The Geometry of the Fast Multipole Methods

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Outline

- The N-body problem and the fast multipole method

- Other related algorithms

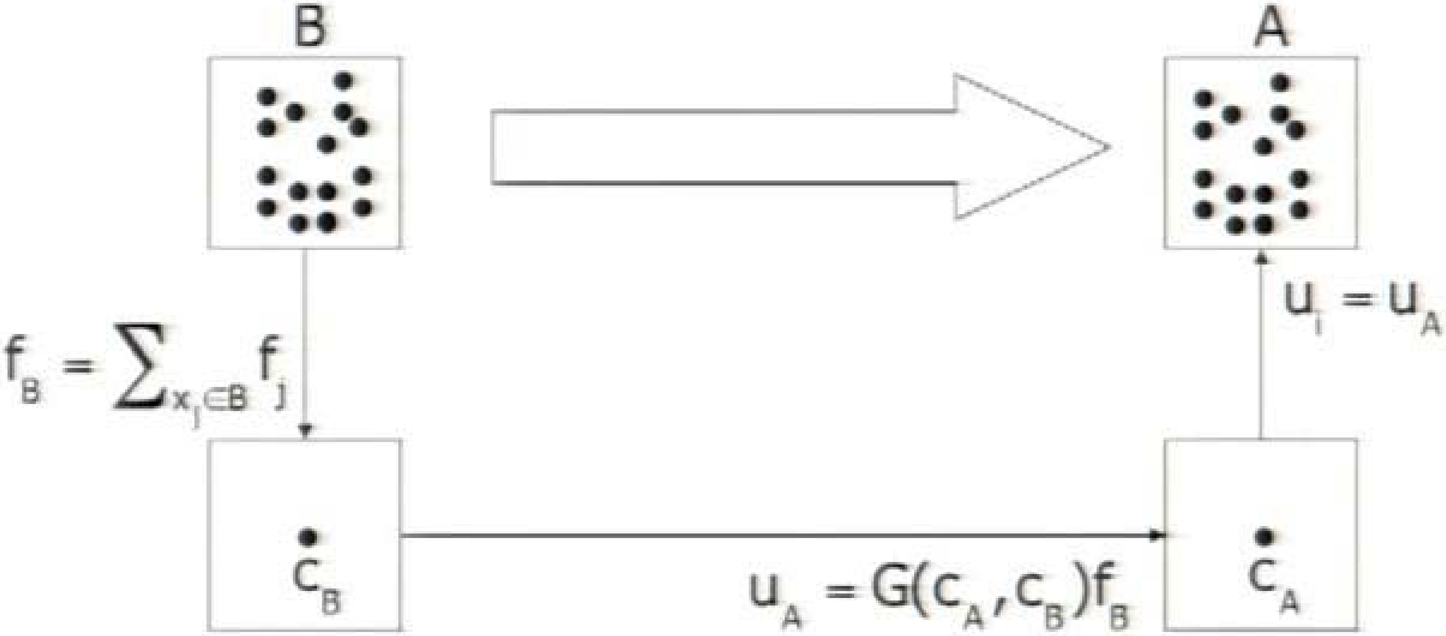
Computation time

- Direct computation $O(N^2)$ steps. Too expensive
- Goal: Calculate them more efficiently.
- Fast multipole method
  - by Greengard and Rokhlin in 1987.
  - Ranked among the top 10 algorithms in the past century
  - Bring the complexity down to $O_\varepsilon(N)$ for any prescribed accuracy ε

