Implementation of the fast multipole method

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Consider evaluating all pairwise interactions between a given set of N electrically charged particles in two dimensions.

$$u_i = \sum_{j=1}^{N} G(\boldsymbol{x}_i, \boldsymbol{x}_j) q_j, \quad i = 1, 2, \ldots, N, \tag{1}$$

$\{\boldsymbol{x}_i\}_{i=1}^N$: a given set of point locations in a square Ω
$\{q_i\}_{i=1}^N$: a given set of corresponding sources
$\{u_i\}_{i=1}^N$: a set of potential values to be determined
$G(\boldsymbol{x}, \boldsymbol{y}) = \log(\boldsymbol{x} - \boldsymbol{y})$: kernel
Using $\mathbf{A}(i,j) = G(\boldsymbol{x}_i, \boldsymbol{x}_j), \mathbf{q}(i) = q_i$ and $\mathbf{u}(i) = u_i$, write (1) as a matrix vector multiplication:

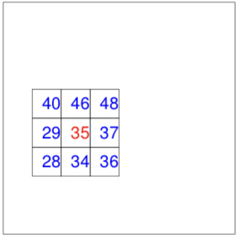
$$\mathbf{u} = \mathbf{Aq}$$

However, direct evaluation cost is $O(N^2)$.

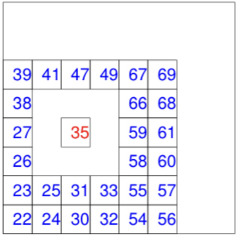
Review of FMM

To evaluate (1) in linear complexity, the fast multipole method (FMM) uses a multilevel technique, splitting the computational domain Ω into a tree of boxes. Denote the level to be $l = 0, 1, \ldots, L-1$, $l = 0$ denotes the root and $l = L-1$ denotes the leaf boxes. Given a box τ in the hierarchical tree, define the index vectors for box τ:

- **parent**: the box on the next coarsest level that contains τ.
- **children list** $\mathcal{L}_\tau^{\text{child}}$: the set contains the boxes whose parent is τ.
- **neighbor list** $\mathcal{L}_\tau^{\text{nei}}$: the set contains the boxes on the same level that directly touch τ
- **interaction list** $\mathcal{L}_\tau^{\text{int}}$: the set contains all boxes σ such that (1) σ and τ are on the same level, (2) σ and τ do not touch, and (3) the parents of σ and τ do touch.



For $\tau = 35$ (red), the neighbor list $\mathcal{L}_\tau^{\text{nei}}$ is shown in blue.



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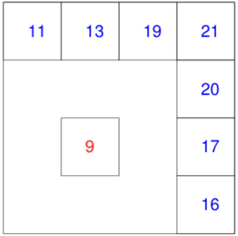


For $\tau = 9$ (red), the interaction list $\mathcal{L}_\tau^{\text{int}}$ is shown in blue.

Evaluating multipole expansions hierarchically.

- **Upward pass**: Compute the outgoing expansion of each box in a pass over all boxes, going from smaller boxes to larger ones.
  - For a leaf box, compute the expansion directly from the sources in the box: $\hat{\mathbf{q}}_\tau = \mathbf{T}^{\text{ofs}}_\tau \, \mathbf{q}(I_\tau)$
  - For a parent box, use the outgoing expansions of its children: $\hat{\mathbf{q}}_\tau = \sum_{\sigma \in \mathcal{L}^{\text{child}}_\tau} \mathbf{T}^{\text{ofo}}_{\tau,\sigma} \, \hat{\mathbf{q}}_\sigma$
- **Downward pass**: Compute the incoming expansion for every box in a pass over all boxes, going from larger boxes to smaller ones. For each box, combine the incoming expansion of its parent ν with the contributions from the outgoing expansions of all boxes in its interaction list:

$$\hat{\mathbf{u}}_\tau = \mathbf{T}^{\text{ifi}}_{\tau,\nu} \, \hat{\mathbf{u}}_\nu + \sum_{\sigma \in \mathcal{L}^{\text{int}}_\tau} \mathbf{T}^{\text{ifo}}_{\tau,\sigma} \, \hat{\mathbf{q}}_\sigma$$

- Compute the potential on every leaf by expanding its incoming potential and then adding the contributions from its near field via direct evaluation:

$$\mathbf{u}(I_\tau) = \mathbf{T}^{\text{tfi}}_\tau \, \hat{\mathbf{u}}_\tau + \mathbf{A}(I_\tau, I_\tau) \, \mathbf{q}(I_\tau) + \sum_{\sigma \in \mathcal{L}^{\text{nei}}_\tau} \mathbf{A}(I_\tau, I_\sigma) \, \mathbf{q}(I_\sigma)$$

Transition operator $\mathbf{T}^{\text{ofo}}_{\tau,\sigma}, \mathbf{T}^{\text{ifo}}_{\tau,\sigma}, \mathbf{T}^{\text{ifi}}_{\tau,\sigma} \in \mathbb{C}^{P \times P}$ are independent of $\{\boldsymbol{x}_i\}_{i=1}^N$. $\mathbf{T}^{\text{ofs}}_\tau \in \mathbb{C}^{P \times N_\tau}$ and $\mathbf{T}^{\text{tfi}}_\tau \in \mathbb{C}^{N_\tau \times P}$ are computed for each leaf box τ.

