

05/09	Class 9	Dense direct solvers	Understand the principle of LU decomposition and the optimization and parallelization techniques that lead to the LINPACK benchmark.
05/12	Class 10	Dense eigensolvers	Determine eigenvalues and eigenvectors and understand the fast algorithms for diagonalization and orthonormalization.
05/16	Class 11	Sparse direct solvers	Understand reordering in AMD and nested dissection, and fast algorithms such as skyline and multifrontal methods.
05/19	Class 12	Sparse iterative solvers	Understand the notion of positive definiteness, condition number, and the difference between Jacobi, CG, and GMRES.
05/23	Class 13	Preconditioners	Understand how preconditioning affects the condition number and spectral radius, and how that affects the CG method.
05/26	Class 14	Multigrid methods	Understand the role of smoothers, restriction, and prolongation in the V-cycle.
05/30	Class 15	Fast multipole methods, H-matrices	Understand the concept of multipole expansion and low-rank approximation, and the role of the tree structure.

the Top 10 Algorithms



- ▶ 1946 — The Monte Carlo method.
- ▶ 1947 — Simplex Method for Linear Programming.
- ▶ 1950 — Krylov Subspace Iteration Method.
- ▶ 1951 — The Decompositional Approach to Matrix Computations.
- ▶ 1957 — The Fortran Compiler.
- ▶ 1959 — QR Algorithm for Computing Eigenvalues.
- ▶ 1962 — Quicksort Algorithms for Sorting.
- ▶ 1965 — Fast Fourier Transform.
- ▶ 1977 — Integer Relation Detection.
- ▶ 1987 — Fast Multipole Method

*Dongarra & Sullivan, IEEE Comput. Sci. Eng.,
Vol. 2(1):22-- 23 (2000)*

Hierarchical N-body methods

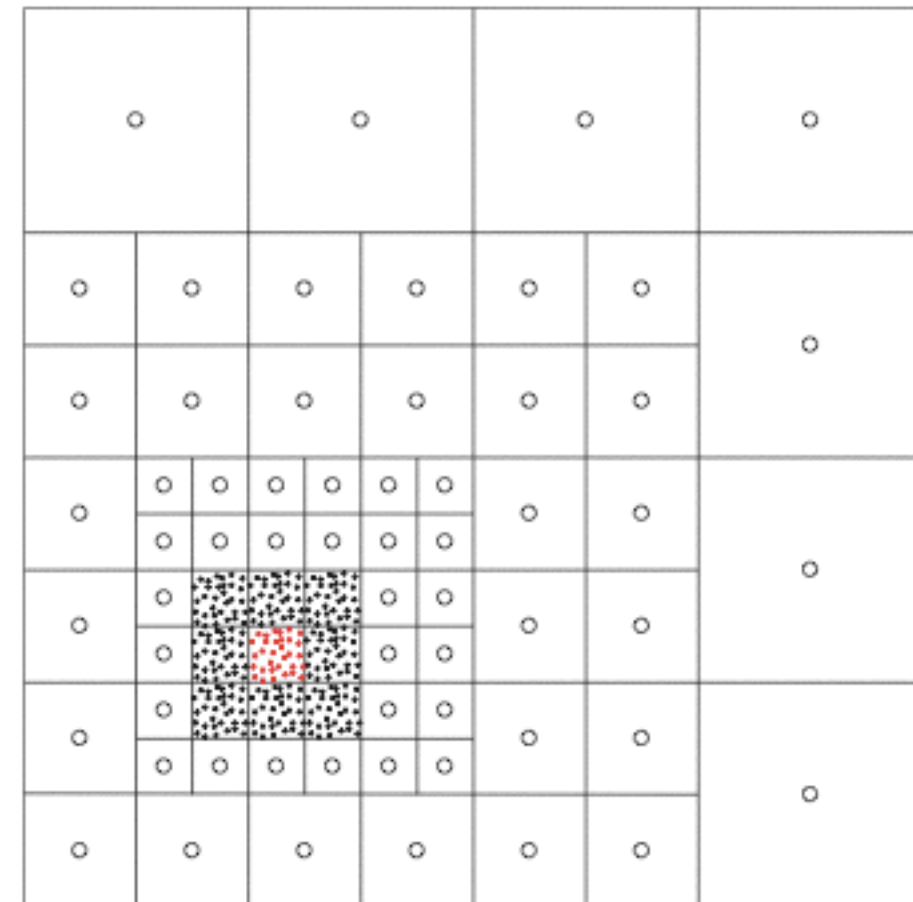
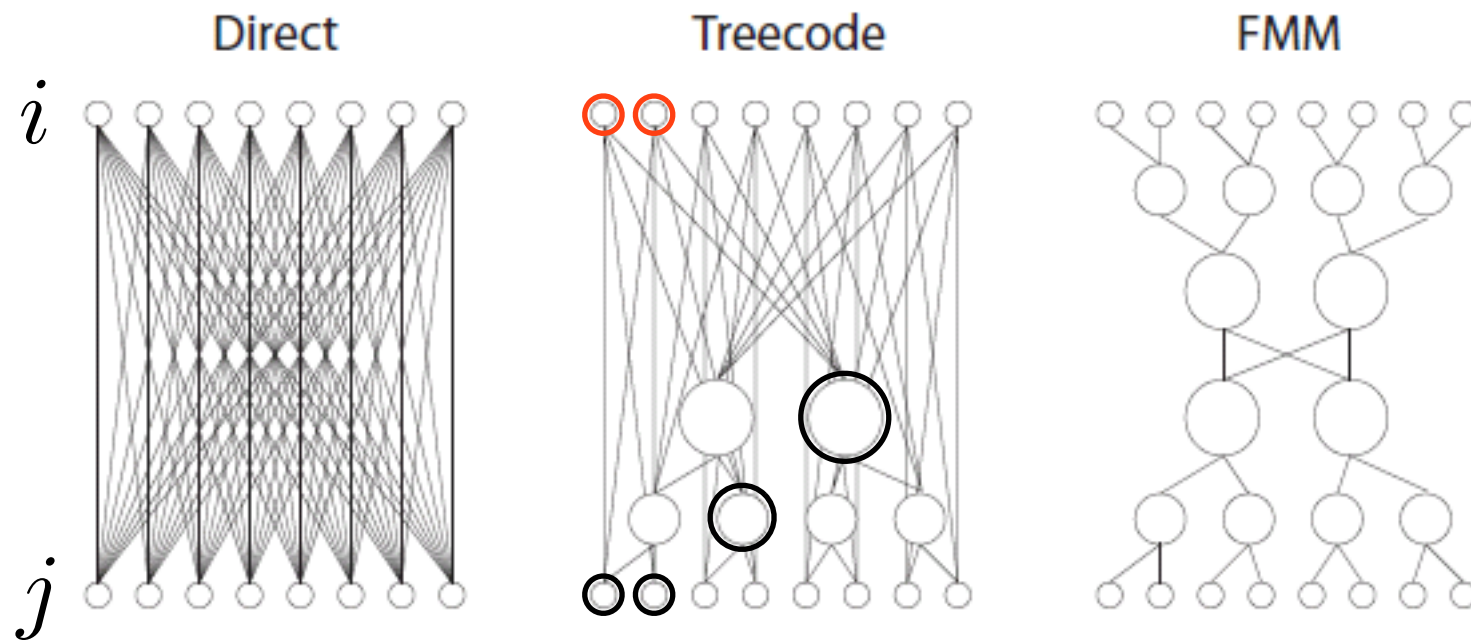
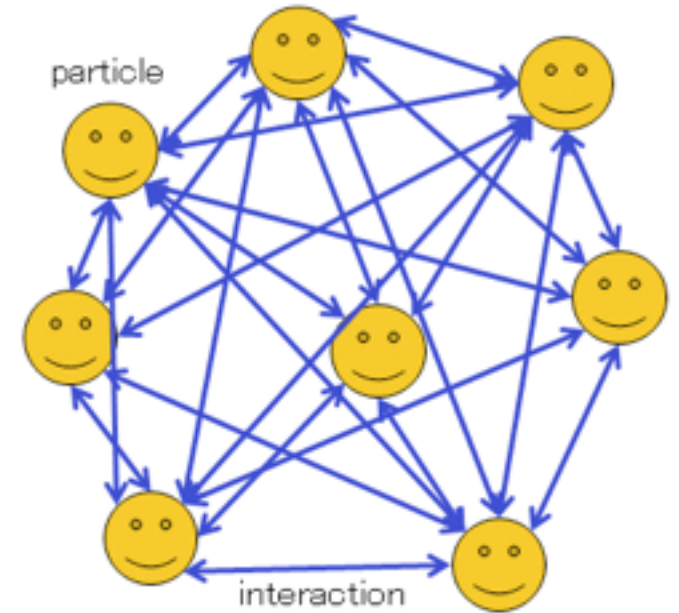
Particles interact with each other
Stars, Galaxies, Atoms, etc.

Computational cost

Direct sum - $O(N^2)$

Treecode - $O(N \log N)$

Fast Multipole Method - $O(N)$



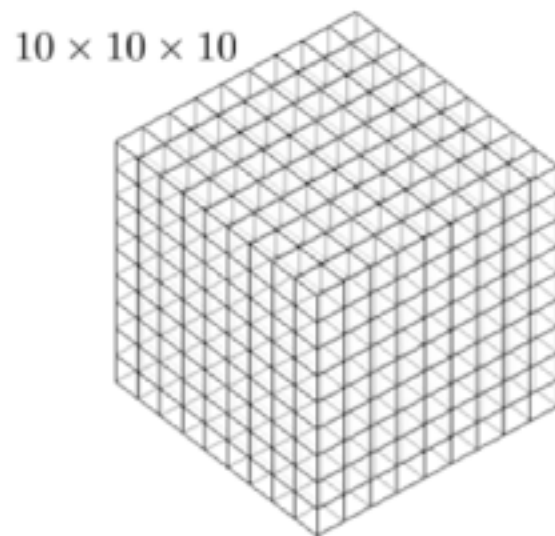
FMM as a Matrix

$$u(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y})$$

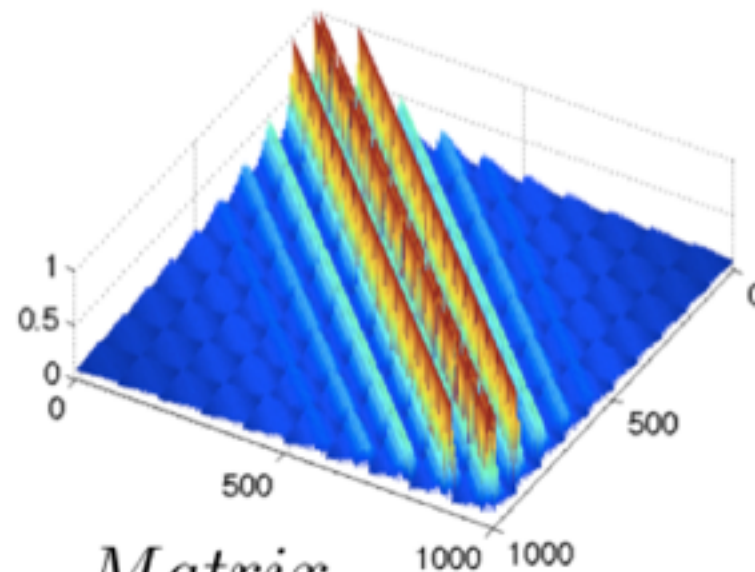
$$\mathbf{u} = \mathbf{A}^{-1} \mathbf{b} = \mathbf{G} \mathbf{b}$$

Laplace

$$G(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi|\mathbf{x} - \mathbf{y}|}$$