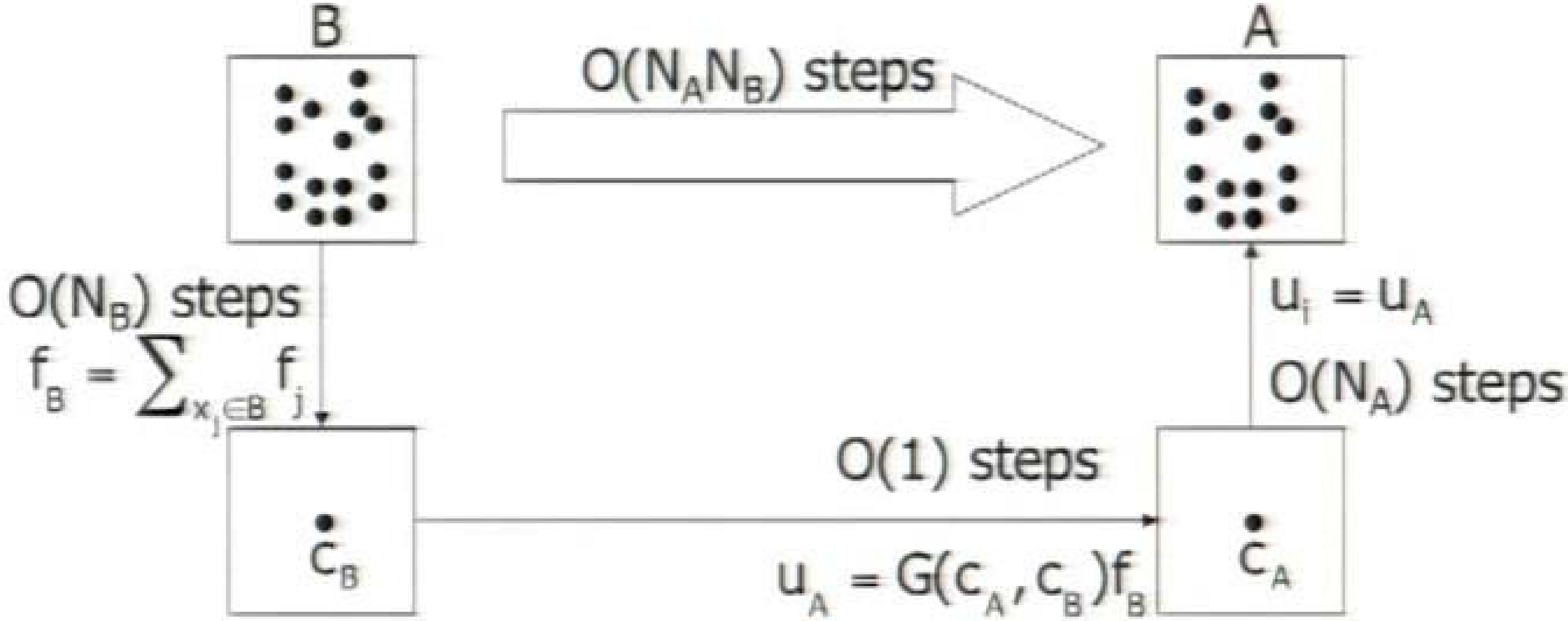
Idea 1: well-separated regions

- Suppose B and A are well-separated.
- Consider the influence from B to A: at each x_i in A, evaluate

