CS601: Software Development for Scientific Computing

Autumn 2021

Week13:

Hierarchical Methods (FMM) and Sparse Matrices

Course Progress..

- Last week
  - Tree-based codes (hierarchical methods)
    - Barnes-Hut
    - Fast Multipole Method (FMM)

- This week
  - FMM
  - Sparse matrices and
  - PA4 discussion

FMM Algorithm

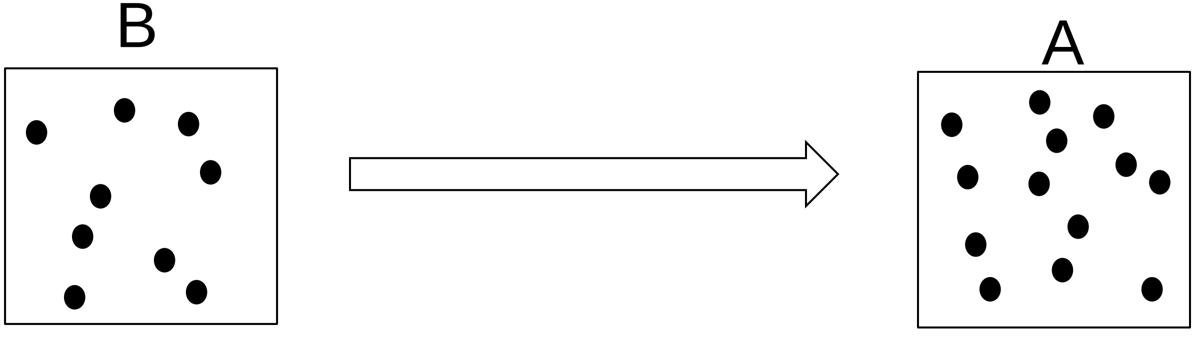
1. Build the quadtree containing all the points.
2. Traverse the quadtree from bottom to top, computing Outer(n) for each square n in the tree.
3. Traverse the quadtree from top to bottom, computing Inner(n) for each square in the tree.
4. For each leaf, add the contributions of nearest neighbors and particles in the leaf to Inner(n)

what is Outer(n) and Inner(n) ?

Well Separated Regions

- Compute the influence of all particles in source region (B) on every particle in target region (A)

  (assumption: A and B are well-separated)



- At each point p_i in A, compute potential:

$$\Phi(x_i, y_i) = \sum_{p_j \in B} m_i \log |p_i - p_j|$$

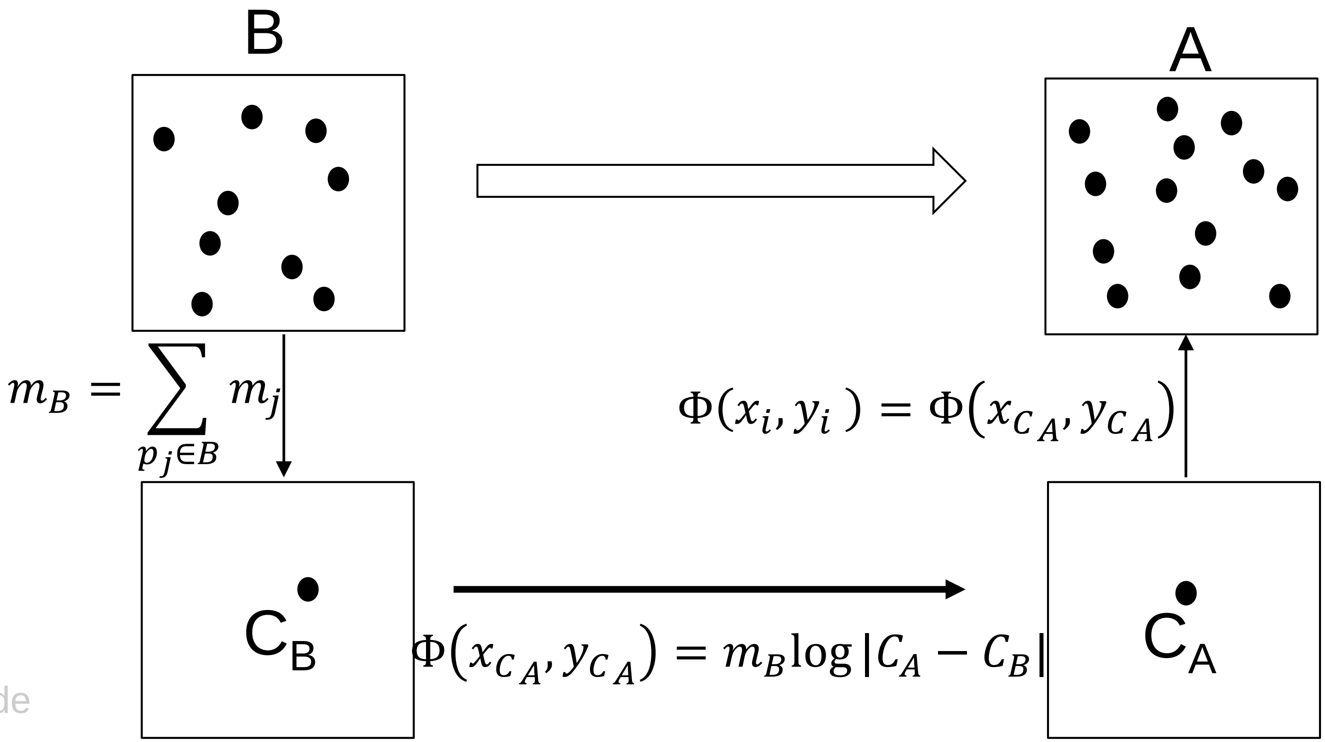
$$i = 1 \; to \; N_A, \qquad j = 1 \; to \; N_B$$