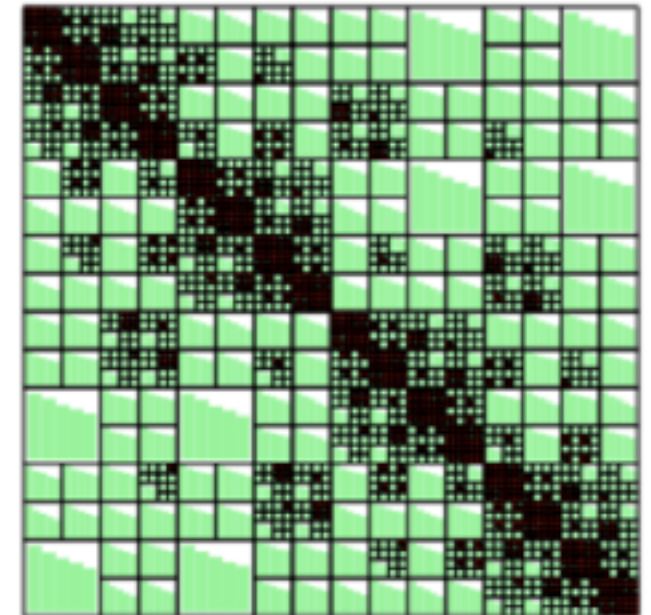


Geometry

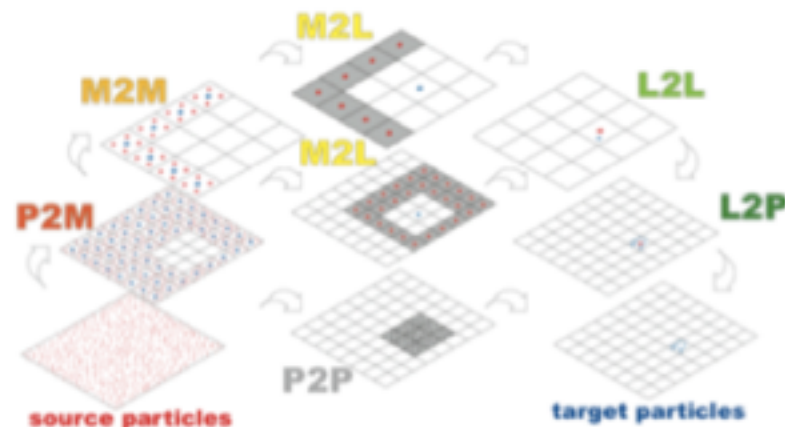


Matrix

H-matrix

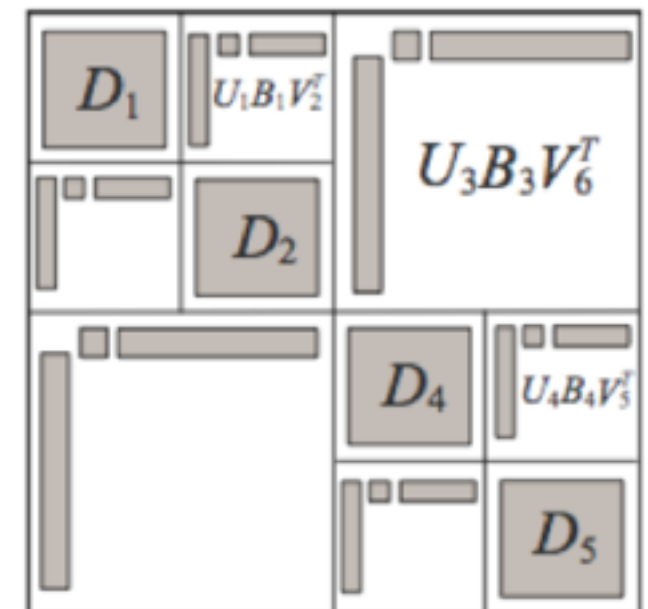


FMM

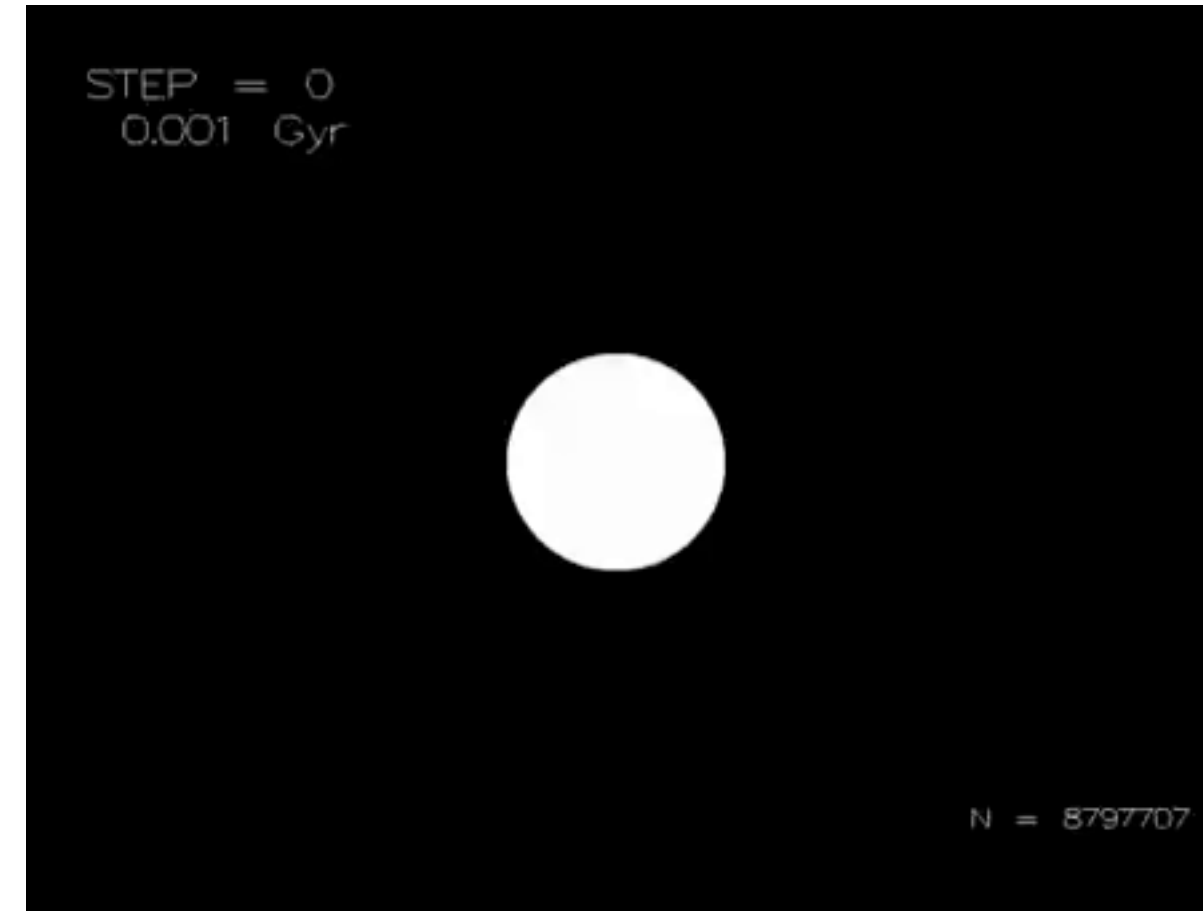
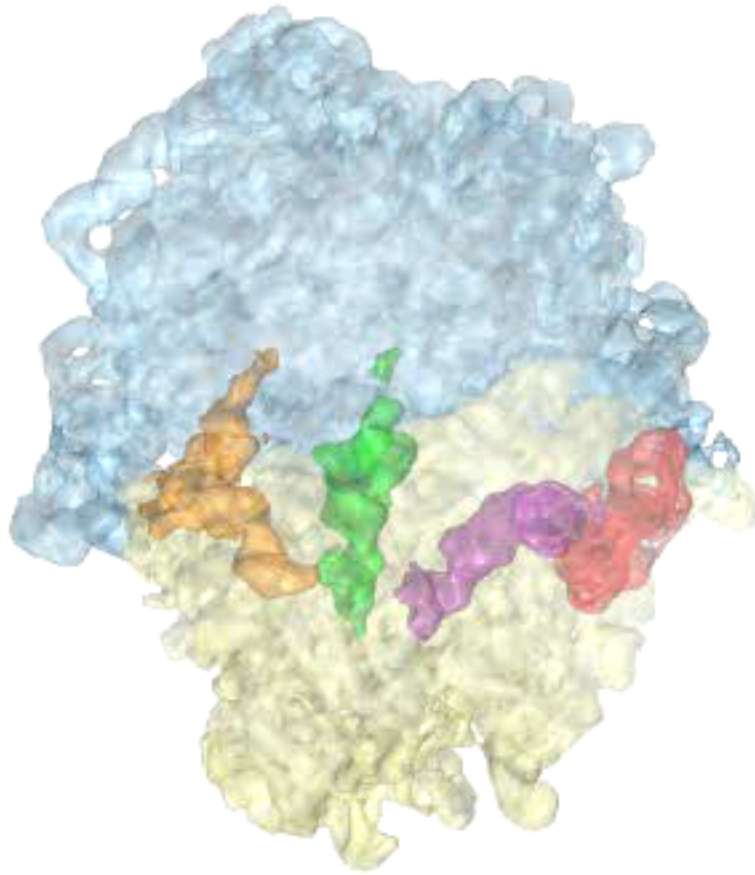


$$G(\mathbf{x}_{ij}) = \sum_{n=0}^p \frac{1}{n!} (\mathbf{x}_{iA} + \mathbf{x}_{Mj})^n \nabla^{(n)} G(\mathbf{x}_{AM})$$

$$= \sum_{k=0}^p \frac{1}{k!} \mathbf{x}_{iA}^k \underbrace{\sum_{n=0}^{p-k} \nabla^{(n+k)} G(\mathbf{x}_{AM})}_{\mathbf{L}} \underbrace{\frac{1}{n!} \mathbf{x}_{Mj}^n}_{\mathbf{M}}$$



N-body problems



Hierarchical N-body methods

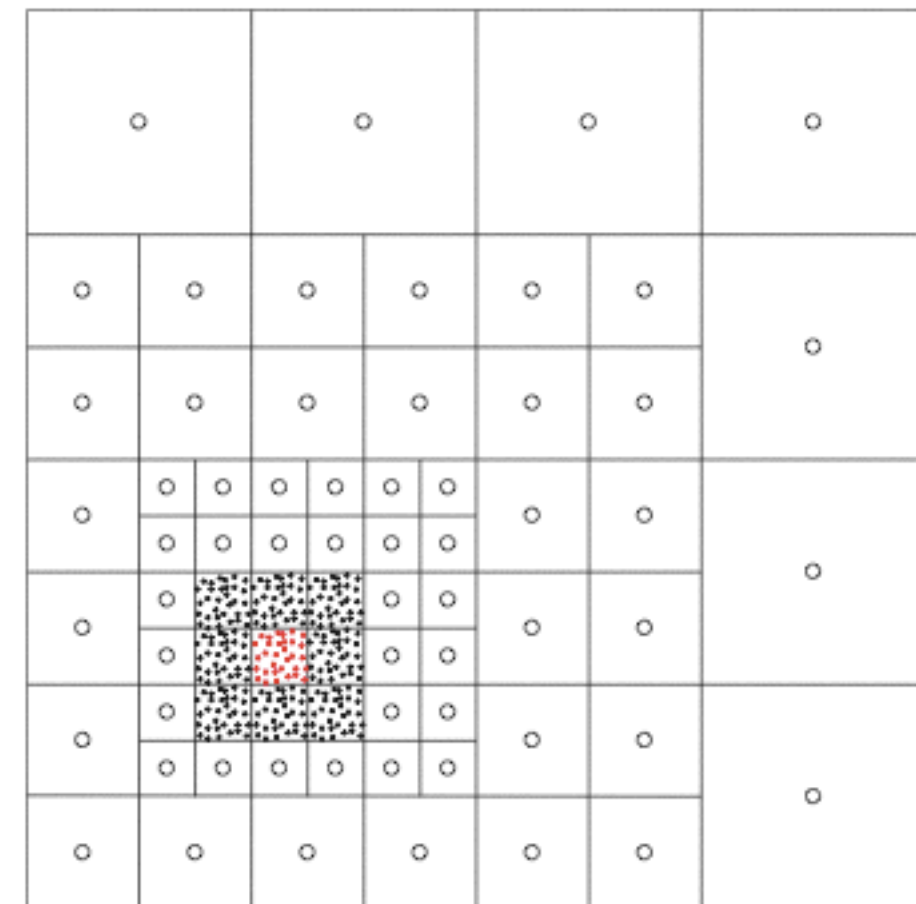
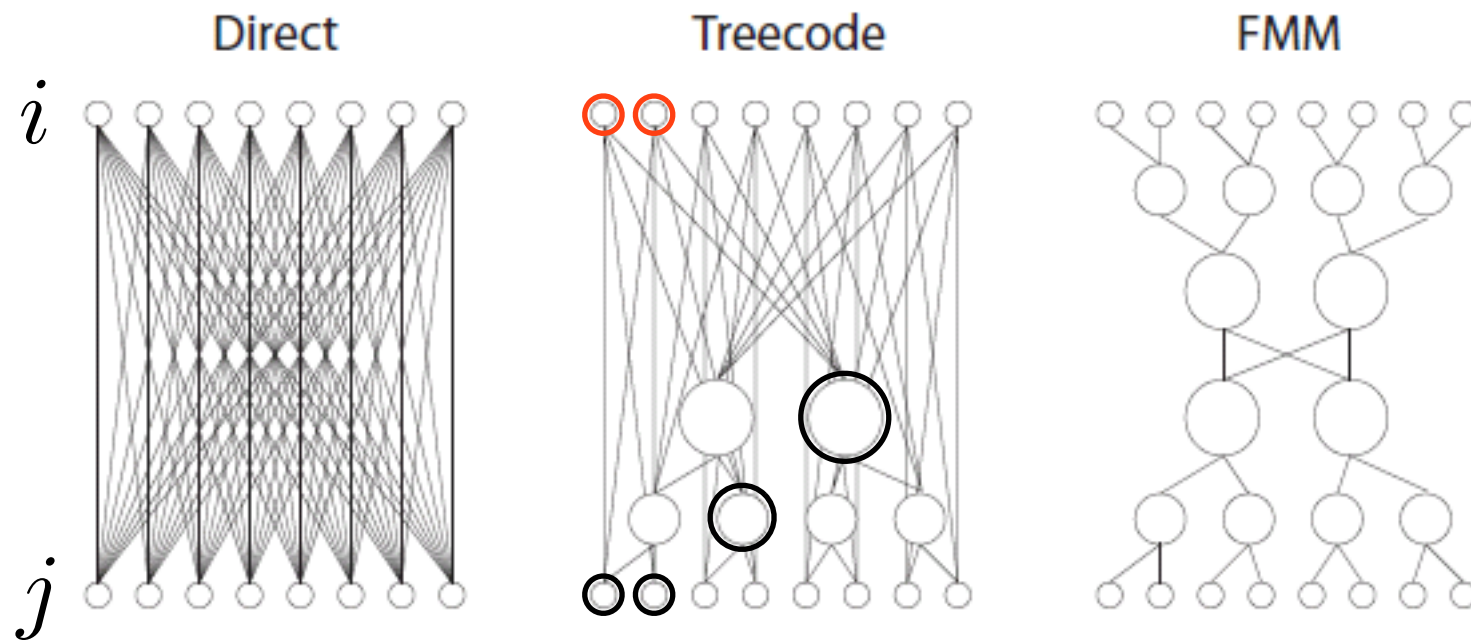
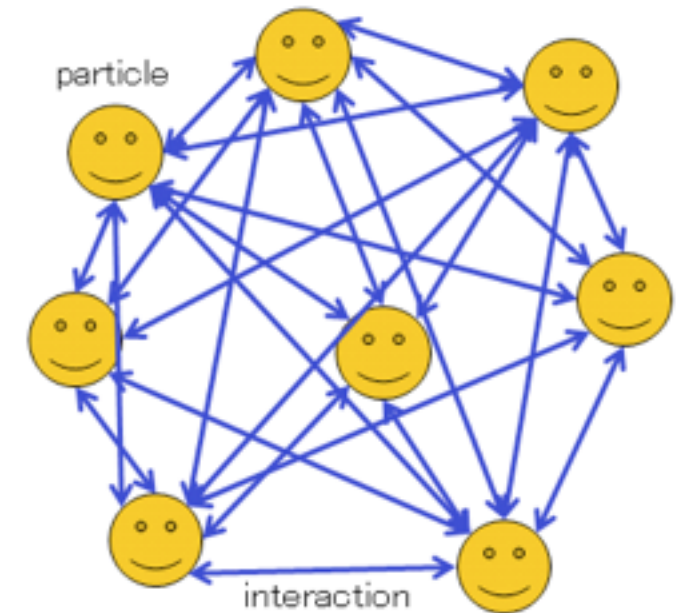
Particles interact with each other
Stars, Galaxies, Atoms, etc.