$$u_i = \sum_{x_j \in B} G(x_i, x_j) f_j$$



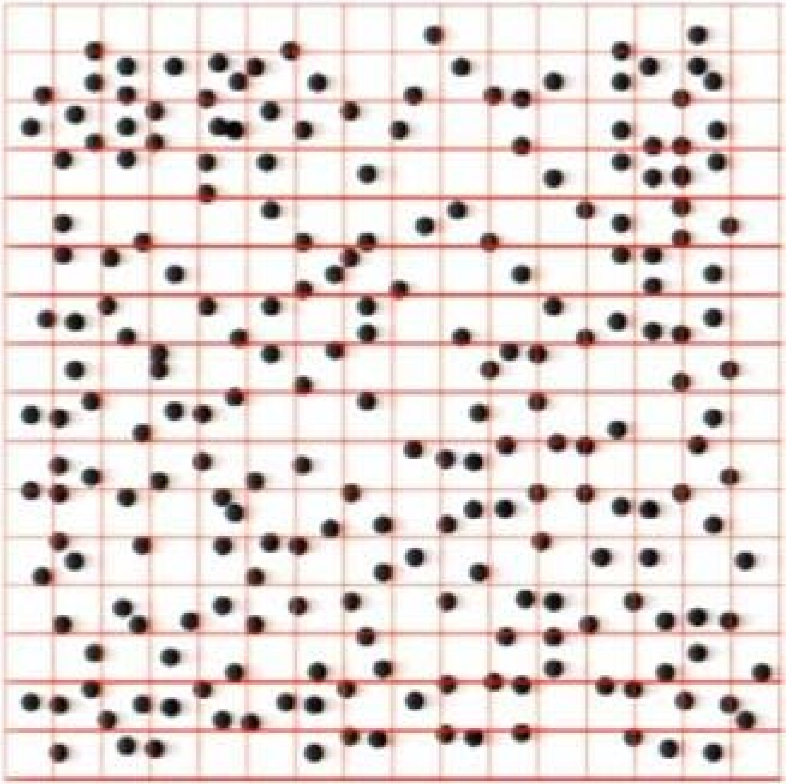
Three-step approximation



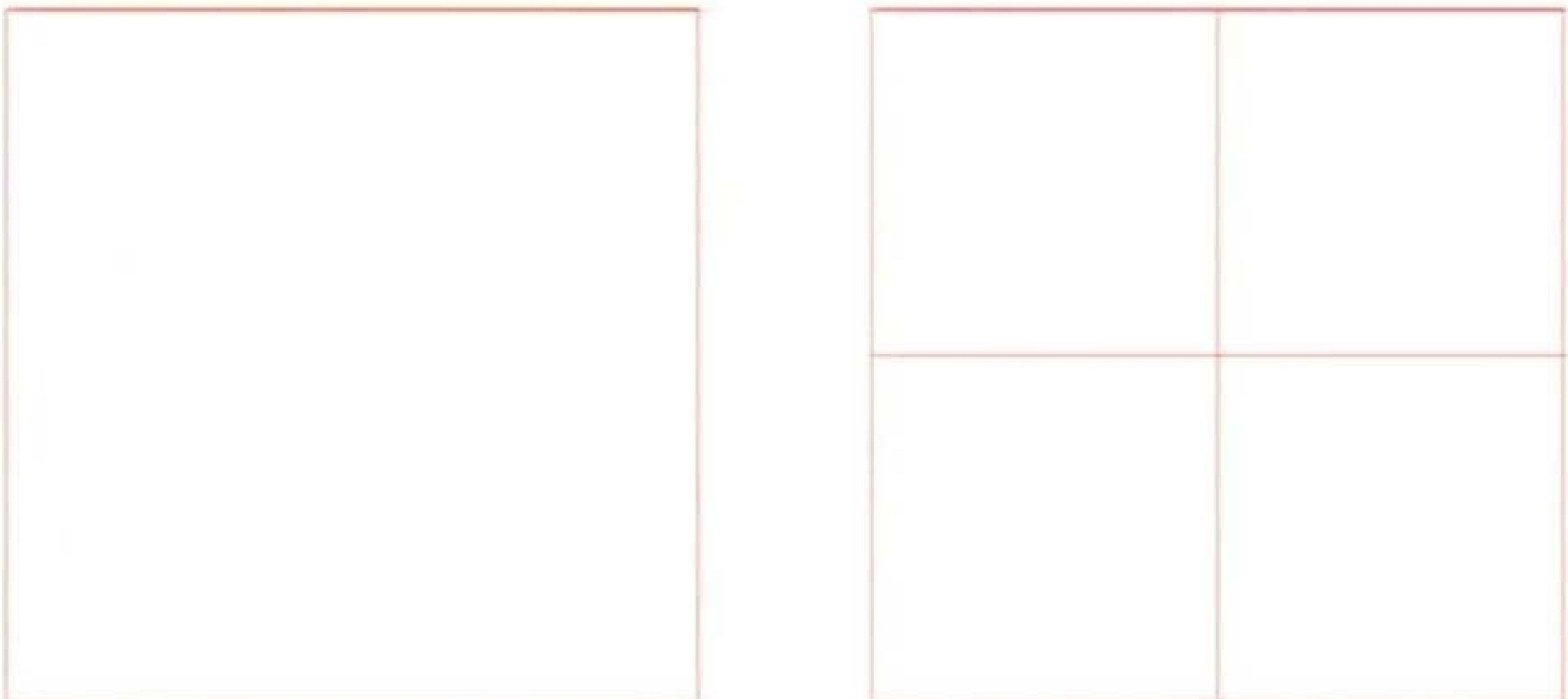
- Reduce $O(N_A N_B)$ steps to $O(N_A + N_B)$ steps
- Good accuracy when A and B are far away
- But we will use it whenever A and B are well-separated

Hierarchical decomposition

- Partition the domain hierarchically until each leaf box contains O(1) number of points
- N: the # of points
- # of levels=$O(\log_4 N)$
- # of boxes on level l=$O(4^l)$
- Total # of boxes=O(N)