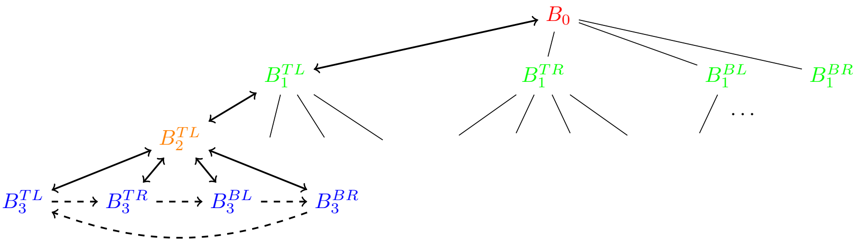
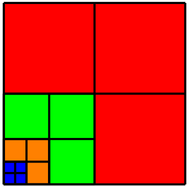


Figure 1: Diagram of the quadtree data structure. L=4.



- Step 1: Build quadtree data structure.
- Step 2: Build the parent, child, neighbor, interaction list
- Step 3: Build the translation operators $\mathbf{T}^{\text{ofo}}_{\tau,\sigma}, \mathbf{T}^{\text{ifo}}_{\tau,\sigma}, \mathbf{T}^{\text{ifi}}_{\tau,\sigma}$.
- Step 4: Sort the particles into leaf boxes.
- Step 5: Calculate the potential using FMM.

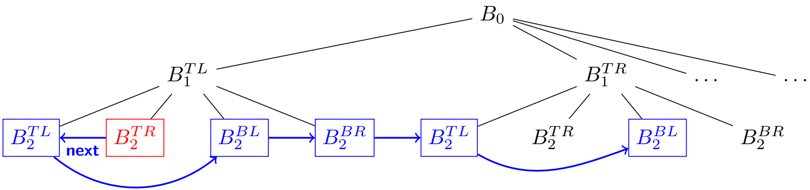
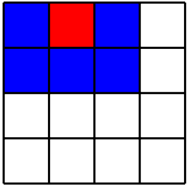


Figure 1: Linked list data structure for neighbor list for the red node (box).



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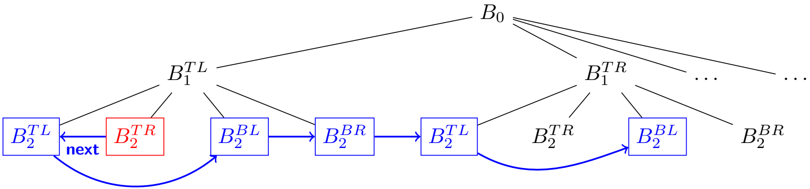
Implementation



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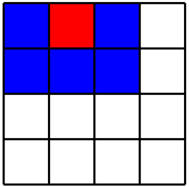

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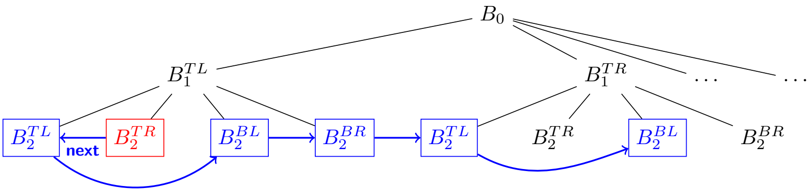

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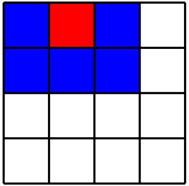

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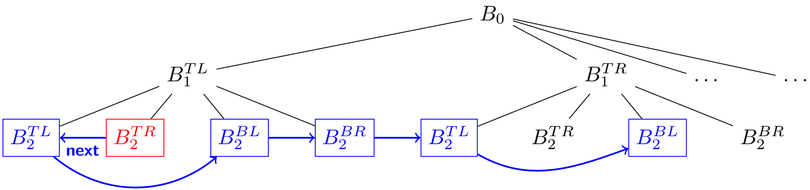

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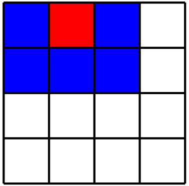