Computational cost

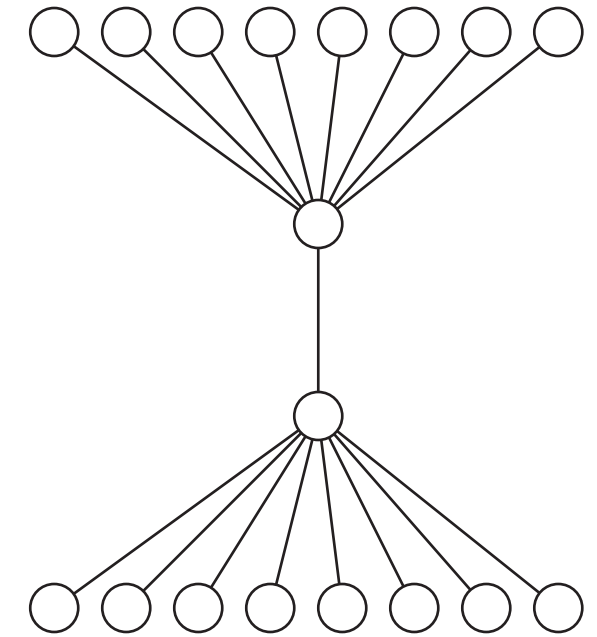
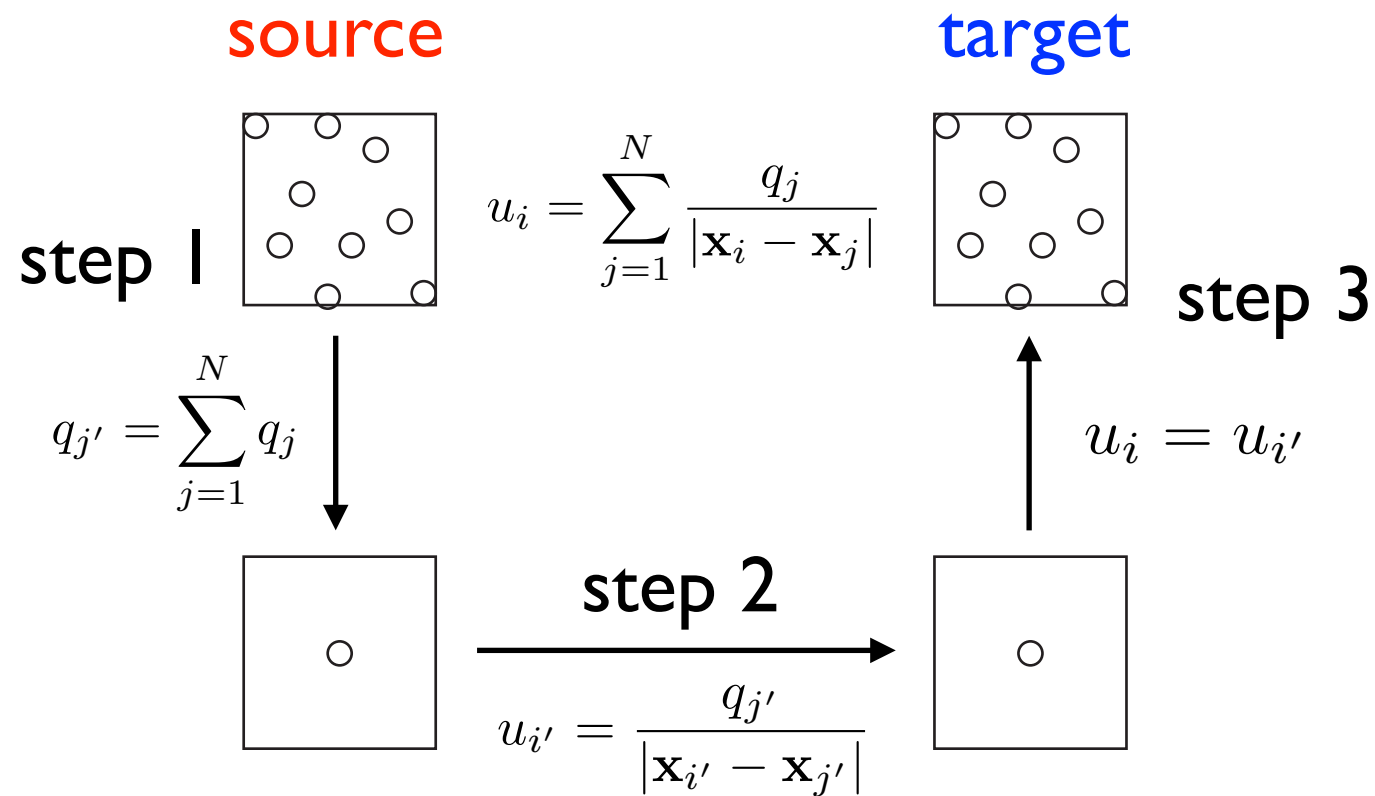
Direct sum - $O(N^2)$

Treecode - $O(N \log N)$

Fast Multipole Method - $O(N)$

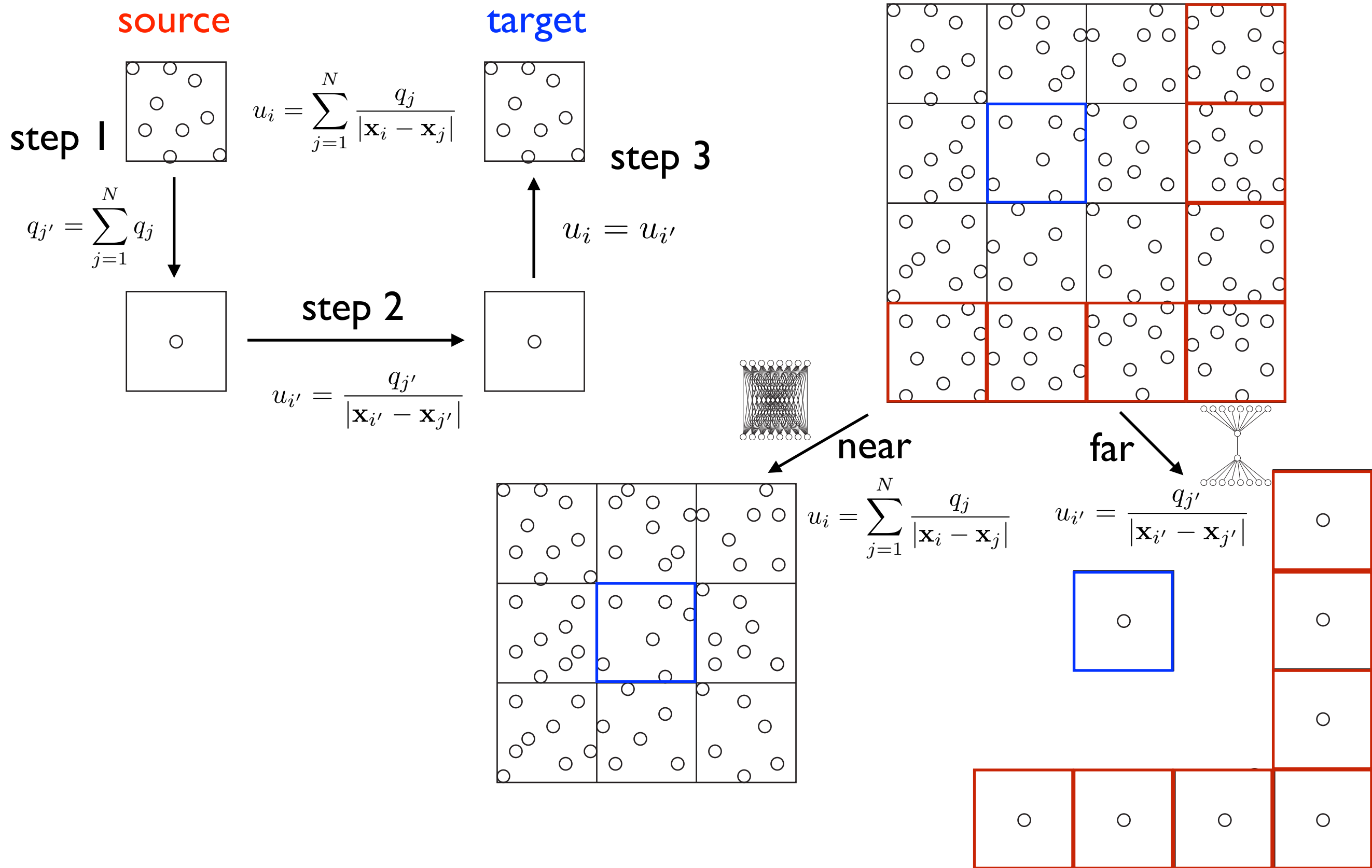


Approximating the interaction

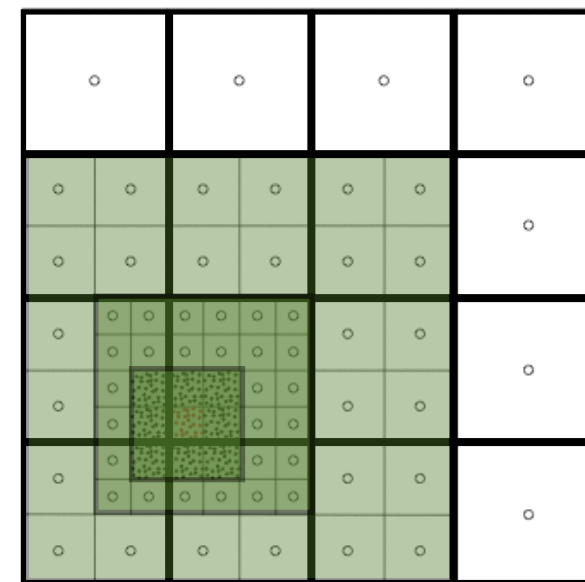
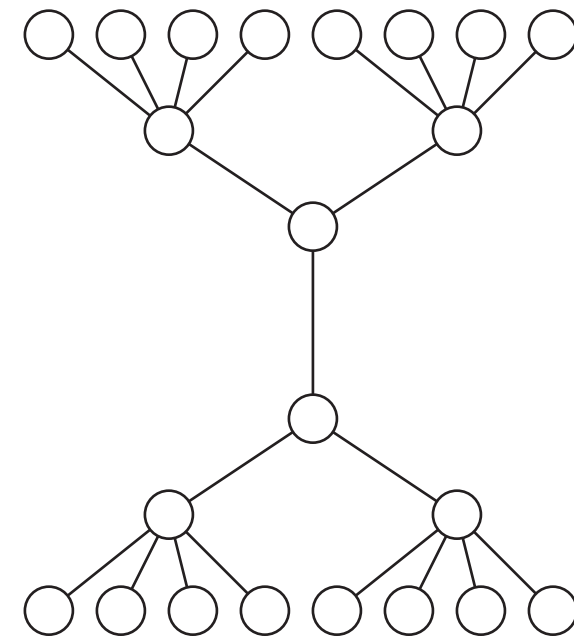
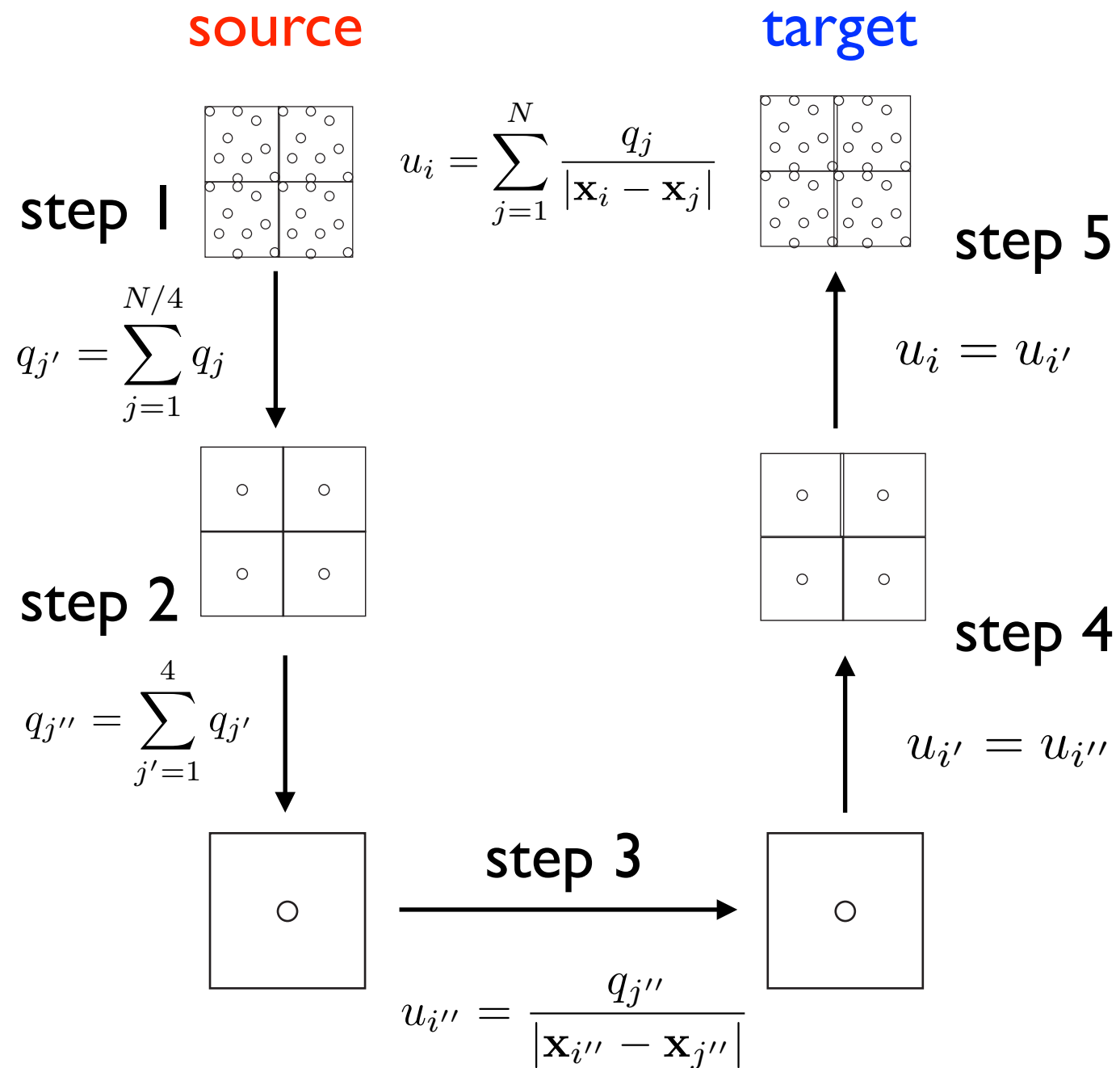