- Cost: $O(N_A N_B)$

Well Separated Regions

- Compute the influence of all particles in source region (B) on every particle in target region (A)

$$\Phi\left(x_{p_i}, y_{p_i}\right) = \sum_{p_j \in B} m_i \log|p_i - p_j| \;, p_i \in A$$



Applying the 3-step Approximation

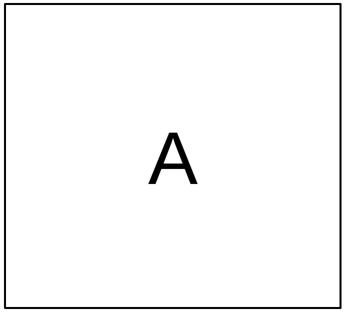
- In N-body simulation every point serves as source as well as target.

  How to identify source and target (boxes A and B in previous slide) i.e. well-separated regions?

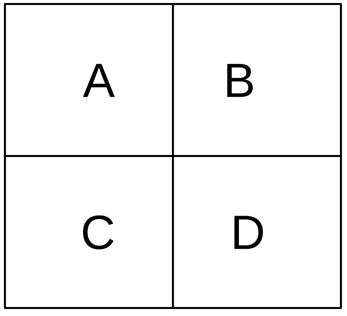
  Hierarchical decomposition

Hierarchical Decomposition

- *Level-0 decomposition*



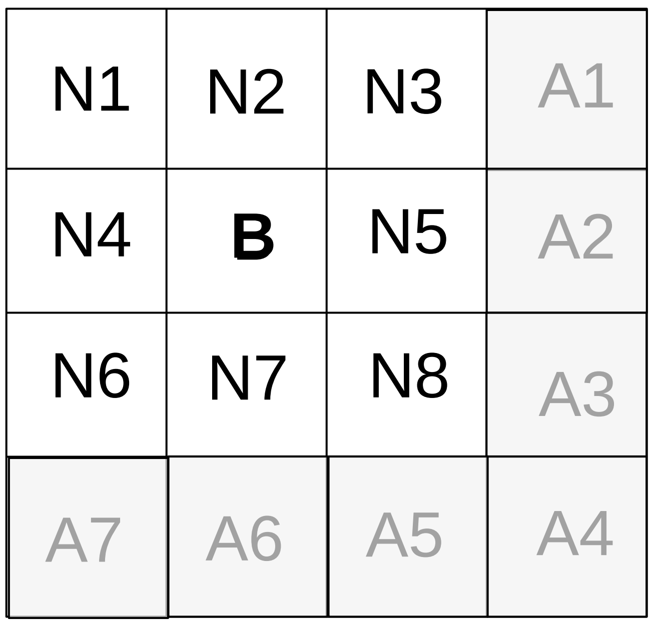
- *Level-1 decomposition*



No well-separated boxes

Hierarchical Decomposition

- *Level-2 decomposition*



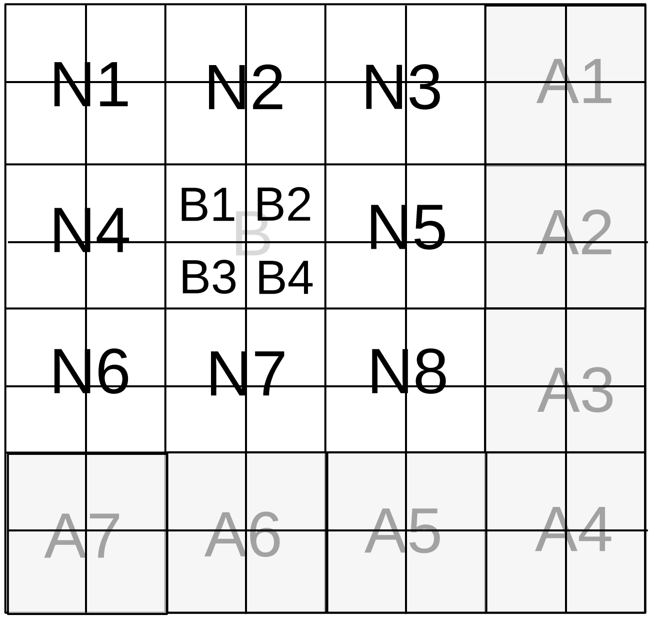
