

Parallel Fast Multipole

Paul Beckman, Mariya Savinov

NYU Courant

May 1, 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

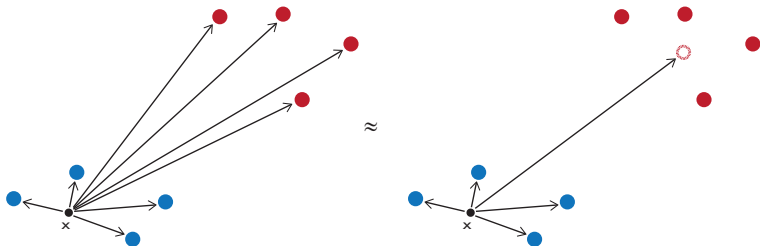
$$u(x) = \sum_{j=1}^n \frac{q_j}{|x - x_j|} = \sum_{j=1}^n q_j \phi(x - x_j)$$

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
 - Take *aggregate* effect of far-field charges via **Taylor series expansion**



Tree Algorithm by Barnes and Hut, complexity $O(N \log N)$

Tree Algorithm by Barnes and Hut, complexity $O(N \log N)$

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

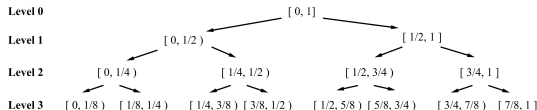
$$\sum_{j \in \text{far-field}} q_j \phi(x - x_j) \approx \sum_{m=0}^p \underbrace{\left[\sum_{j \in \text{far-field}} q_j a_m(x_j - x^*) \right]}_{\text{weight } m} S_m(x^* - x) + O(\delta^{p+1})$$

Tree Algorithm by Barnes and Hut, complexity $O(N \log N)$

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

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

- For N particles, partition $[0, 1]$ uniformly at $O(\log N)$ levels:

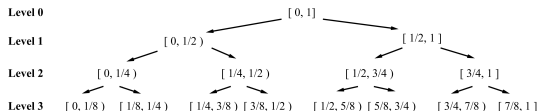


Tree Algorithm by Barnes and Hut, complexity $O(N \log N)$

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

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

- For N particles, partition $[0, 1]$ uniformly at $O(\log N)$ levels:



- For each $T_{\ell,k}$ cell, compute weights $w_{\ell,k,m}$. **COST?**

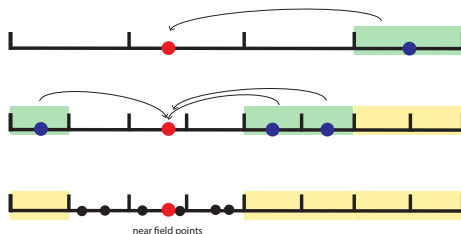
Tree Algorithm by Barnes and Hut: Interaction List

Tree Algorithm by Barnes and Hut: Interaction List

- At each level, only 'interact' with up to 3 far-field cells *not already included at higher levels*

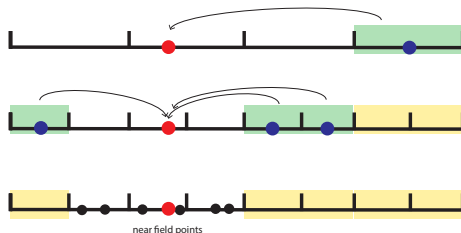
Tree Algorithm by Barnes and Hut: Interaction List

- At each level, only 'interact' with up to 3 far-field cells *not already included at higher levels*



Tree Algorithm by Barnes and Hut: Interaction List

- At each level, only 'interact' with up to 3 far-field cells *not already included at higher levels*

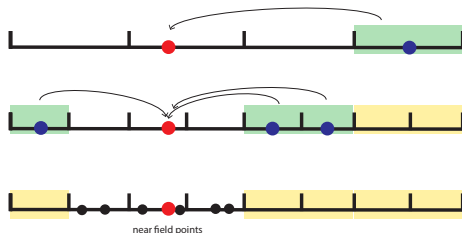


- Then for a point x , the potential is approximately **ACCURACY?**

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

Tree Algorithm by Barnes and Hut: Interaction List

- At each level, only 'interact' with up to 3 far-field cells *not already included at higher levels*