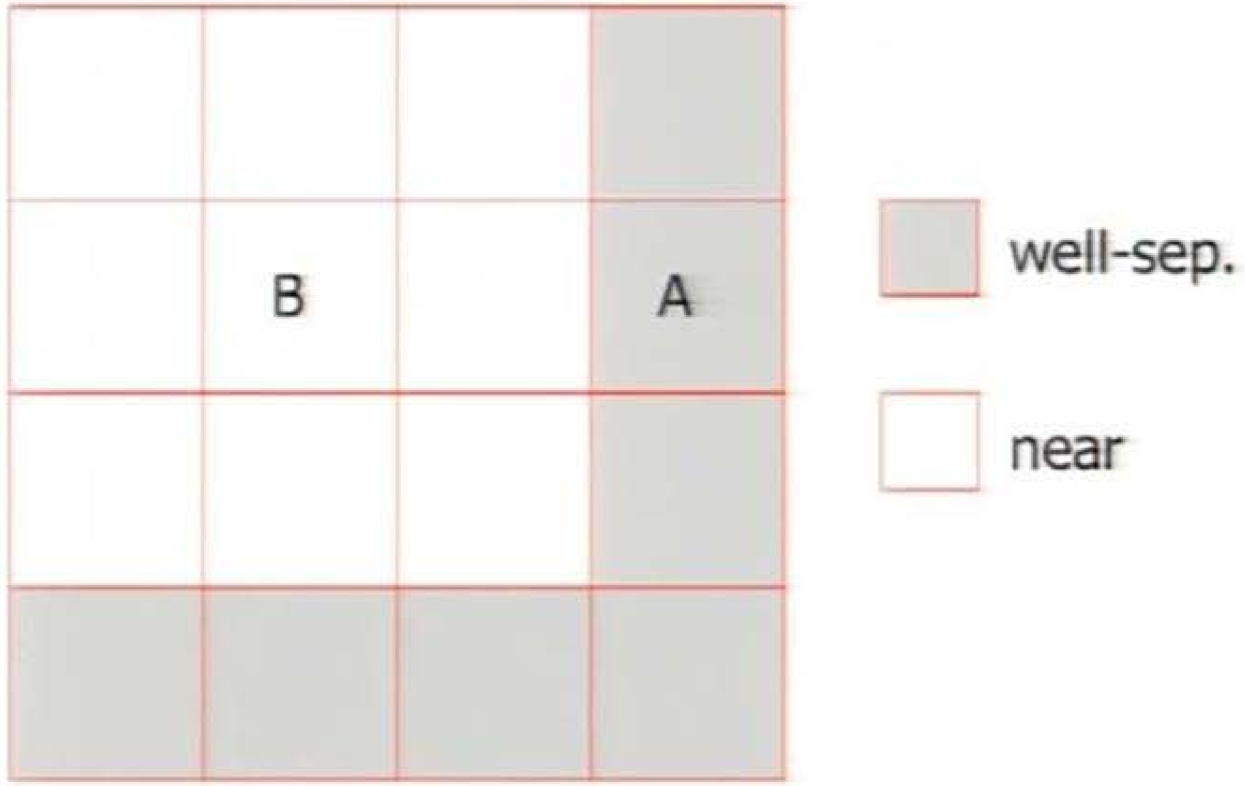


Levels 0 and 1



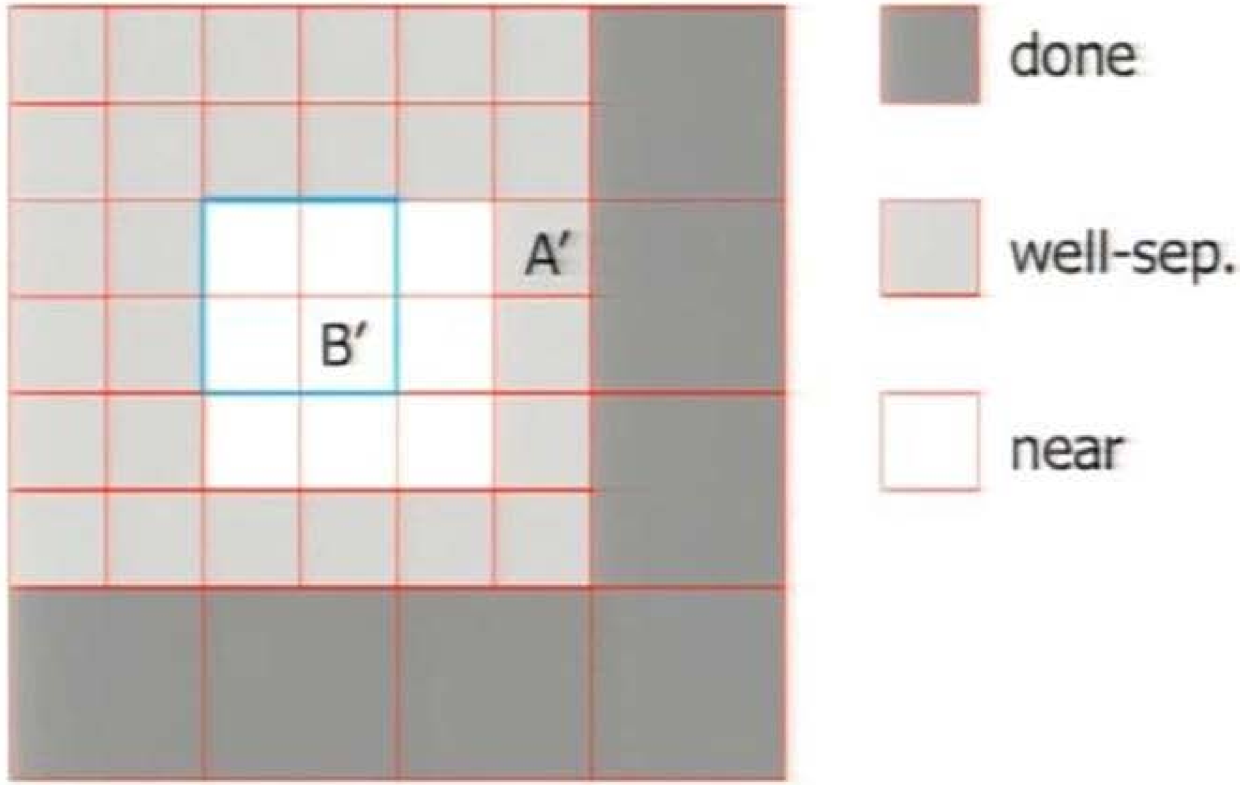
- The boxes are adjacent to each other. So cannot use the 3-step approximation

Level 2



- B and A are well-separated
  - Use the 3-step approx. for the influence from B to A
- Q: Influence between B and its near field (neighbors)?
  - Go to the next level

Level 3

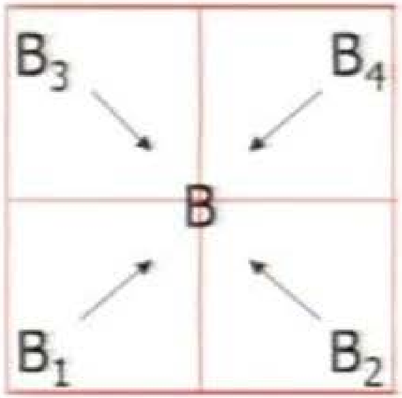


- B′ and A′ are well-separated
  - Use the 3-step approx. for the influence from B′ to A′
  - influence list of B = all such A′s, at most 6^2-3^2=27 boxes

Algorithm 1

- 1. For each box B in the tree
  - $f_B \Leftarrow \sum_{x_j \in B} f_j$
- 2. For L=2 to last level
  - For each B on level L
    - For each A in B's influence list