Well-separated from B

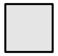
Can approximate the influence of points in `B` on points in `Ai` s

What do we do about **B**’s influence on Ni s?

Hierarchical Decomposition

- *Level-3 decomposition*

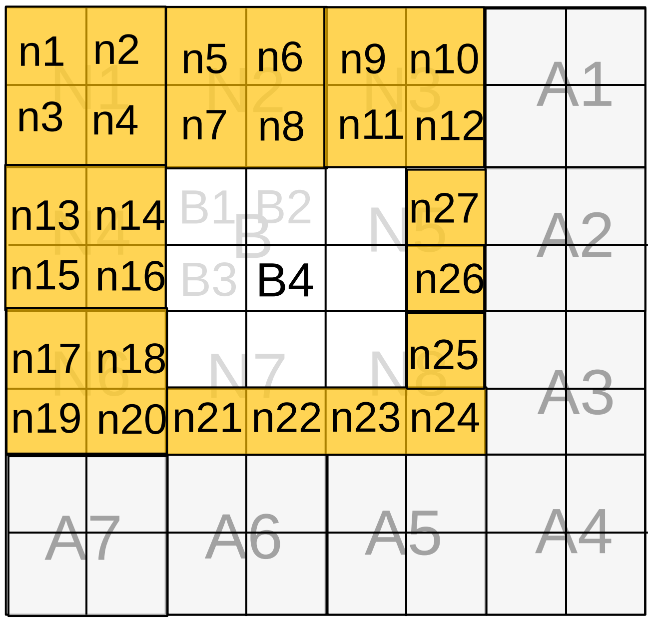


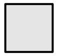


Influence of points in `Bi` s on those in `Ai` s already computed at the previous level (level-2)

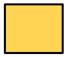
Hierarchical Decomposition

- *Level-3 decomposition*





Influence of points in `Bi` s on those in `Ai` s already computed at the previous level (level-2)



Well-separated from B4

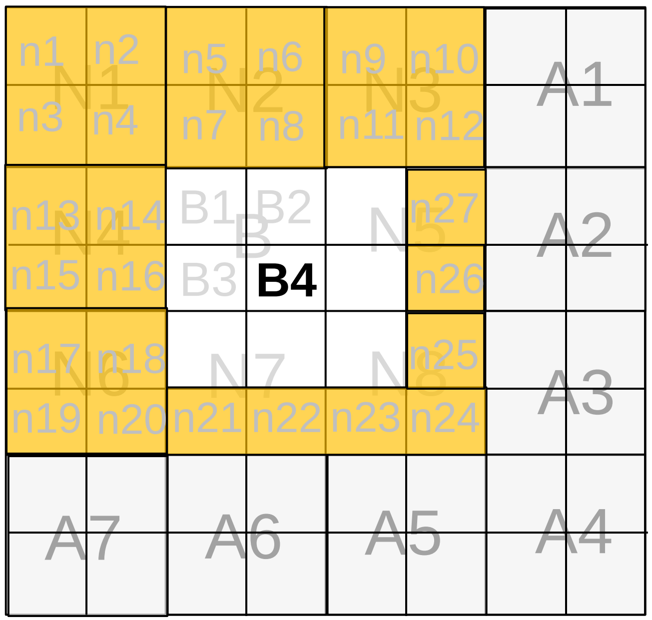
Influence of `B4’s` points on `nx’s` points can be approximated

`nx’s` constitute the <u>interaction list</u> for `B4`.