1. Sum all charges
2. Calculate effect of center source on center target
3. Assume all targets in the box have equal potential

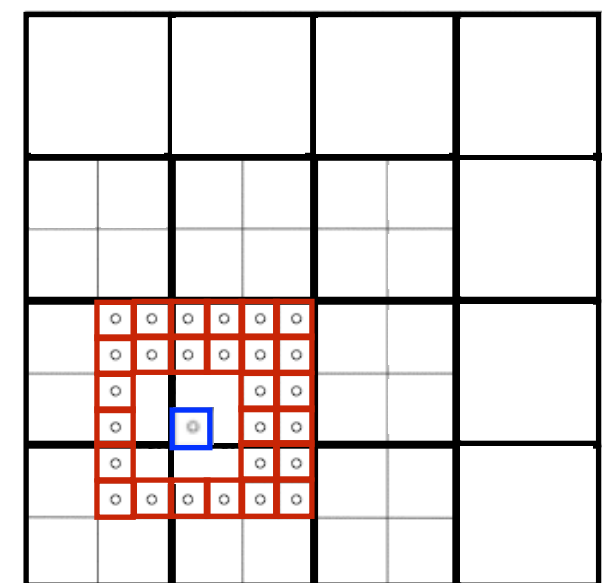
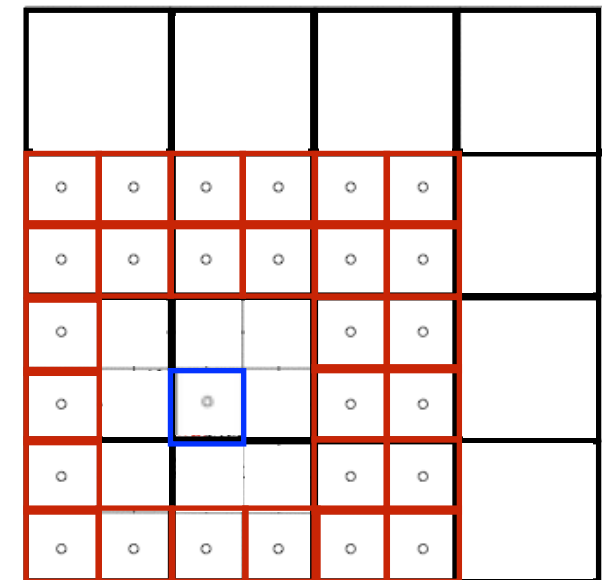
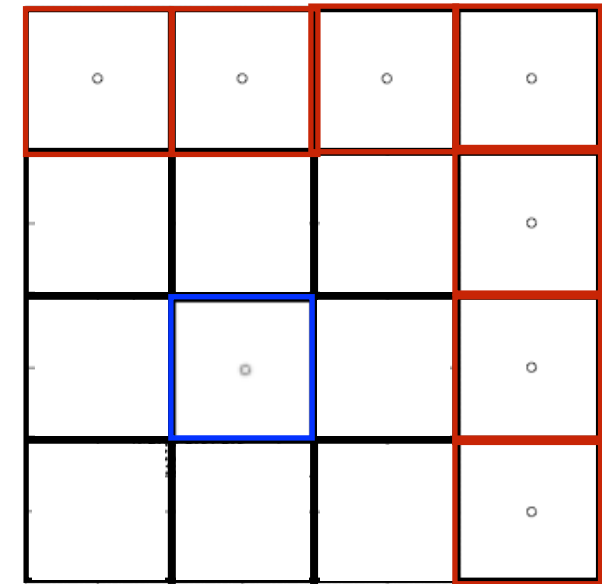
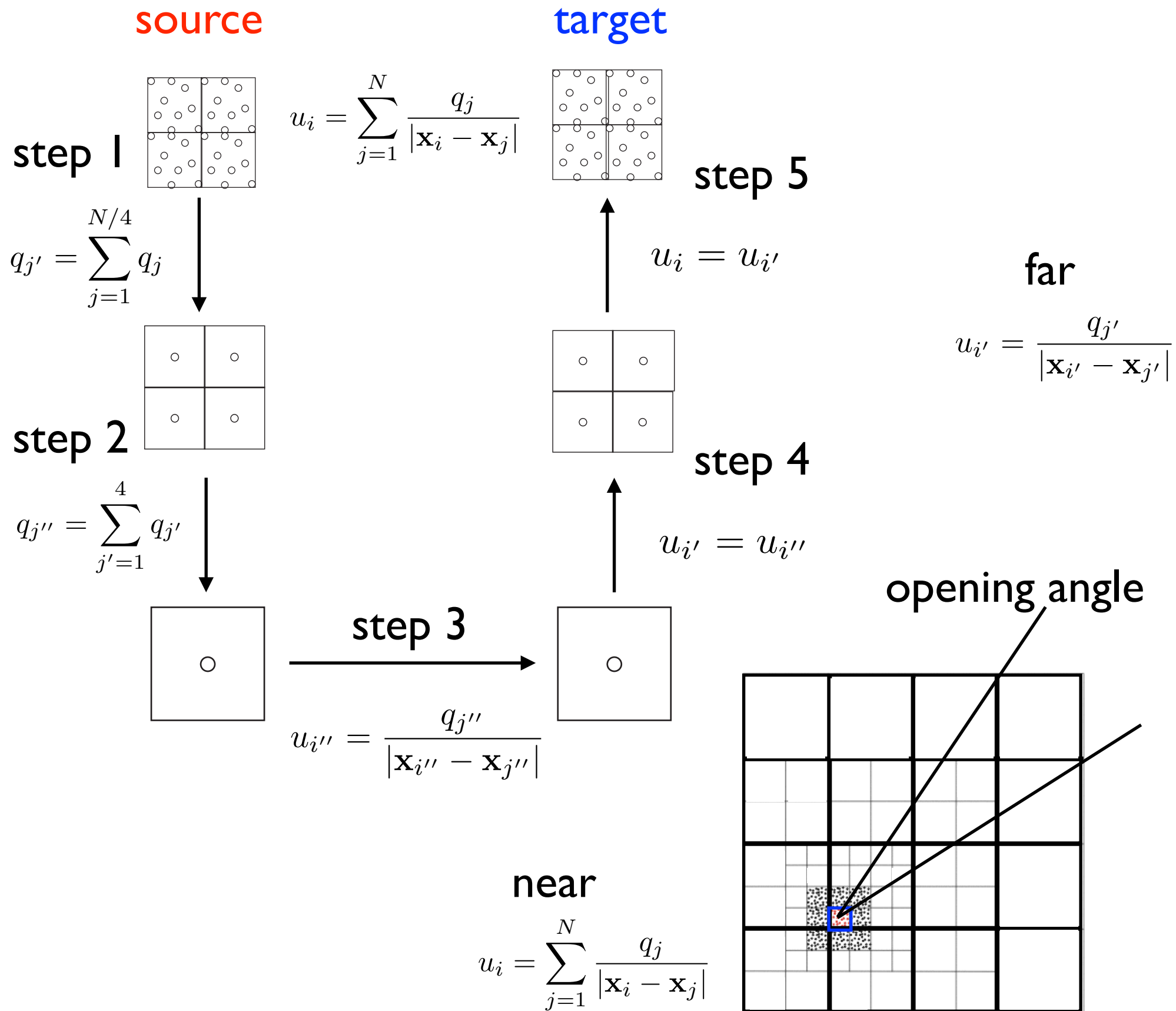
Near-far decomposition



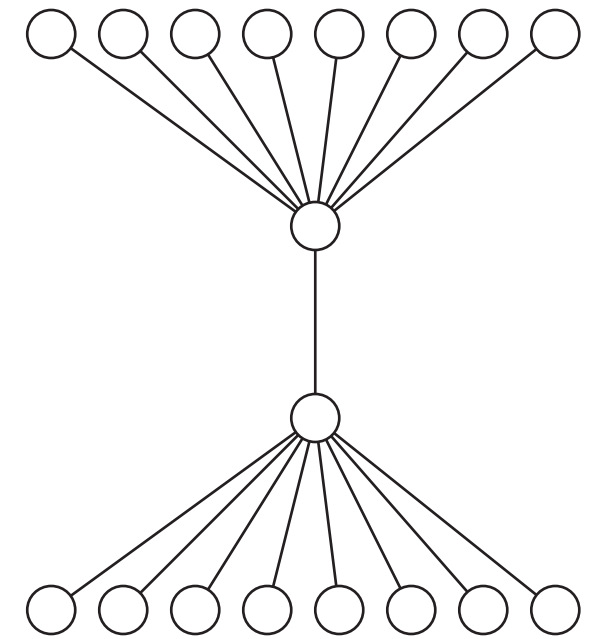
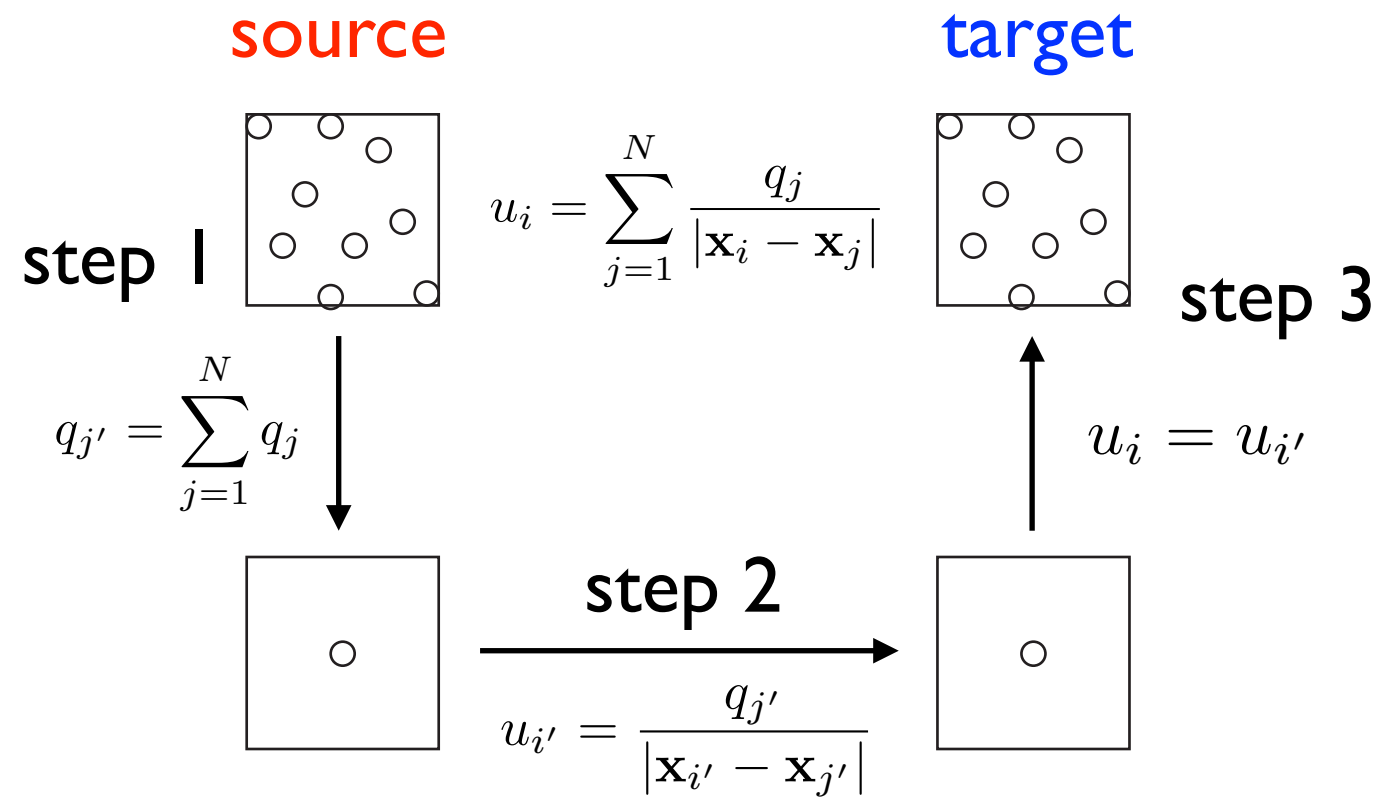
Hierarchical decomposition