      - $u_A \Leftarrow u_A + G(c_A, c_B) f_B$
- 3. For each box A in the tree
  - $u_i \Leftarrow u_i + u_A$, for $x_i \in A$
- 4. For each box B on the last level
  - $u_i \Leftarrow u_i + \sum_{x_j \in Nbhd(B)} G(x_i, x_j) f_j$, for $x_i \in B$

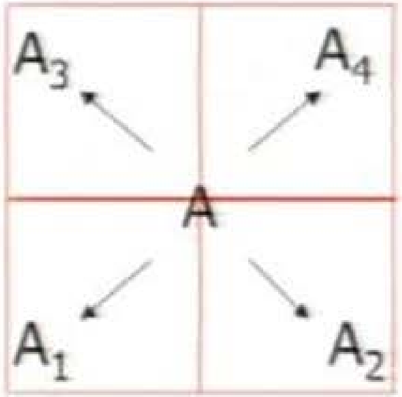
Idea 3: reuse the computation



$$f_B = \sum_{x_j \in B} f_j = \sum_{x_j \in B_1} f_j + \sum_{x_j \in B_2} f_j + \sum_{x_j \in B_3} f_j + \sum_{x_j \in B_4} f_j = f_{B_1} + f_{B_2} + f_{B_3} + f_{B_4}$$

- Compute f_B from its children
  - O(1) cost
  - Traverse the quadtree bottom-up

$$u_i \Leftarrow u_i + u_A,\ \text{for } x_i \in A$$



- Similarly, can add u_A only to its children
  - O(1) cost
  - Traverse the quadtree top-down

