

# Parallel Multipole Methods

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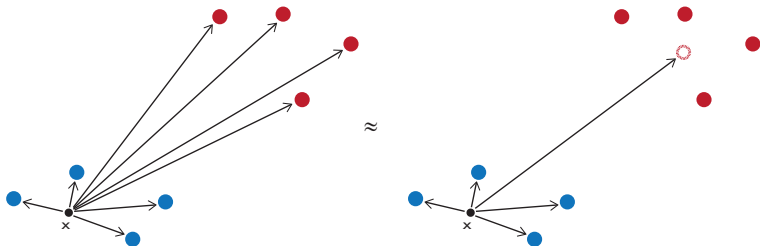
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  - Take *aggregate* effect of far-field charges via **Taylor series expansion**



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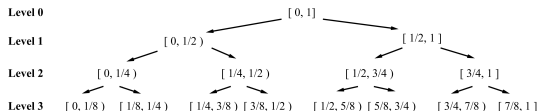


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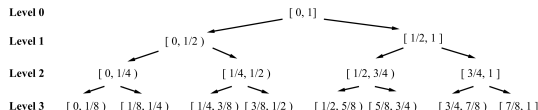


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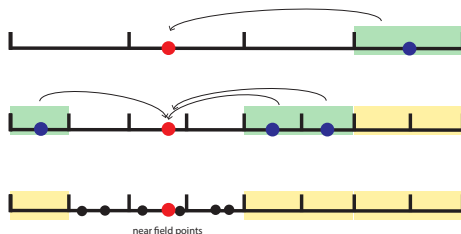
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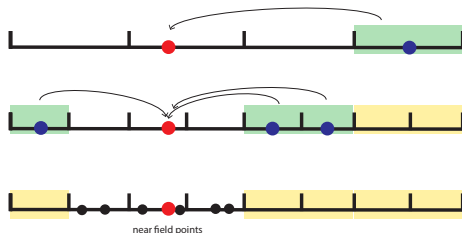
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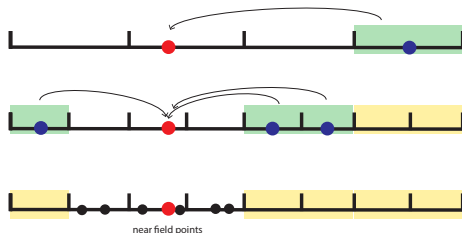


- Then for a point  $x$ , the potential is approximately

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

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- Total cost is  $O(N \log N)$

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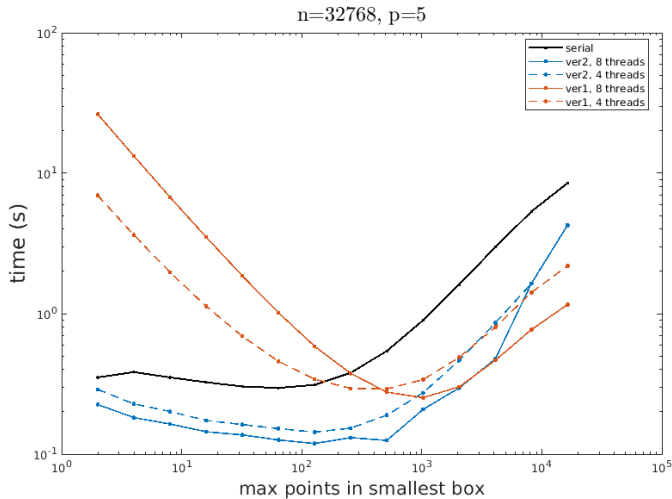
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  - ▶ *Potential Problem:* Nested parallelism

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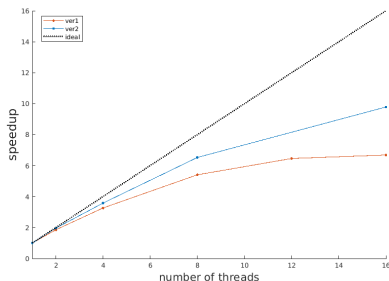
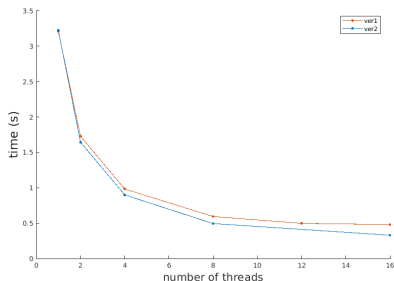


crack1e1: Intel Xeon E5630 (2.53 GHz)

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

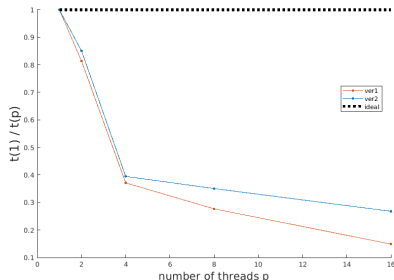
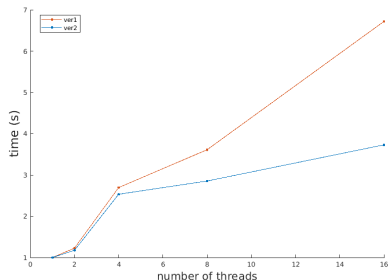


crunchy1: AMD Opteron 6272 (2.1 GHz)

# Results: Weak Scaling

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



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# Supplemental Slides

## Approximating far-field

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

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

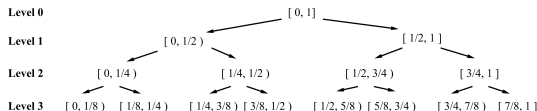
- Then potential from  $x_j \in \text{far-field}$  is

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

- 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  $\ell$  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

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