Hierarchical near-far decomposition

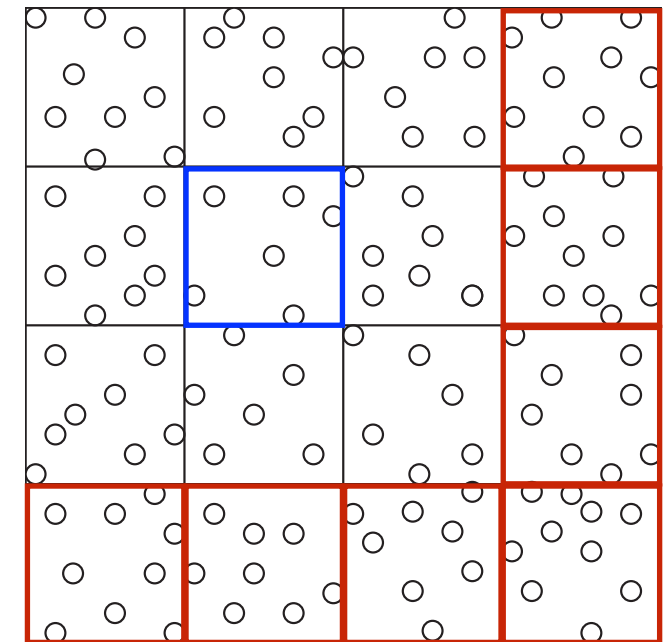
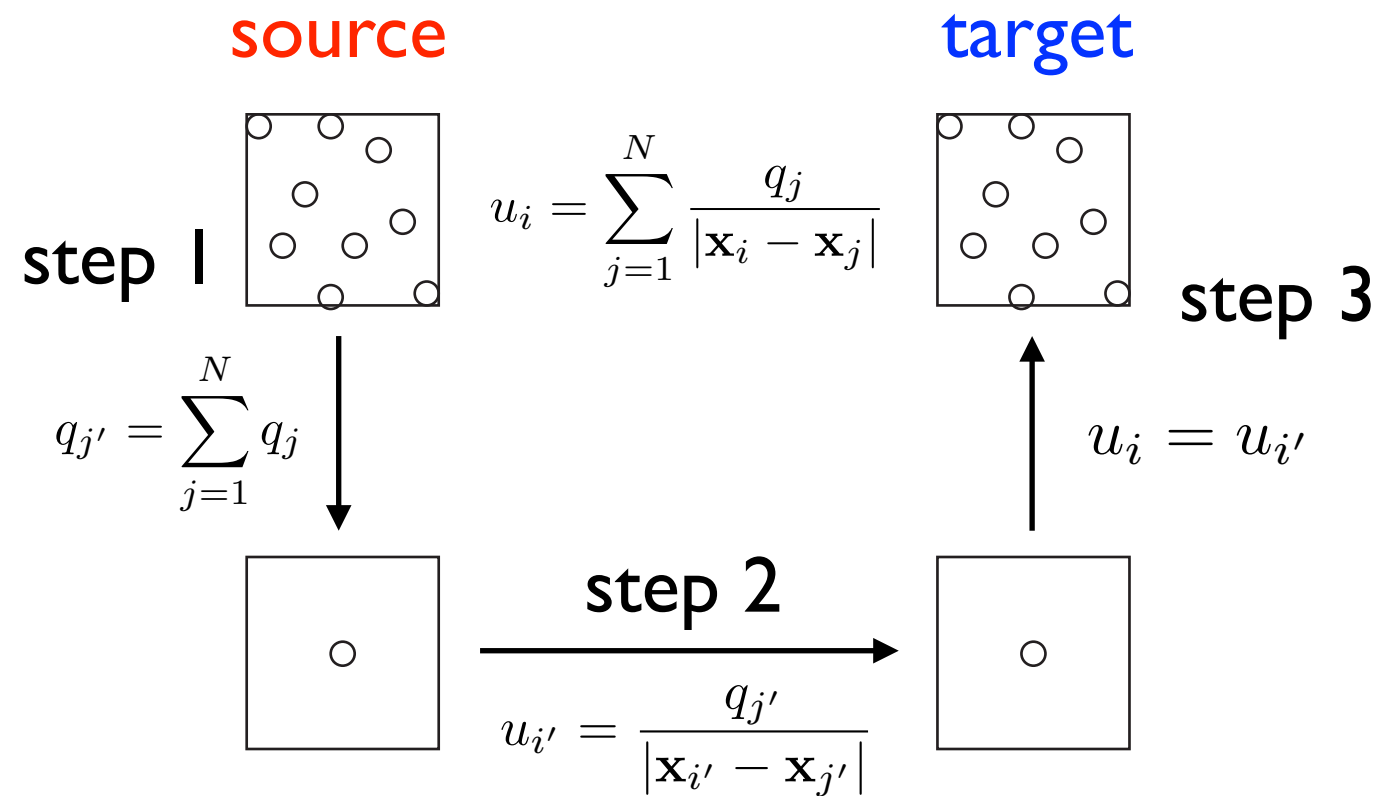


Approximating the interaction



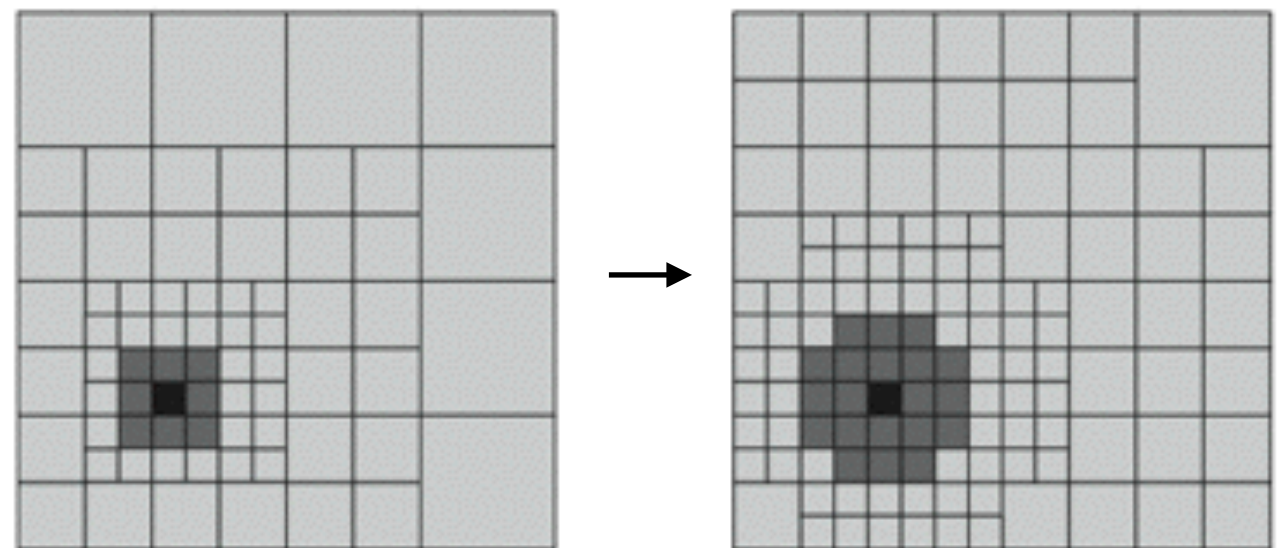
How accurate is the solution?

It depends on the well-separatedness



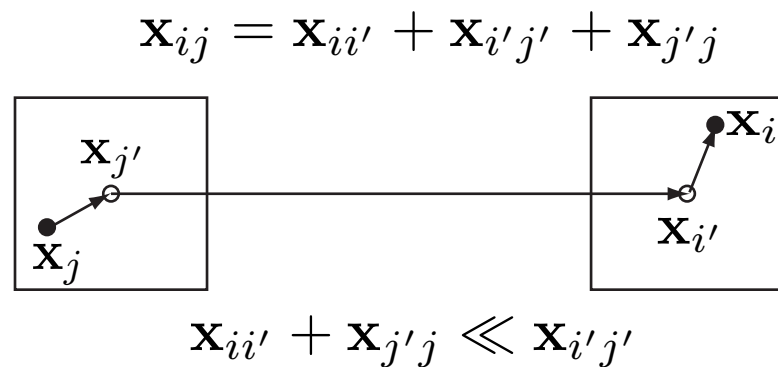
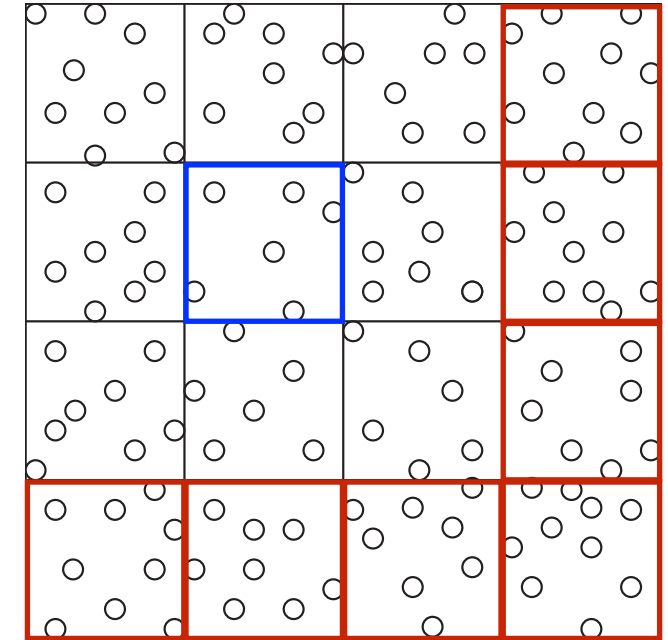
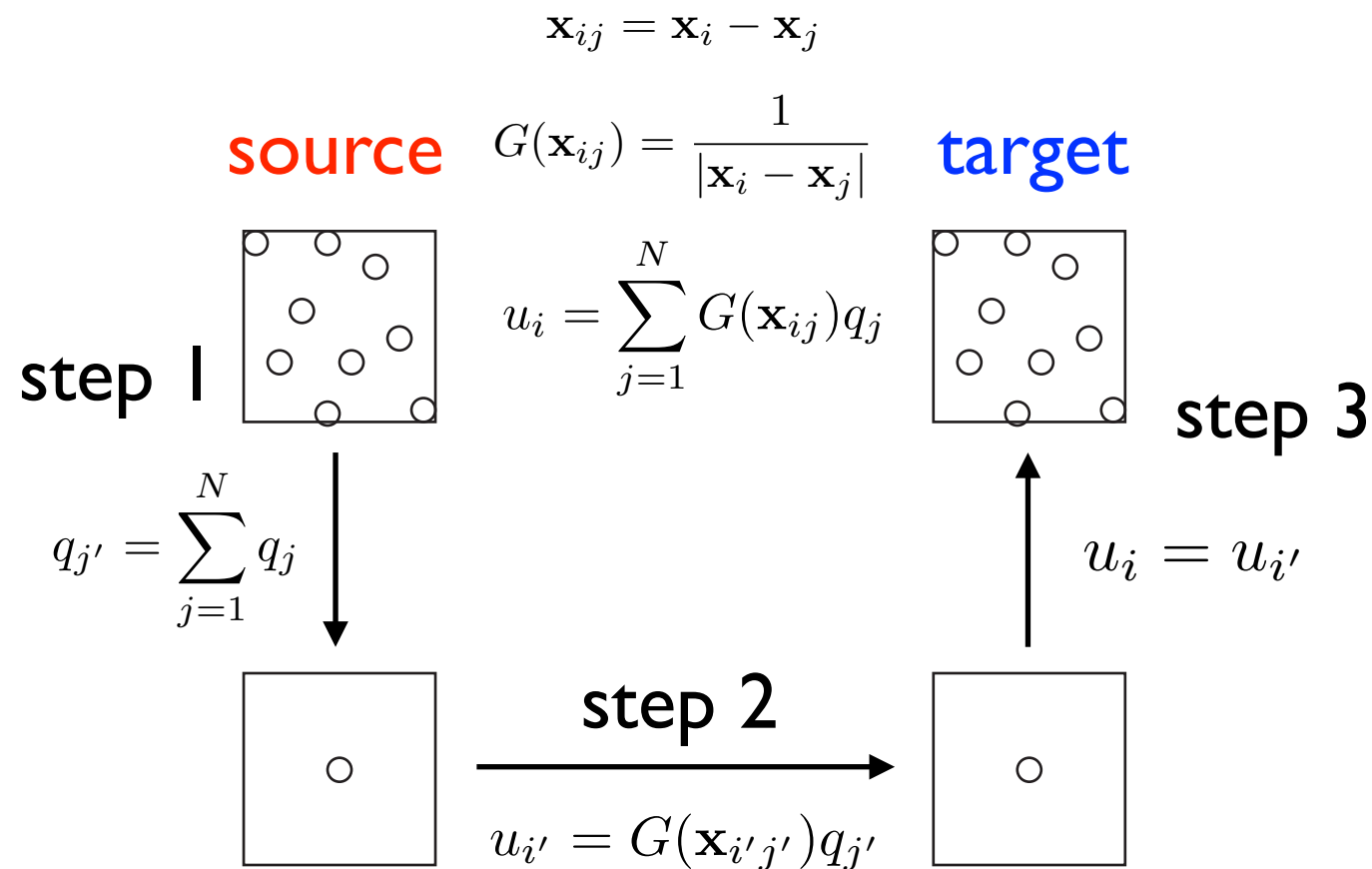
We can separate them more to get an accurate solution

Less approximation



but more boxes to calculate

Higher order approximations



$$G(\mathbf{x}_{ij}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{x}_{ii'} + \mathbf{x}_{j'j})^n \nabla^{(n)} G(\mathbf{x}_{i'j'})$$