Algorithm 2 (FMM): cost analysis

- 1. Go up the tree, for each box B
  - If B is a leaf box,

    $f_B \Leftarrow \sum_{x_j \in B} f_j$ Cost = O(N)

    else

    $f_B \Leftarrow f_{B_1} + f_{B_2} + f_{B_3} + f_{B_4}$ Cost = O(N)
- 2. Same as Step 2 of Algorithm 1 Cost = O(N)
- 3. Go down the tree, for each box A
  - If A is a leaf box

    $u_i \Leftarrow u_i + u_A$, for $x_i \in A$ Cost = O(N)

    else

    $u_{A_1} \Leftarrow u_{A_1} + u_A$, same for A_2, A_3, A_4 Cost = O(N)
- 4. Same as Step 4 of Algorithm 1

Total cost = O(N)

Idea 4: better source/target reps

- Currently
  - f_B is the sum of charges in B, and
  - u_A is the potential at c_A
  - Low accu. if A & B are well-sep. but close to each other
- More generally
  - f_B is a compact rep of the sources in B (for the pts well-separated from B)
  - u_A is a compact rep of the potential in A (induced by pts well-separated from A)
- Better accuracy (2D): treat x, y as points in complex plane **C**
  - $G(x,y) = \mathrm{Re}(\ln(x-y))$
  - Multipole and local expansions: O(1) numbers
  - Equivalent sources: O(1) numbers

Summary of FMM

- Low rank influence between well-separated regions
- Hierarchical decomposition: quadtree in 2D, octree in 3D
- Reuse of computation
- More accurate compact reps for f_B and u_A
- Adaptive algorithm for non-uniform dist. is also available.

Hierarchical matrix algebra

- This matrix decomposition is general. It can represent elliptic operators, their inverses (Green's function), square roots, etc.
- Hierarchical matrix algebra by Hackbusch et al
  - A framework to represent, manipulate, and apply operators in this hierarchical form.
- Highly efficient. For $N \times N$ matrices,

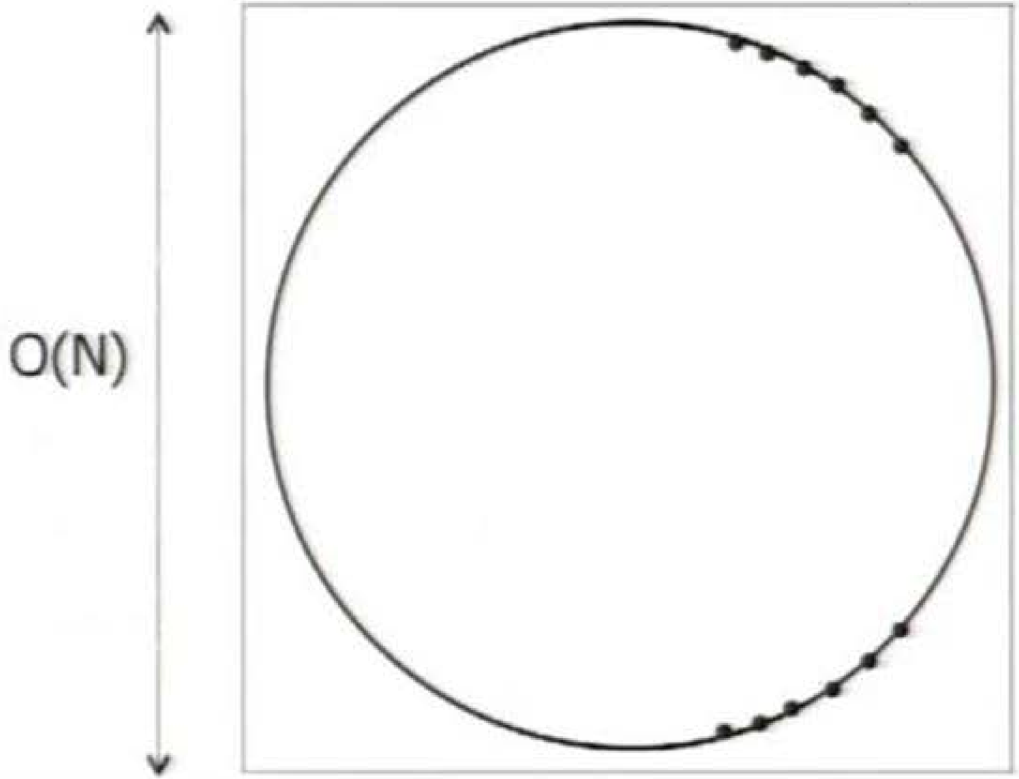
	Std. Mat. Alg.	Hier. Mat. Alg.
Mat representation	$O(N^2)$	$O(N \log N)$
Mat addition	$O(N^2)$	$O(N \log N)$
Mat multiplication	$O(N^3)$	$O(N \log^2 N)$
Mat inversion	$O(N^3)$	$O(N \log^3 N)$