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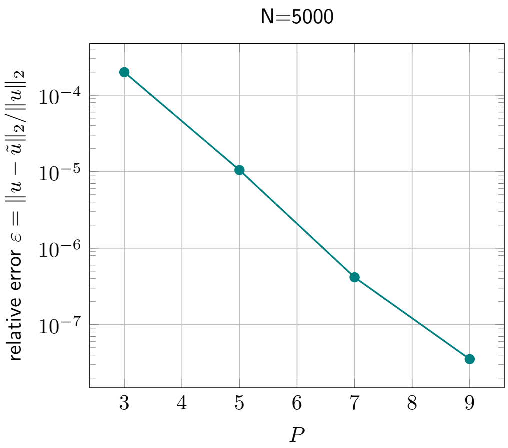
Set up

- Uniformly distributed particles. $\mathbf{x}_i$ are i.i.d. uniform random in $[0,1]^2$.
- Given ε, the length of the outgoing expansion length P is chosen such that

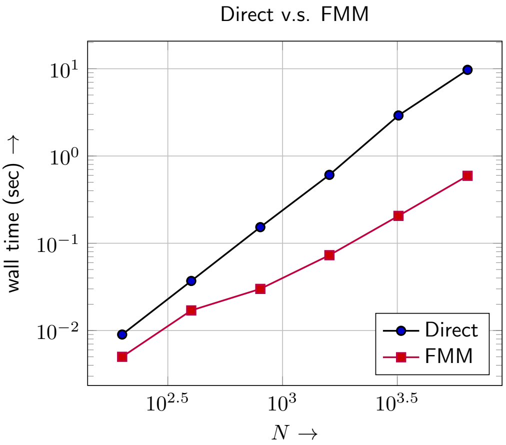
$$\varepsilon \sim \eta_{\text{2D}}^P, \quad \eta_{\text{2D}} = \frac{\sqrt{2}}{4-\sqrt{2}}.$$

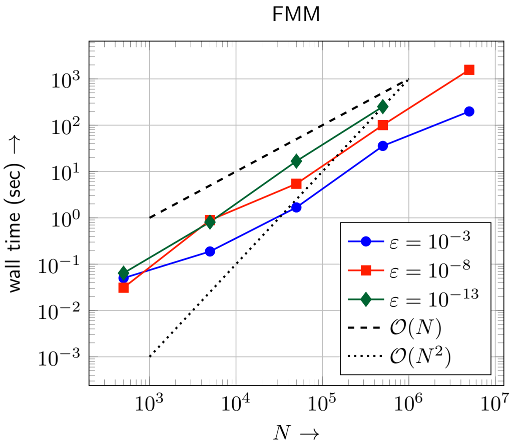
- The depth of the tree L is chosen such that each box contains roughly P number of particles,

$$4^{L-1} \approx N/P$$

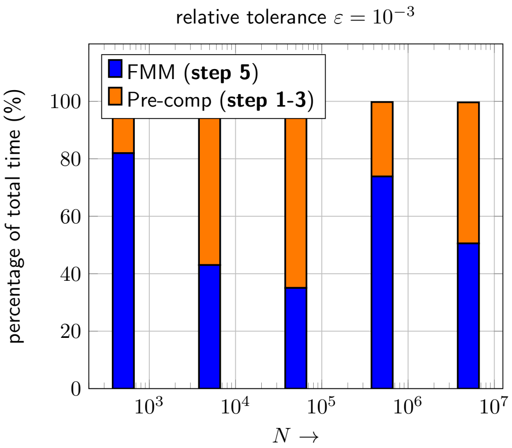


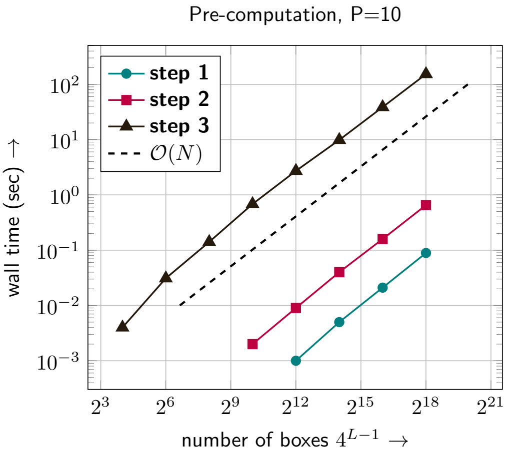
- The calculated P is larger than needed, e.g. for $\varepsilon = 10^{-4}$, $P = 15$.


Direct v.s. FMM
10^{1}
10^{0}
10^{-1}
10^{-2}
wall time (sec) →
$10^{2.5}$
10^{3}
$10^{3.5}$
$N \rightarrow$
Direct
FMM


FMM
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
wall time (sec) →
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
$N \rightarrow$
$\varepsilon = 10^{-3}$
$\varepsilon = 10^{-8}$
$\varepsilon = 10^{-13}$
$\mathcal{O}(N)$
$\mathcal{O}(N^2)$

Performance tests





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