Binomial theorem

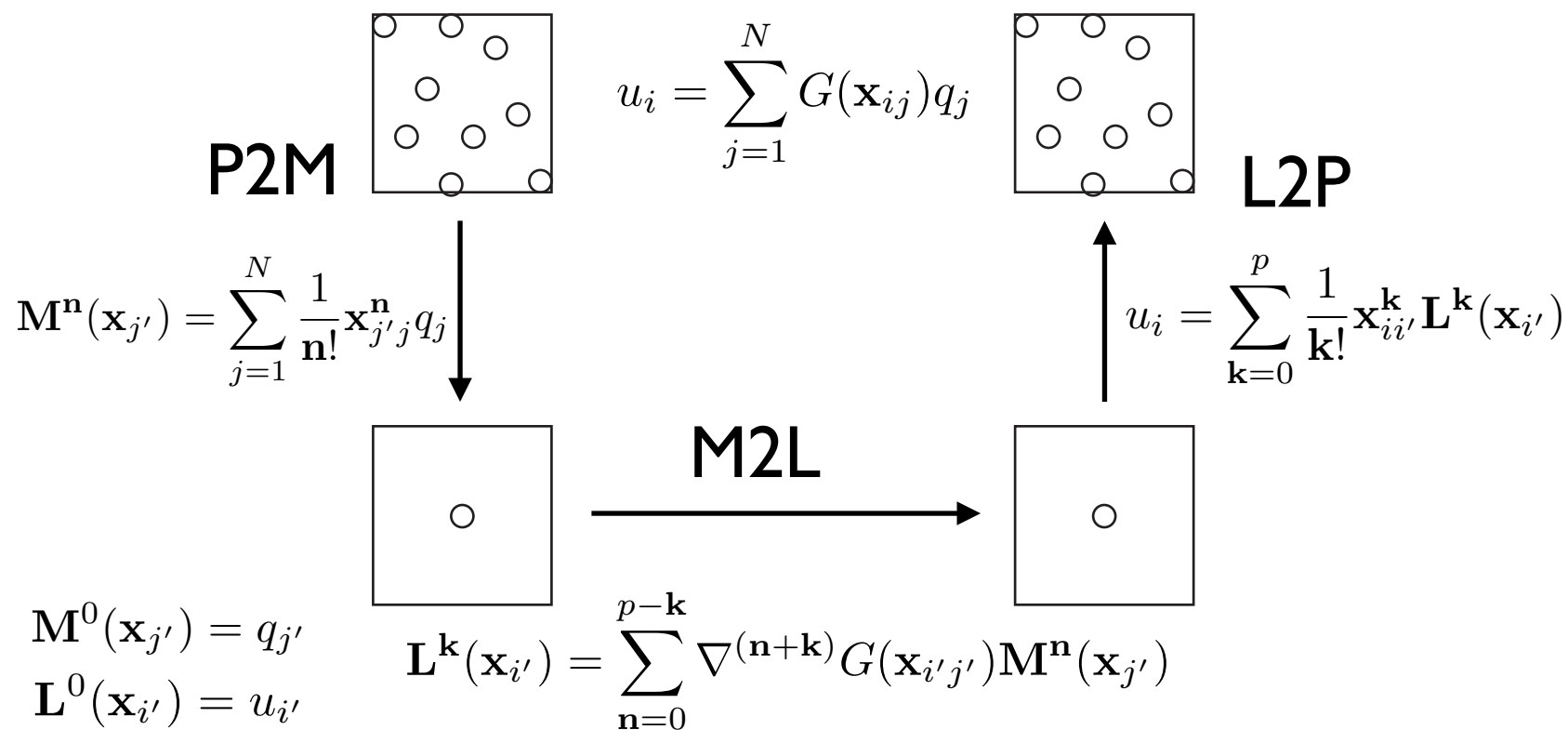
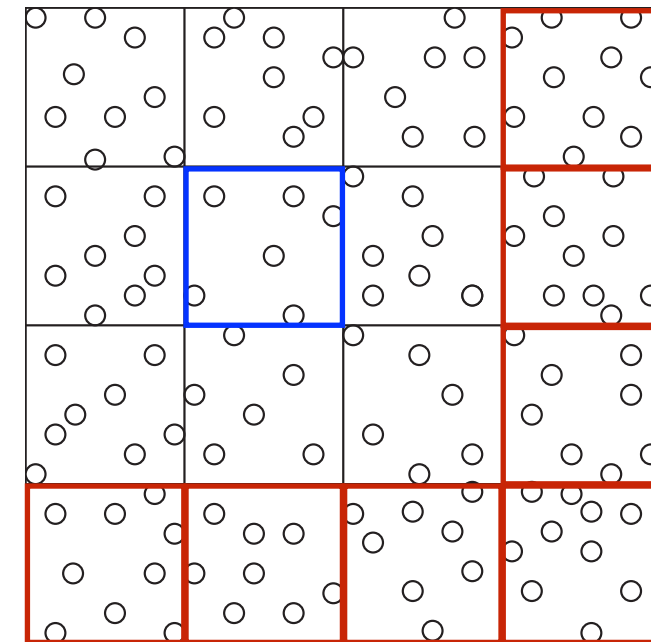
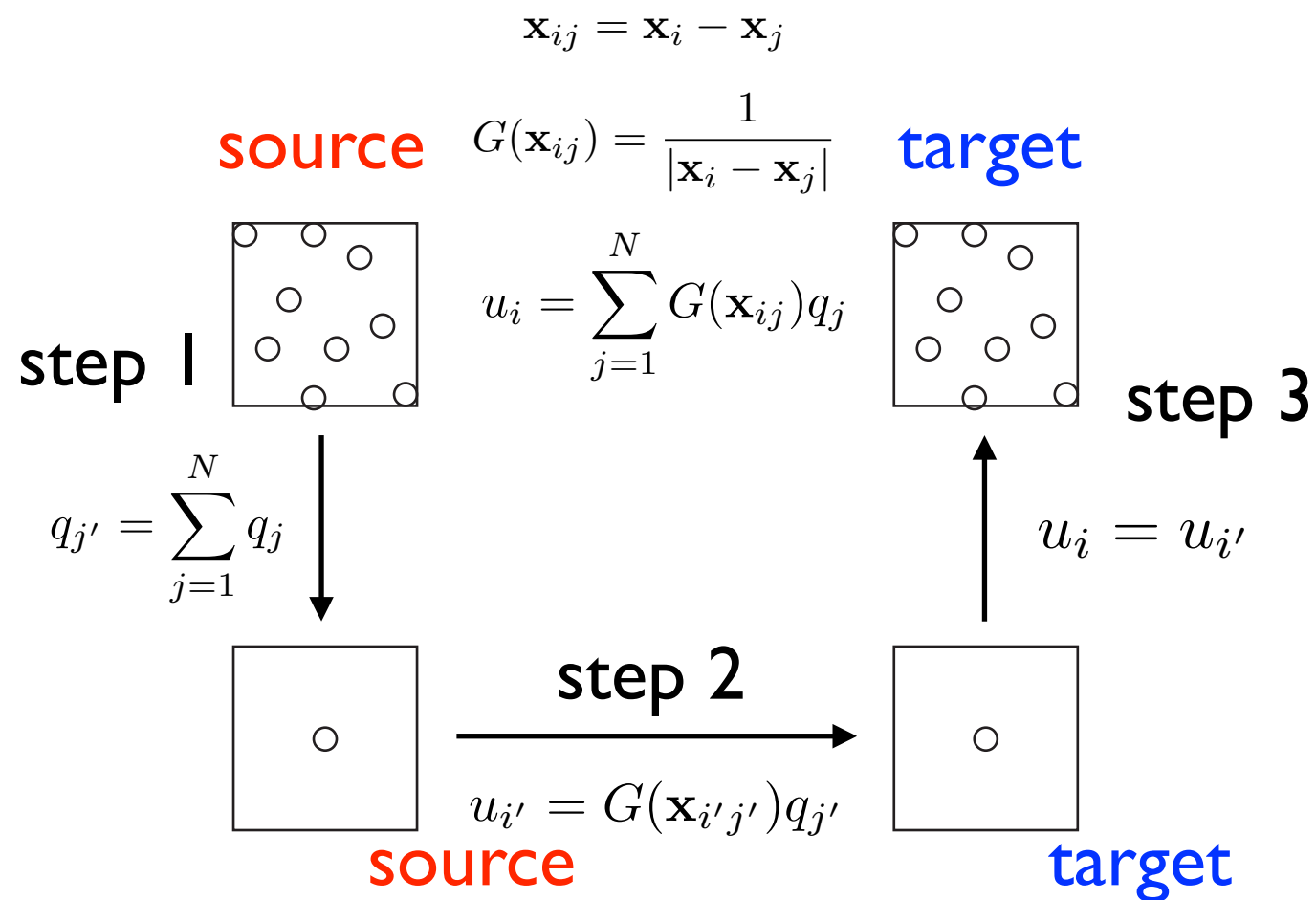
$$(x + y)^n = \sum_{k=0}^n \frac{n!}{(n-k)!k!} x^{n-k} y^k$$

$$\begin{aligned} G(\mathbf{x}_{ij}) &= \sum_{n=0}^p \frac{1}{n!} (\mathbf{x}_{ii'} + \mathbf{x}_{j'j})^n \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\ &\rightarrow = \sum_{n=0}^p \frac{1}{n!} \sum_{k=0}^n \frac{n!}{(n-k)!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^{n-k} \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\ &\xrightarrow{\text{Cancel } n!} = \sum_{n=0}^p \sum_{k=0}^n \frac{1}{(n-k)!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^{n-k} \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\ &\xrightarrow{\text{Swap loop order between } n \text{ and } k} = \sum_{k=0}^p \sum_{n=k}^p \frac{1}{(n-k)!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^{n-k} \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\ &\xrightarrow{\text{Redefine } n-k \text{ to } n} = \sum_{k=0}^p \sum_{n=0}^{p-k} \frac{1}{n!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^n \nabla^{(n+k)} G(\mathbf{x}_{i'j'}) \\ &= \underbrace{\sum_{k=0}^p \frac{1}{k!} \mathbf{x}_{ii'}^k}_{\mathbf{L}} \underbrace{\sum_{n=0}^{p-k} \nabla^{(n+k)} G(\mathbf{x}_{i'j'}) \frac{1}{n!} \mathbf{x}_{j'j}^n}_{\mathbf{M}} \end{aligned}$$

Taylor expansion

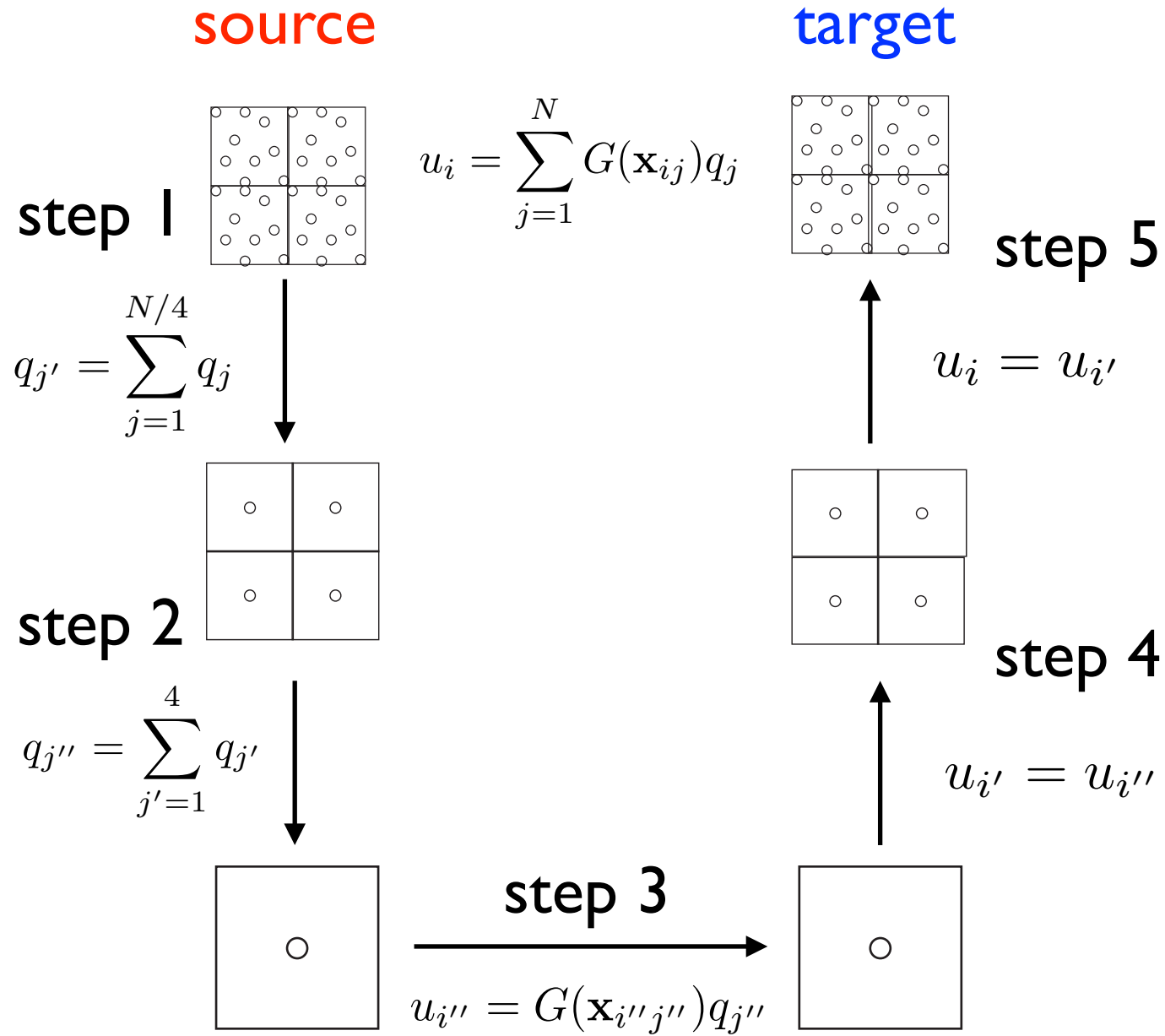
$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x - a)^n$$

Higher order approximations



$$\begin{aligned}
 G(\mathbf{x}_{ij}) &= \sum_{n=0}^p \frac{1}{n!} (\mathbf{x}_{ii'} + \mathbf{x}_{j'j})^n \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\
 &= \sum_{n=0}^p \frac{1}{n!} \sum_{k=0}^n \frac{n!}{(n-k)!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^{n-k} \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\
 &= \sum_{n=0}^p \sum_{k=0}^n \frac{1}{(n-k)!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^{n-k} \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\
 &= \sum_{k=0}^p \sum_{n=k}^p \frac{1}{(n-k)!k!} \mathbf{x}_{ii'}^k \mathbf{x}_{j'j}^{n-k} \nabla^{(n)} G(\mathbf{x}_{i'j'}) \\
 &= \sum_{k=0}^p \frac{1}{k!} \mathbf{x}_{ii'}^k \sum_{n=0}^{p-k} \nabla^{(n+k)} G(\mathbf{x}_{i'j'}) \underbrace{\frac{1}{n!} \mathbf{x}_{j'j}^n}_M \\
 &\quad \underbrace{\hspace{10em}}_L
 \end{aligned}$$