- Then for a point x , the potential is approximately **ACCURACY?**

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

- TOTAL COST?** Total cost is $O(N \log N)$

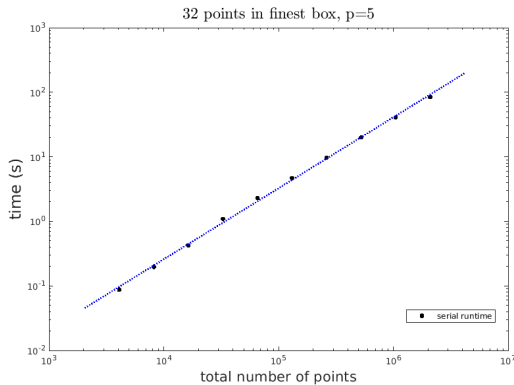
Serial implementation

Serial implementation

- Successfully implemented the serial code for the algorithm, making use of a tree data type

Serial implementation

- Successfully implemented the serial code for the algorithm, making use of a tree data type
- Confirmation of $O(N \log N)$ cost:



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

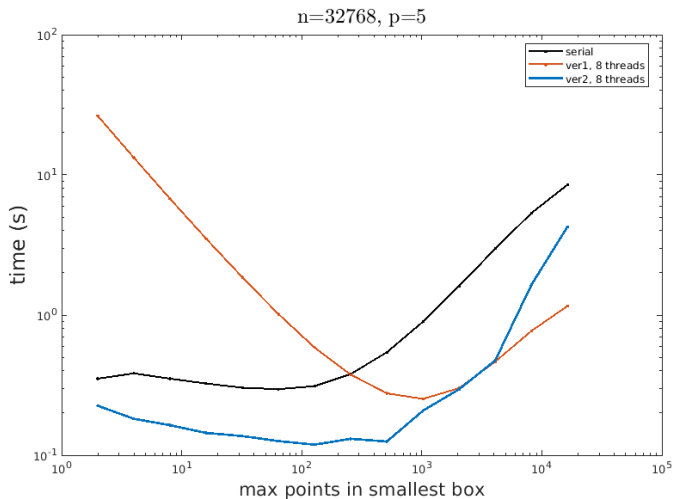
- Parallelizing with OpenMP
 - ▶ *Challenge:* Recursive tree code may prevent significant speedup
- Two options of how to parallelize
- **OPTION 1:** Parallelize the loops in the code
 - ▶ computing weights, adding near-field terms, and adding far-field terms
 - ▶ *Potential Problem:* Loops of varying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

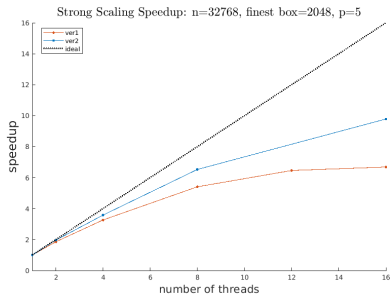
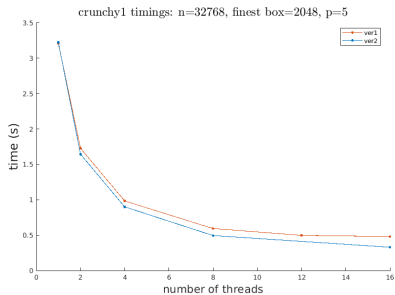
Results: Comparing Parallel Options

Results: Comparing Parallel Options



Results: Strong Scalability

Results: Strong Scalability



Results: Weak Scalability

Results: Weak Scalability

Starting with $n = 8192$, max pts = 512, and $p = 5$, as work doubles we double thread number p

Supplemental Slides

Approximating far-field

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

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

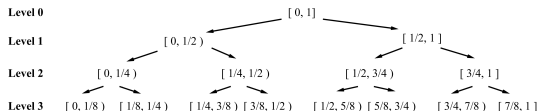
- Then potential from $x_j \in \text{far-field}$ is

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

- Accuracy depends on choice of x^* and thus size of $\delta = \frac{x_j - x^*}{x^* - x}$

Tree Algorithm by Barnes and Hut, complexity $O(N \log N)$

- For N particles, partition $[0, 1]$ uniformly at $O(\log N)$ levels:



- Let $T_{\ell,k}$ be the cell at level ℓ with index $k = 1 : 2^\ell$ with center $x_{\ell,k}^*$.
- Compute weight at each cell, total cost $O(N \log N)$

$$w_{\ell,k,m} = \sum_{x_j \in T_{\ell,k}} q_j a_m(x_j - x_{\ell,k}^*)$$

- For a point x : far-field components added at increasingly *coarse* levels

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

Interaction List

- At each level, only 'interact' with up to 3 far-field cells *not already included at higher levels*