What is the max size of interaction list? i.e. max number of `nx` *s that we can have for any* `Bi`*?*

Hierarchical Decomposition

- *Level-3 decomposition*



Influence of points in `Bi` s on those in `Ai` s already computed at the previous level (level-2)

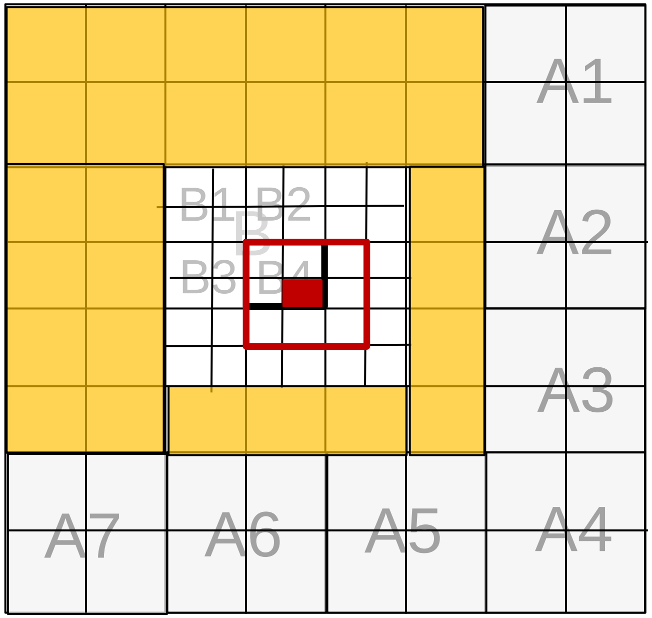
Well-separated from B4

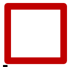
Influence of `B4’s` points on `nx’s` points can be approximated

What do we do about **B4**’s influence on its neighbors (white/unshaded boxes)?

Hierarchical Decomposition

- *Level-4 decomposition*



Any unshaded box outside  can be the *target* for computing the influence of points in  (*source*)

1. Computing Potential for Well-Separated Regions

for level L=2 **to** last_level
    for each Box B at level L
        iList = GetInteractionList(B)
        for each well-separated box A in iList
            //Compute potential
            potential $= m_B \log|C_A - C_B|$
            //Accumulate potential
            $\Phi\left(x_{C_A}, y_{C_A}\right) +=$ potential

Cost?

1. Computing Potential for Well-Separated Regions

```
1. for level L=2 to last_level
2.    for each Box B at level L
3.          iList = GetInteractionList(B)
4.          for each well-separated box A in iList
                //Compute potential
5.                potential  = m_B log|C_A − C_B|
                //Accumulate potential
6.                Φ(x_{C_A}, y_{C_A}) += potential
```

Prereqs: we need $\mathrm{m_B}, \mathrm{C_A}, \mathrm{C_B}$ details. (step 0)

2. Assigning Potential to Points

```
1. for each Box A at level L=0 to last_level
```

2. $\Phi_{p_i} = \Phi_{p_i} + \Phi_{C_A}$ (where $p_i \in A$ and C_A is A's CM)

Cost?

3. Assigning Potential to Points (last level)

1. **for** each Box B at last_level
2. $\Phi_{p_i} = \Phi_{p_i} + \sum_{p_j \in Neighbors(B)} m_B \log|p_i - p_j|$ (where $p_i \in B$)

Cost?

0. Computing Prereqs

```
1. for each Box B at level L=0 to last_level
2.        m_B = Σ_{p_j∈B} m_j
3.    //similarly compute C_B
```

Cost?

Total Cost (steps 0 + 1 + 2 + 3)

`O(N log N) + O (N) + O(N log N) + O(N)`

Can we do better?

0’. Computing Prereqs

- Traverse the tree bottom up instead of top-down

```
for each Box B starting from last_level to L=0
      if B is a leaf box
```

$$m_B = \sum_{p_j \in B} m_j$$

```
      else
```

$$m_B = m_{B_1} + m_{B_2} + m_{B_3} + m_{B_4}$$

//B_1-B_4 are children of B

Cost?