Multi-level case



$$G(\mathbf{x}_{ij}) = \sum_{k=0}^p \frac{1}{k!} \mathbf{x}_{ii''}^k \underbrace{\sum_{n=0}^{p-k} \nabla^{(n+k)} G(\mathbf{x}_{i''j''}) \frac{1}{n!} \mathbf{x}_{j''j}^n}_{\mathbf{L}^k(\mathbf{x}_{i''})}$$

$$\mathbf{x}_{j''j} = \mathbf{x}_{j''j'} + \mathbf{x}_{j'j}$$

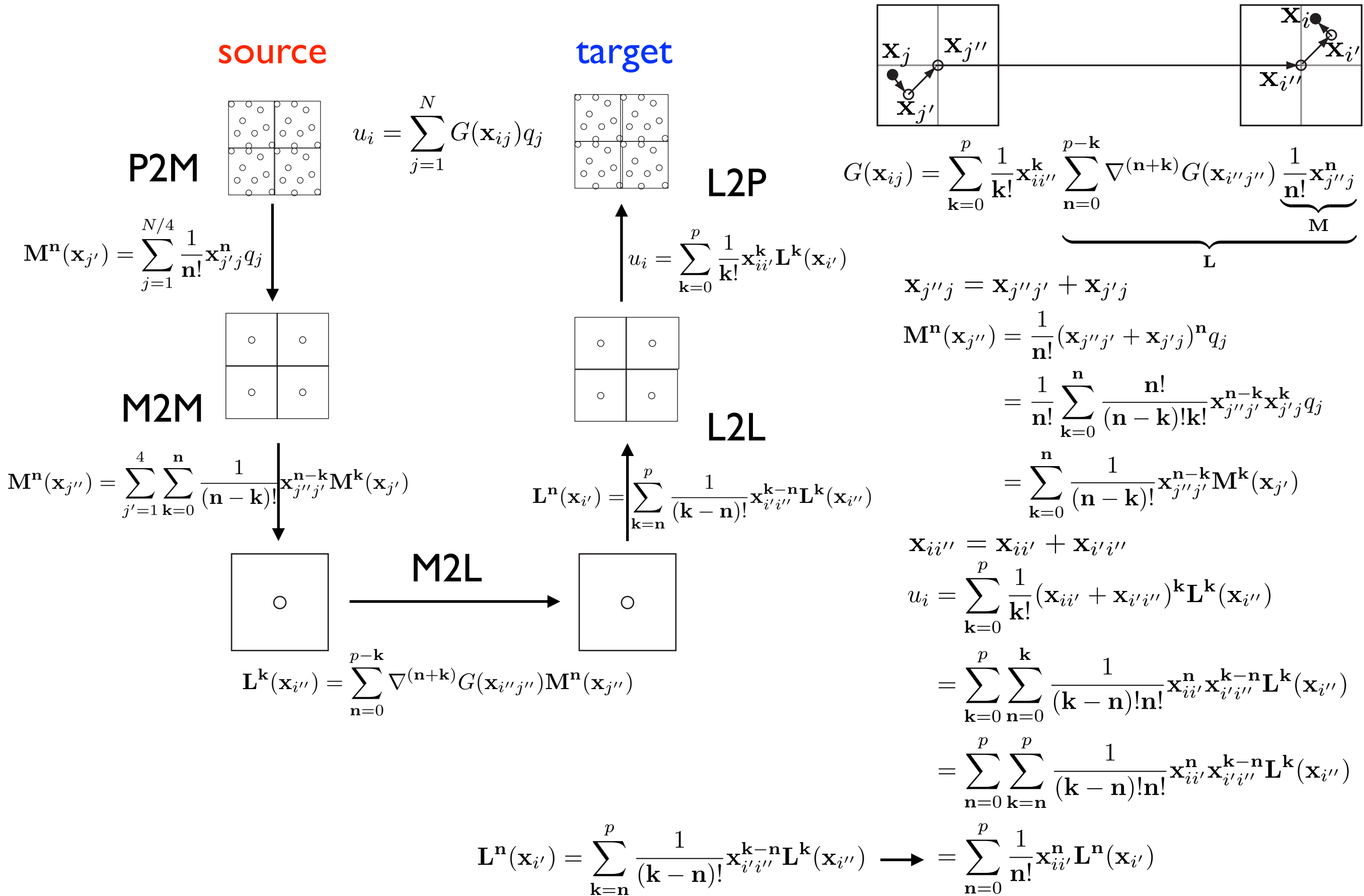
$$\begin{aligned} \mathbf{M}^n(\mathbf{x}_{j''}) &= \frac{1}{n!} (\mathbf{x}_{j''j'} + \mathbf{x}_{j'j})^n q_j \\ &= \frac{1}{n!} \sum_{k=0}^n \frac{n!}{(n-k)!k!} \mathbf{x}_{j''j'}^{n-k} \mathbf{x}_{j'j}^k q_j \\ &= \sum_{k=0}^n \frac{1}{(n-k)!} \mathbf{x}_{j''j'}^{n-k} \mathbf{M}^k(\mathbf{x}_{j'}) \end{aligned}$$

$$\mathbf{x}_{ii''} = \mathbf{x}_{ii'} + \mathbf{x}_{i'i''}$$

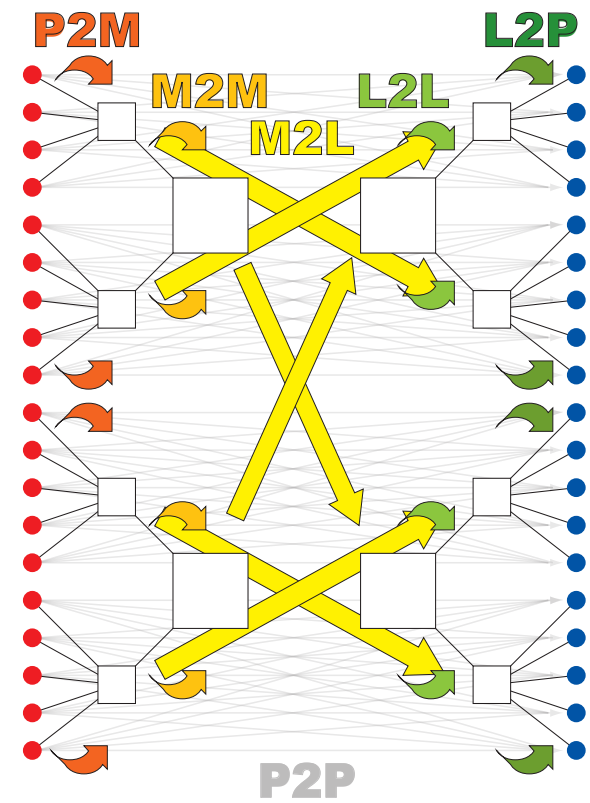
$$\begin{aligned} u_i &= \sum_{k=0}^p \frac{1}{k!} (\mathbf{x}_{ii'} + \mathbf{x}_{i'i''})^k \mathbf{L}^k(\mathbf{x}_{i''}) \\ &= \sum_{k=0}^p \sum_{n=0}^k \frac{1}{(k-n)!n!} \mathbf{x}_{ii'}^n \mathbf{x}_{i'i''}^{k-n} \mathbf{L}^k(\mathbf{x}_{i''}) \\ &= \sum_{n=0}^p \sum_{k=n}^p \frac{1}{(k-n)!n!} \mathbf{x}_{ii'}^n \mathbf{x}_{i'i''}^{k-n} \mathbf{L}^k(\mathbf{x}_{i''}) \end{aligned}$$

$$\mathbf{L}^n(\mathbf{x}_{i'}) = \sum_{k=n}^p \frac{1}{(k-n)!} \mathbf{x}_{i'i''}^{k-n} \mathbf{L}^k(\mathbf{x}_{i''}) \rightarrow \sum_{n=0}^p \frac{1}{n!} \mathbf{x}_{ii'}^n \mathbf{L}^n(\mathbf{x}_{i'})$$

Multi-level case



Flow of Calculation



$$\mathbf{L}^k(\mathbf{x}_{i''}) = \sum_{n=0}^{p-k} \nabla^{(n+k)} G(\mathbf{x}_{i''j''}) \mathbf{M}^n(\mathbf{x}_{j''})$$

$$\mathbf{M}^n(\mathbf{x}_{j''}) = \sum_{j'=1}^4 \sum_{k=0}^n \frac{1}{(n-k)!} \mathbf{x}_{j''j'}^{n-k} \mathbf{M}^k(\mathbf{x}_{j'})$$

$$\mathbf{L}^n(\mathbf{x}_{i'}) = \sum_{k=n}^p \frac{1}{(k-n)!} \mathbf{x}_{i'i''}^{k-n} \mathbf{L}^k(\mathbf{x}_{i''})$$

$$\mathbf{M}^n(\mathbf{x}_{j'}) = \sum_{j=1}^{N/4} \frac{1}{n!} \mathbf{x}_{j'j}^n q_j$$

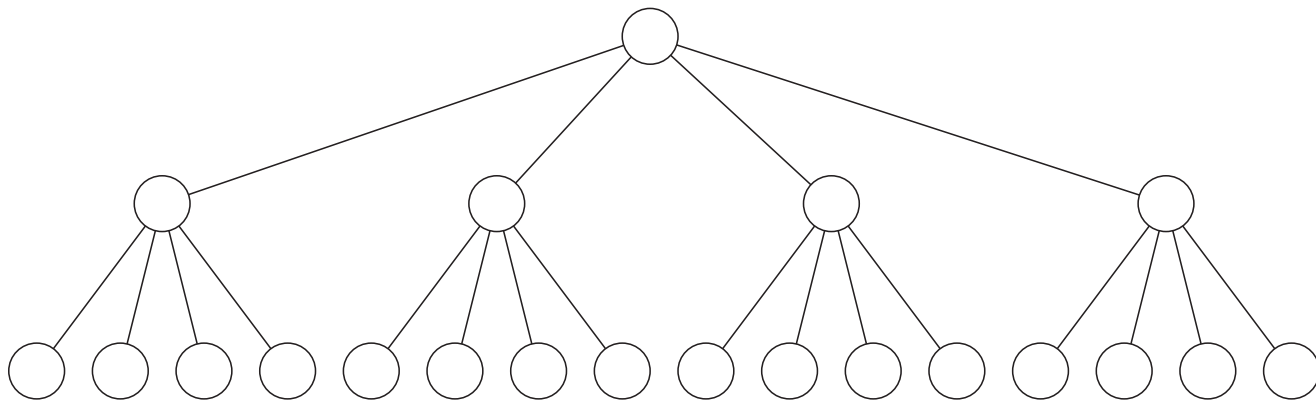
$$u_i = \sum_{k=0}^p \frac{1}{k!} \mathbf{x}_{ii'}^k \mathbf{L}^k(\mathbf{x}_{i'})$$

source particles

target particles

$$u_i = \sum_{j=1}^N G(\mathbf{x}_{ij}) q_j$$

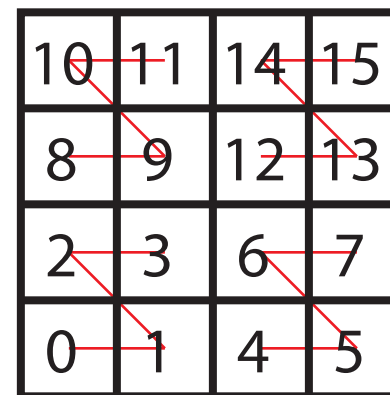
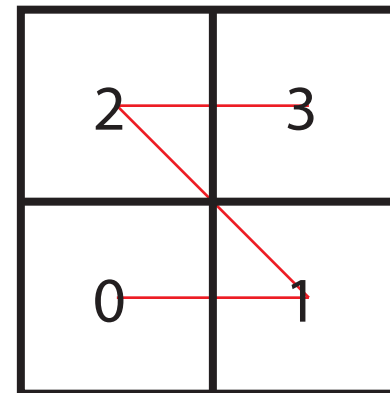
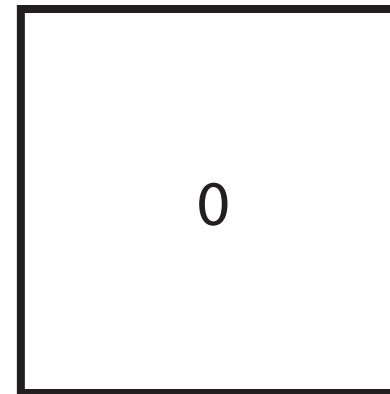
Linked tree



```
struct Cell {  
    Cell *parent;  
    Cell *child[4];  
    double Multipole;  
}
```

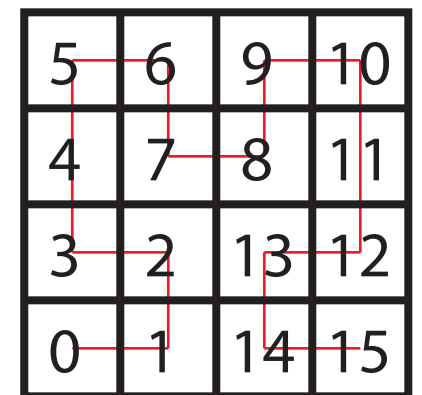
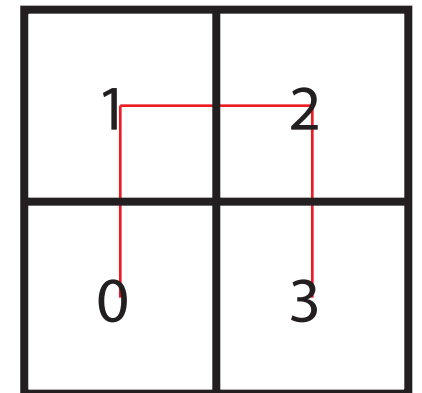
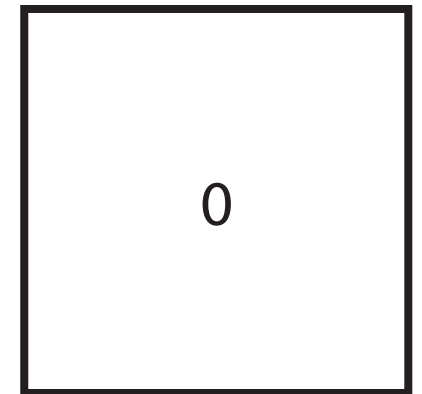
Tree Structure

Morton



Indexed tree

Hilbert



```
int parent = i/4;  
int child[c] = i*4+c;  
Multipole[i]
```

Bit interleaving and space filling curves

42	43	46	47	58	59	62	63
40	41	44	45	56	57	60	61
34	35	38	39	50	51	54	55
32	33	36	37	48	49	52	53
10	11	14	15	26	27	30	31
8	9	12	13	24	25	28	29
2	3	6	7	18	19	22	23
0	1	4	5	16	17	20	21

←
x4

10	11	14	15
8	9	12	13
2	3	6	7
0	1	4	5

←
x4

2	3
0	1

Morton



2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1

2	3	2	3
0	1	0	1
2	3	2	3
0	1	0	1

x4

+

x4

+

A 2x2 grid with black borders. The top-left cell contains the number 2, the top-right cell contains the number 3, the bottom-left cell contains the number 0, and the bottom-right cell contains the number 1. Red lines connect the numbers: a horizontal line from 2 to 3, a horizontal line from 0 to 1, and a diagonal line from 2 to 1.