2: Directional FMM

- N-body problem with Helmholtz kernel

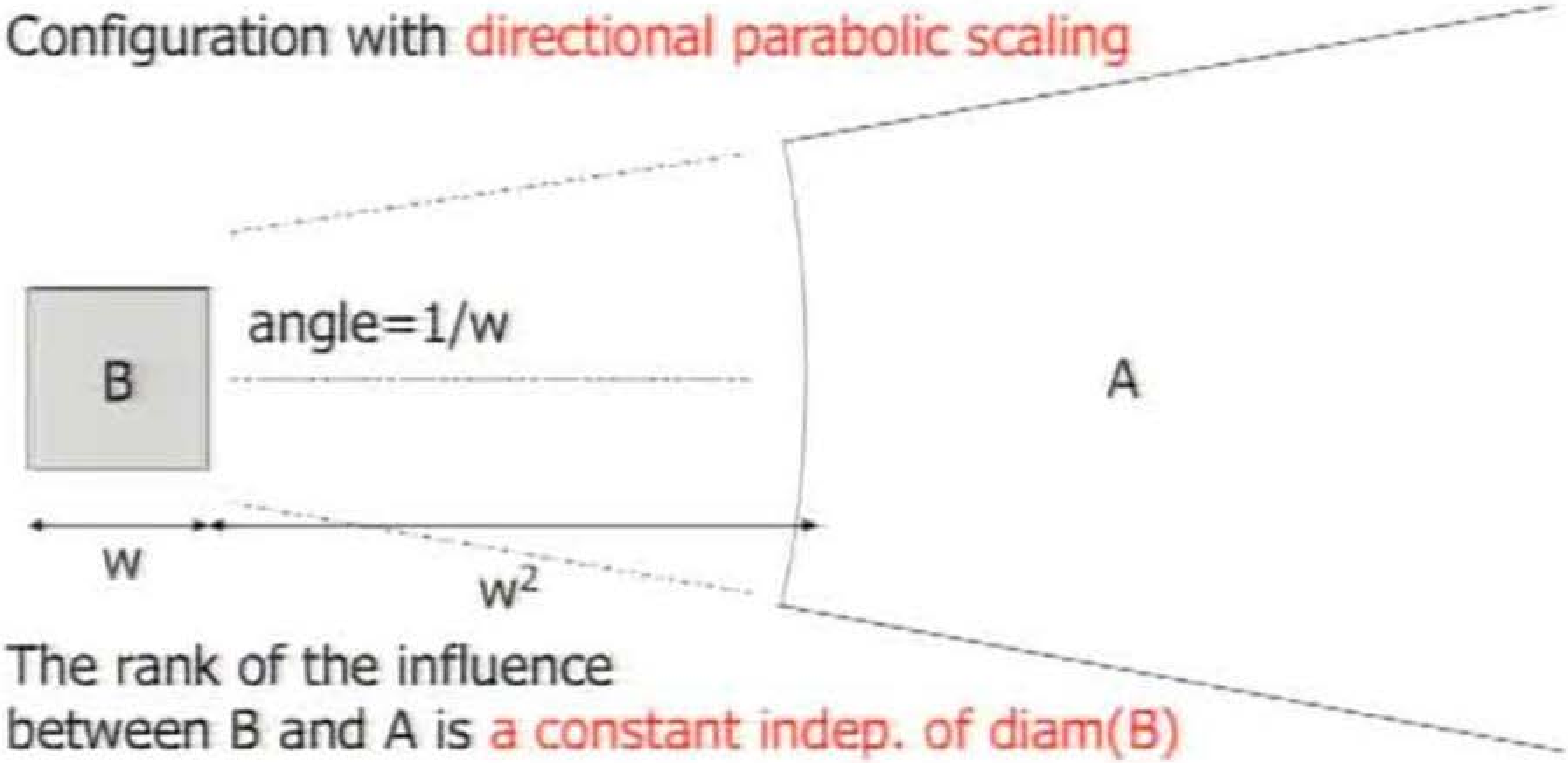
$$u_i = \sum_{j=1}^{N} G(x_i, x_j) f_j$$

$$G(x,y) = H_0^1(|x-y|) \text{ (in 2D)}, \quad G(x,y) = \frac{\exp(i|x-y|)}{|x-y|} \text{ (in 3D)}$$



