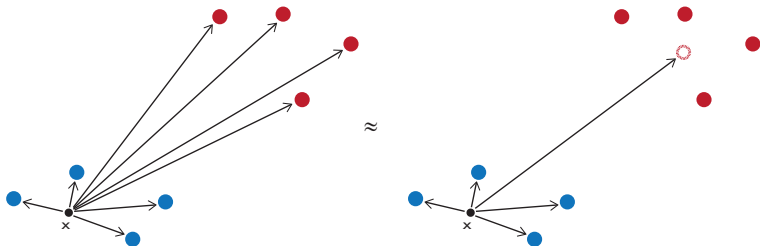
- Separate sum into **near-field** and **far-field** contributions

## Motivating Problem

- Consider a collection of interacting particles with a potential
- Total potential** at a point  $x$  due to **particles**  $x_j$  with **charges**  $q_j$  is

$$u(x) = \sum_{j=1}^n \frac{q_j}{|x - x_j|} = \sum_{j=1}^n q_j \phi(x - x_j)$$

- Separate sum into **near-field** and **far-field** contributions
  - Take *aggregate* effect of far-field charges via **Taylor series expansion**



# Barnes-Hut Tree Code: Taylor Expansion

## Barnes-Hut Tree Code: Taylor Expansion

- Use **Taylor series expansion** of  $\phi$  for small  $\delta = \frac{x_j - x^*}{x^* - y}$ :

$$\begin{aligned}\phi(x_j - y) &= \phi(x^* - y)\phi(1 + \delta) \\ &\approx \phi(x^* - y) \left[ \sum_{m=0}^p \frac{\phi^{(m)}(1)}{m!} \delta^m + O(\delta^{p+1}) \right] \\ &= \sum_{m=0}^p a_m(x_j - x^*) S_m(x^* - y) + O(\delta^{p+1})\end{aligned}$$



## Barnes-Hut Tree Code: Taylor Expansion

- Use **Taylor series expansion** of  $\phi$  for small  $\delta = \frac{x_j - x^*}{x^* - y}$ :

$$\begin{aligned}\phi(x_j - y) &= \phi(x^* - y)\phi(1 + \delta) \\ &\approx \phi(x^* - y) \left[ \sum_{m=0}^p \frac{\phi^{(m)}(1)}{m!} \delta^m + O(\delta^{p+1}) \right] \\ &= \sum_{m=0}^p a_m(x_j - x^*) S_m(x^* - y) + O(\delta^{p+1})\end{aligned}$$

- For a set of points  $x_j$ , potential contribution can be approximated:

$$\sum_{j \in \text{far-field}} q_j \phi(x_j - y) \approx \sum_{m=0}^p \underbrace{\left[ \sum_{j \in \text{far-field}} q_j a_m(x_j - x^*) \right]}_{\text{weight } w} S_m(x^* - y) + O(\delta^{p+1})$$

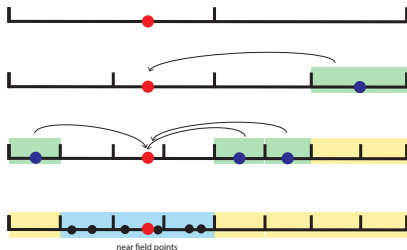
# Barnes-Hut Tree Code: Interaction List

## Barnes-Hut Tree Code: Interaction List

- compute terms involving far-field cells *not included at higher levels*

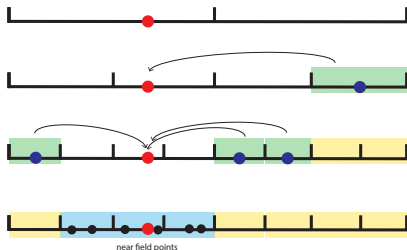
# Barnes-Hut Tree Code: Interaction List

- compute terms involving far-field cells *not included at higher levels*



# Barnes-Hut Tree Code: Interaction List

- compute terms involving far-field cells *not included at higher levels*

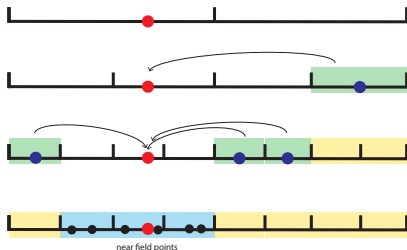


- Then for a point  $x$ , the potential is approximately

$$u(x) = \sum_{\ell=1}^{O(\log N)} \sum_{m=0}^p w_{\ell,k(\ell),m} S_m \left( x_{\ell,k(\ell)}^* - x \right) + O(2^{-p})$$

# Barnes-Hut Tree Code: Interaction List

- compute terms involving far-field cells *not included at higher levels*



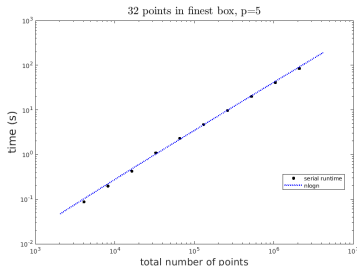
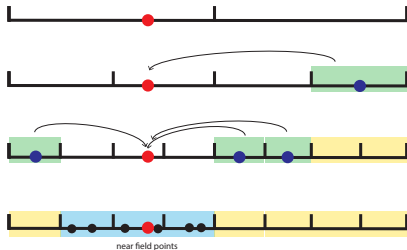
- Then for a point  $x$ , the potential is approximately

$$u(x) = \sum_{\ell=1}^{O(\log N)} \sum_{m=0}^p w_{\ell,k(\ell),m} S_m \left( x_{\ell,k(\ell)}^* - x \right) + O(2^{-p})$$