2'. Assigning Potential to Points

```
1. for each Box A at level L=0 to last_level
2.     if A is a leaf box
```

$\Phi_{p_i} = \Phi_{p_i} + \Phi_{C_A}$ (where $p_i \in A$ and C_A is A's CM)

```
    else
```

$\Phi_{A_1} = \Phi_{A_1} + \Phi_A$

$\Phi_{A_2} = \Phi_{A_2} + \Phi_A$

$\Phi_{A_3} = \Phi_{A_3} + \Phi_A$

$\Phi_{A_4} = \Phi_{A_4} + \Phi_A$

//A_1-A_4 are children of A

Cost?

Total Cost (steps 0’ + 1 + 2’ + 3)

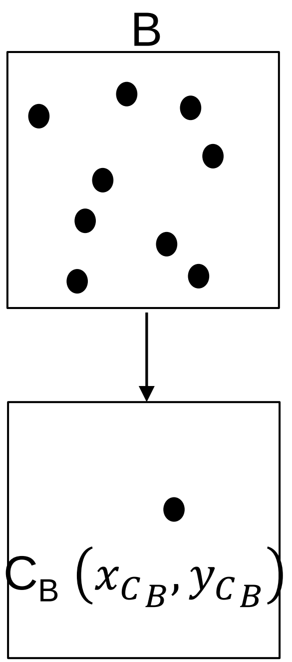
`O(N) + O (N) + O(N) + O(N)`

Problem: low accuracy if source (A) and target (B) are not far away from each other

Solution: more accurate representations for m_B and $\Phi\left(x_{C_A}, y_{C_A}\right)$

Multipole expansion

- Like a Taylor series expansion that is accurate when $x^2 + y^2$ is large (x, y are cartesian coordinates of the point)
- For a quadtree box B centered at $\left(x_{C_B}, y_{C_B}\right)$, we compute and store the terms: $\{\boldsymbol{m_B}, \boldsymbol{\alpha_1}, \boldsymbol{\alpha_2}, \dots, \boldsymbol{\alpha_p}, \boldsymbol{z_{C_B}}\}$

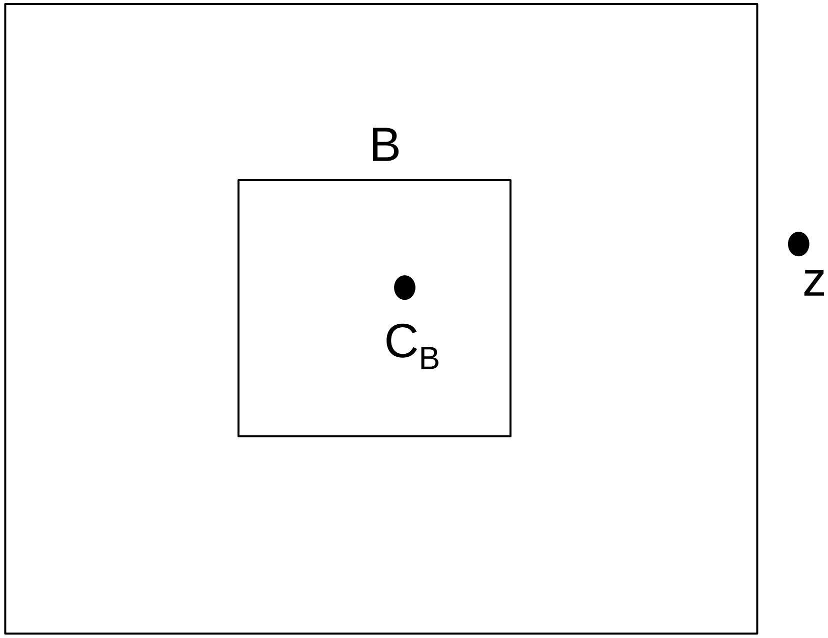


$$\alpha_j = \sum_{i=1}^{N_B} m_i \left(\frac{z_i^j}{j}\right)$$

z_i means $|z_i| = |(x_i, y_i)|$

Multipole expansion

- We approximate the potential at point z due to B by:



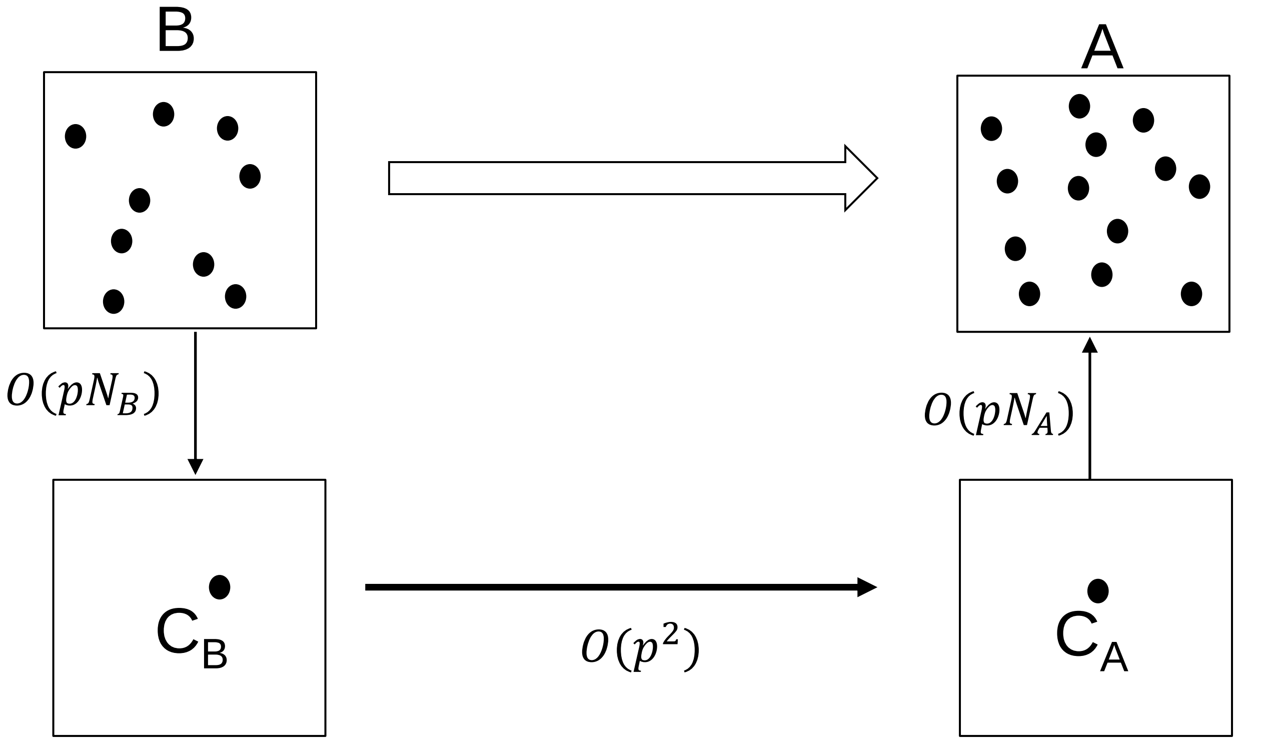
$$\Phi(x_z, y_z) = m_B \log(z - C_B) + \frac{\alpha_1}{z - C_B} + \frac{\alpha_2}{(z - C_B)^2} + \cdots + \frac{\alpha_p}{(z - C_B)^p}$$

- Because $\{\boldsymbol{m_B}, \boldsymbol{\alpha_1}, \boldsymbol{\alpha_2}, \ldots, \boldsymbol{\alpha_p}, \boldsymbol{z_{C_B}}\}$ is used to compute potential outside B, it is called <u>outer expansion</u>

Multipole expansion

- Similarly, we have the inner expansion $\{m_B, \beta_1, \beta_2, \ldots, \beta_p, z_{C_B}\}$
for computing the potential inside the Box due to all other points outside the box
- Computing outer expansions starts from leaf nodes and proceeds upwards in the tree.
- Computing inner expansions starts from root node and proceeds downwards in the tree.

3-Step Approximation (accurate)



FMM Algorithm

1. Build the quadtree containing all the points.
2. Traverse the quadtree from bottom to top, computing Outer(n) for each square n in the tree.
3. Traverse the quadtree from top to bottom, computing Inner(n) for each square in the tree.
4. For each leaf, add the contributions of nearest neighbors and particles in the leaf to Inner(n)

Multipole expansion

- How to obtain the expression for alpha, beta ?
- What is the value of p?
- How to compute alpha and beta?

- Further reading:

  https://people.eecs.berkeley.edu/~demmel/cs267/lecture27/lecture27.html