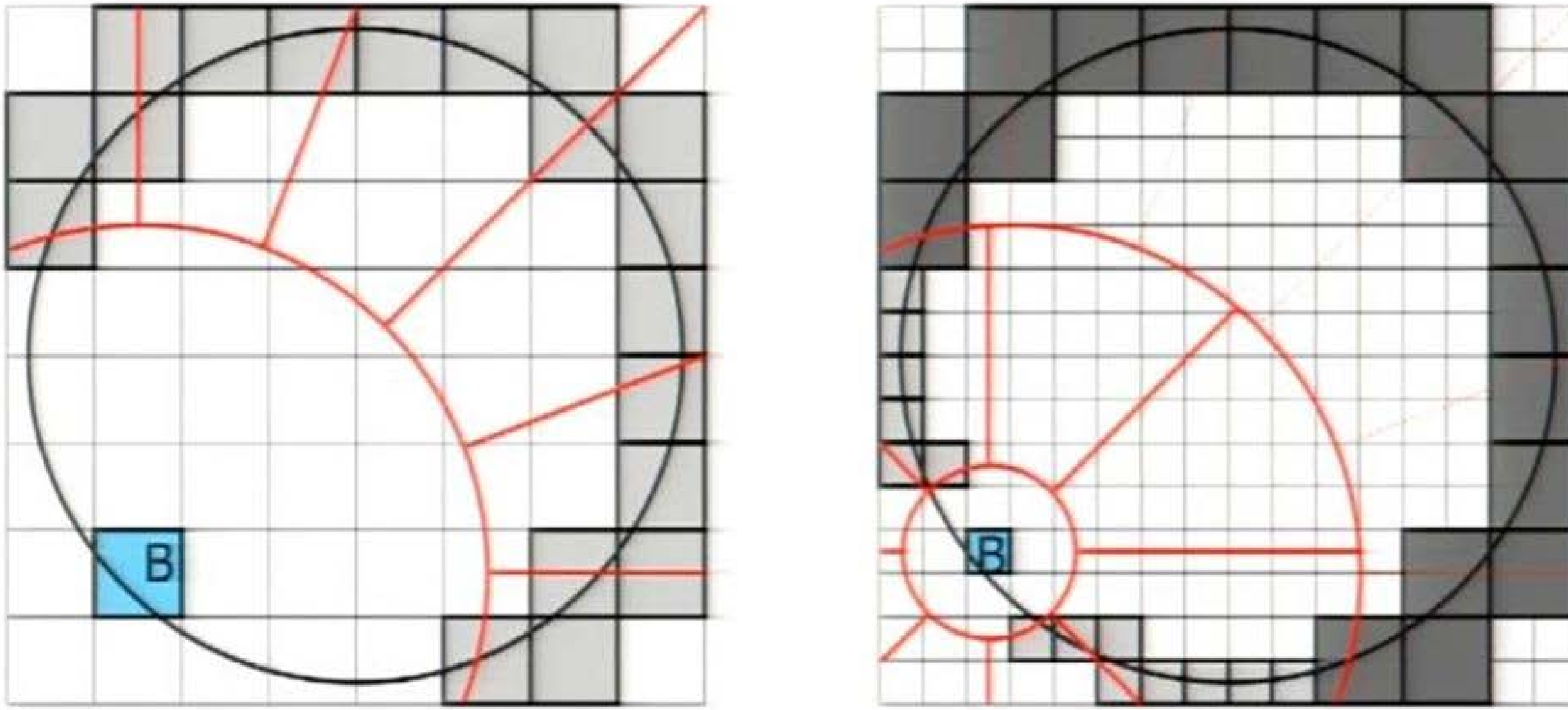
A new geometric configuration

- Configuration with directional parabolic scaling



- The rank of the influence between B and A is a constant indep. of diam(B)
- This is the key of the O(N logN) directional FMM algorithm for surface pt distribution.

Directional FMM algorithm



- The total complexity is O(N logN).

Thank you

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