- For each box, compute weights  $w_{\ell,k,m} \rightarrow$  total cost  $O(N \log N)$

# Barnes-Hut Tree Code: Interaction List

- compute terms involving far-field cells *not included at higher levels*



- Then for a point  $x$ , the potential is approximately

$$u(x) = \sum_{\ell=1}^{O(\log N)} \sum_{m=0}^p w_{\ell,k(\ell),m} S_m \left( x_{\ell,k(\ell)}^* - x \right) + O(2^{-p})$$

- For each box, compute weights  $w_{\ell,k,m} \rightarrow$  total cost  $O(N \log N)$

# Parallelism



# Parallelism

- Parallelizing with OpenMP

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:*

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code
  - ▶ computing weights, adding near-field terms, and adding far-field terms

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code
  - ▶ computing weights, adding near-field terms, and adding far-field terms
  - ▶ *Potential Problem:* Loops of varying sizes, possibly large overhead

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code
  - ▶ computing weights, adding near-field terms, and adding far-field terms
  - ▶ *Potential Problem:* Loops of varying sizes, possibly large overhead
- **OPTION 2:** Distribute the work in the tree among threads



# Parallelism

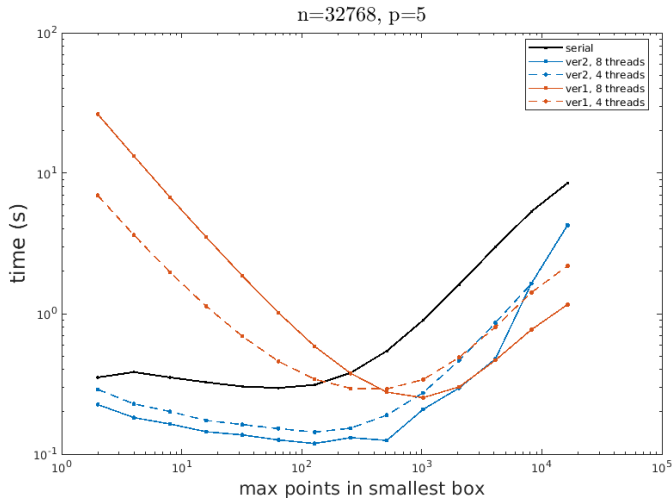
- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code
  - ▶ computing weights, adding near-field terms, and adding far-field terms
  - ▶ *Potential Problem:* Loops of varying sizes, possibly large overhead
- **OPTION 2:** Distribute the work in the tree among threads
  - ▶ At tree levels  $\ell < O(\log r)$  for  $r$  threads, open a new section

# Parallelism

- Parallelizing with OpenMP
  - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code
  - ▶ computing weights, adding near-field terms, and adding far-field terms
  - ▶ *Potential Problem:* Loops of varying sizes, possibly large overhead
- **OPTION 2:** Distribute the work in the tree among threads
  - ▶ At tree levels  $\ell < O(\log r)$  for  $r$  threads, open a new section
  - ▶ *Potential Problem:* Nested parallelism

# Results: Comparing Parallel Options

# Results: Comparing Parallel Options

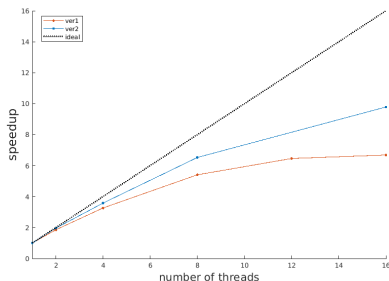
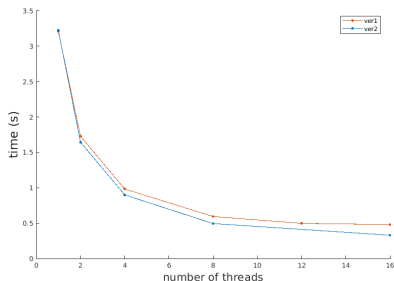


crack1e1: Intel Xeon E5630 (2.53 GHz)

# Results: Strong Scaling

# Results: Strong Scaling

$n = 32768$ , max points in box 2048, and  $p = 5$

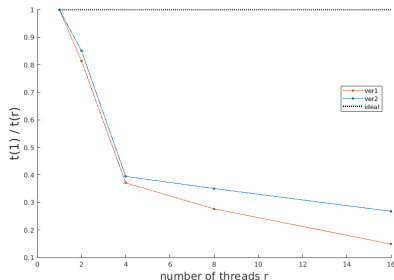
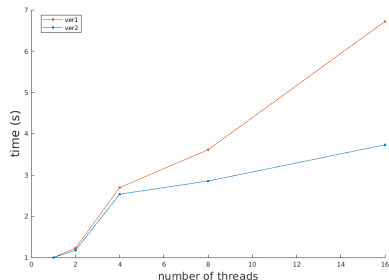


crunchy1: AMD Opteron 6272 (2.1 GHz)

# Results: Weak Scaling

# Results: Weak Scaling




$n = 8192 \cdot r$ , max points in box = 2048, and  $p = 5$



crunchy1: AMD Opteron 6272 (2.1 GHz)



# References

-  Josh Barnes and Piet Hut, *A hierarchical  $O(N\log N)$  force-calculation algorithm*, Nature **324** (1986), no. 6096, 446–449.
-  Long Chen, *Introduction to fast multipole methods*.
-  Leslie Greengard and Vladimir Rokhlin, *A fast algorithm for particle simulations*, Journal of computational physics **73** (1987), no. 2, 325–348.