A 4x4 grid of numbers from 0 to 15. The numbers are arranged in two 2x2 blocks. The top-left block contains 10, 11, 8, 9, 2, 3, 0, 1. The top-right block contains 14, 15, 12, 13, 6, 7, 4, 5. Red lines connect adjacent numbers horizontally and diagonally. Horizontal connections: 10-11, 14-15, 8-9, 12-13, 2-3, 6-7, 0-1, 4-5. Diagonal connections: 10-9, 14-13, 8-7, 12-11, 2-1, 6-5, 0-1, 4-3.

```
level      1
direction  y x
```

$$\begin{matrix} & 1 \\ y & x \end{matrix}$$
$$\begin{array}{cc} 1 & 2 \\ y & x \end{array}$$
$$\begin{array}{cc} 1 & 2 \\ y & x \end{array}$$

1 2 3
y x y x y x

Interleaving the bits

7	42	43	46	47	58	59	62	63
6	40	41	44	45	56	57	60	61
5	34	35	38	39	50	51	54	55
4	32	33	36	37	48	49	52	53
3	10	11	14	15	26	27	30	31
2	8	9	12	13	24	25	28	29
1	2	3	6	7	18	19	22	23
0	0	1	4	5	16	17	20	21
	0	1	2	3	4	5	6	7

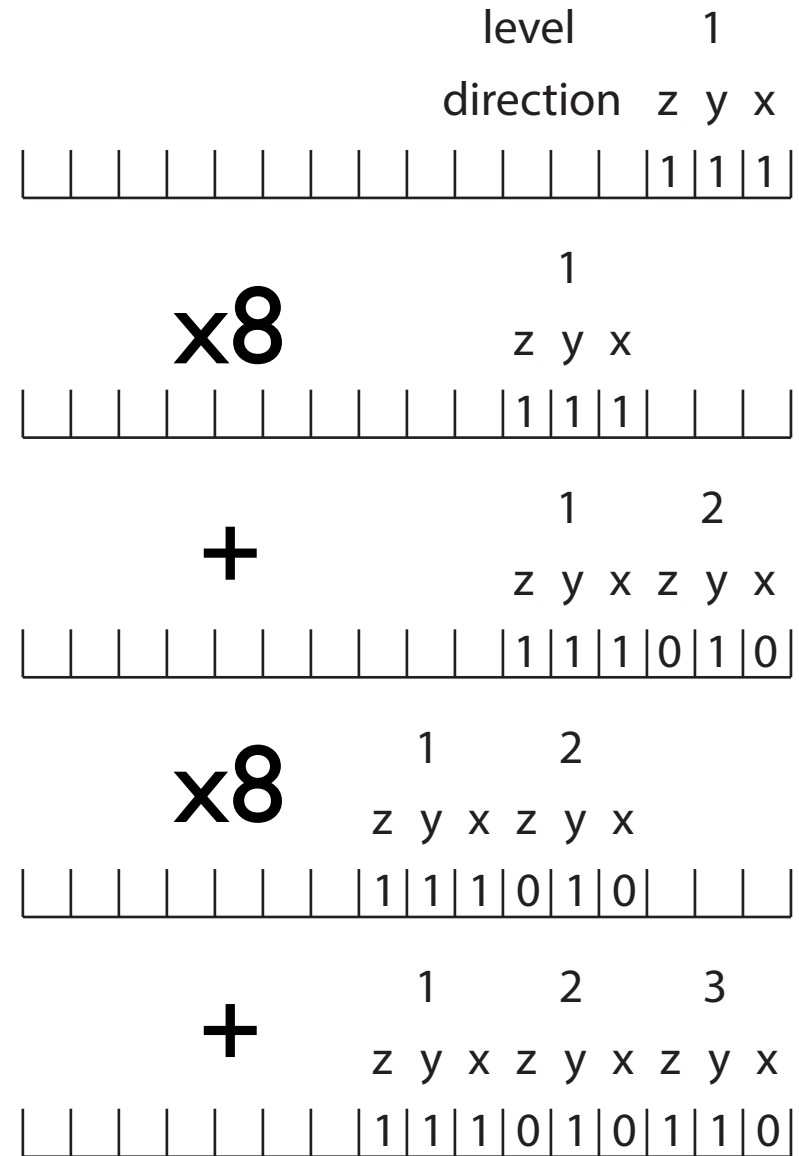
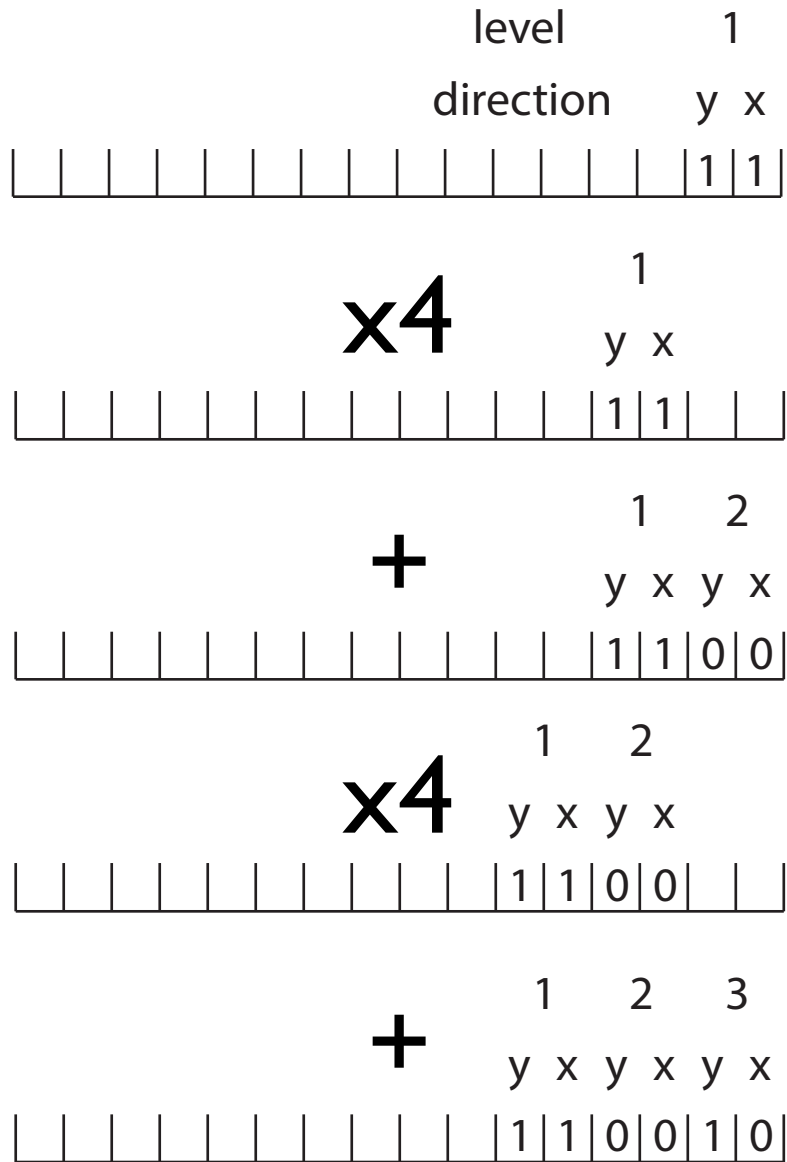
										1	1	0	0	1	0
--	--	--	--	--	--	--	--	--	--	---	---	---	---	---	---

1 2 3
y x y x y x

x															
y															

50 → (4,5)

3-D version


$$(i_x, i_y, i_z) \xrightarrow{\text{interleave bits}} i$$

(ix,iy,iz) ← deinterleave bits i

Neighbor finding

7	21	23	29	31	53	55	61	63
6	20	22	28	30	52	54	60	62
5	17	19	25	27	49	51	57	59
4	16	18	24	26	48	50	56	58
3	5	7	13	15	37	39	45	47
2	4	6	12	14	36	38	44	46
1	1	3	9	11	33	35	41	43
0	0	2	8	10	32	34	40	42
	0	1	2	3	4	5	6	7

Find neighbors of 26

Deinterleave 26 $\rightarrow$ (3,4)

Neighbors
are

(2,5),(3,5),(4,5)
(2,4),(3,4),(4,4)
(2,3),(3,3),(4,3)



25,27,49

24,26,48

13,15,37

Interleave

(ix,iy,iz) $\xrightarrow{\text{interleave bits}}$ i

(ix,iy,iz) $\xleftarrow{\text{deinterleave bits}}$ i

HSS

Stores matrix (algebraic)
Good for multiple r.h.s.
Easy to factorize matrix

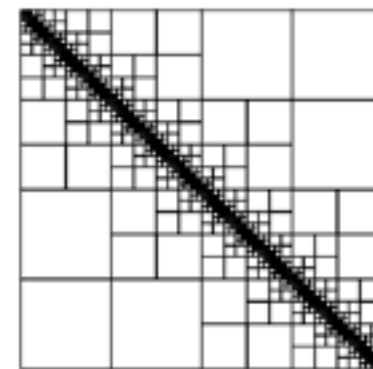
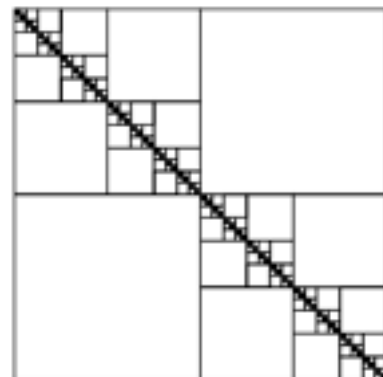
FMM

Matrix-free (geometric)
Low memory footprint
High arithmetic intensity

Weak admissibility
1-D or 2-D problems

Standard admissibility
High dimension problems

HSS2D: Xia, J.
HIF: Ho, K & Ying, L



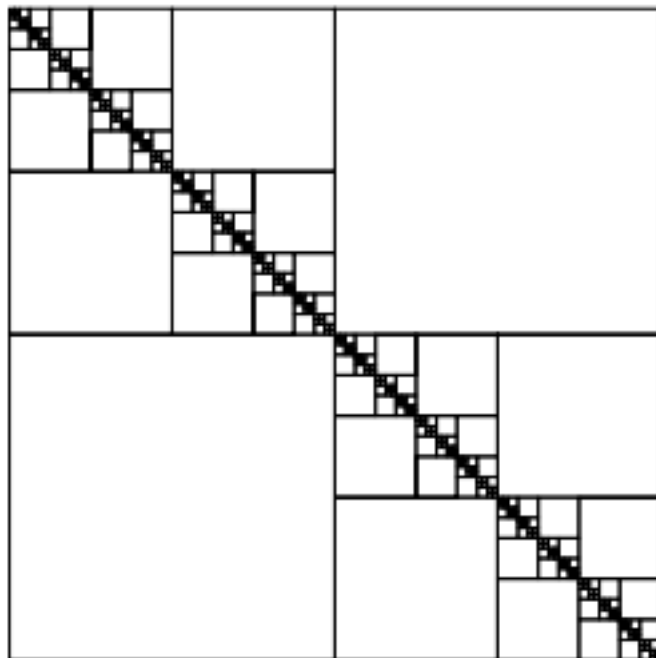
IFMM: Ambikasaran, S
& Darve, E.

Requires:
Numerically low-rank
off-diagonal blocks

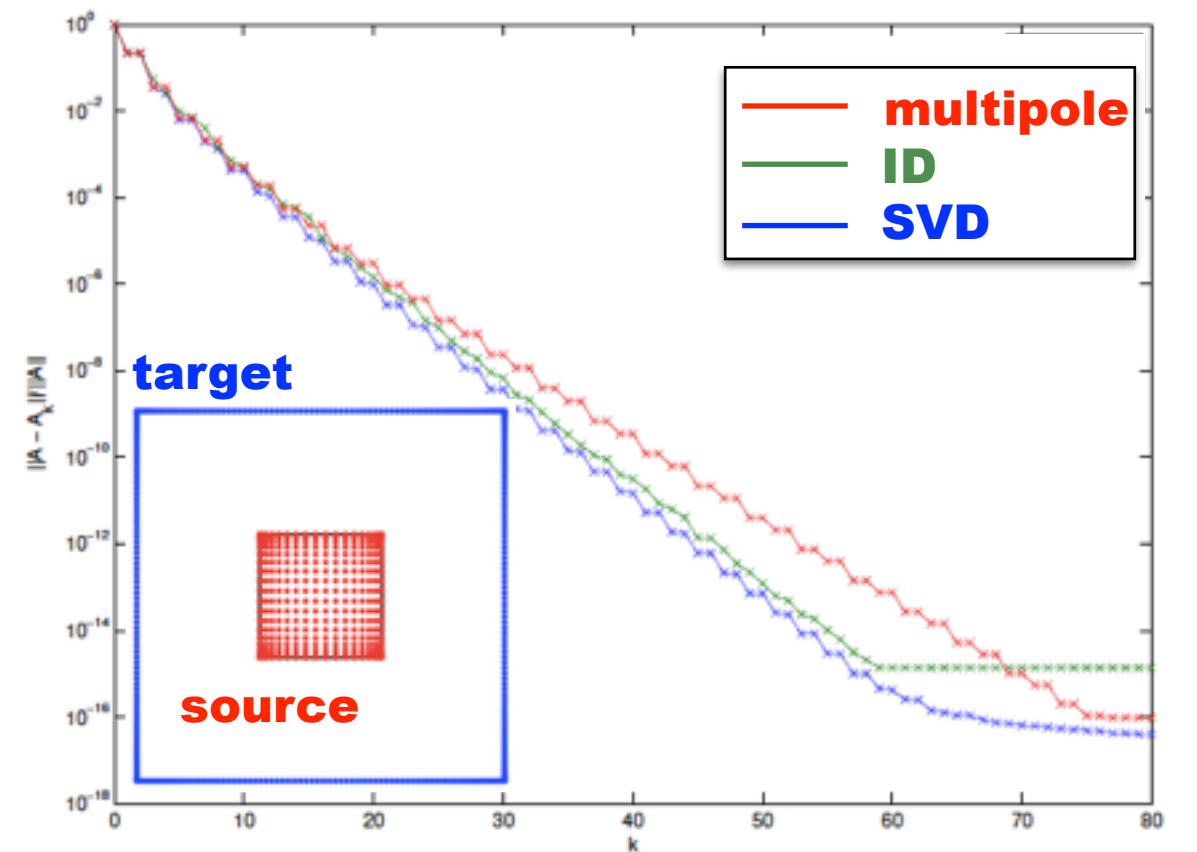
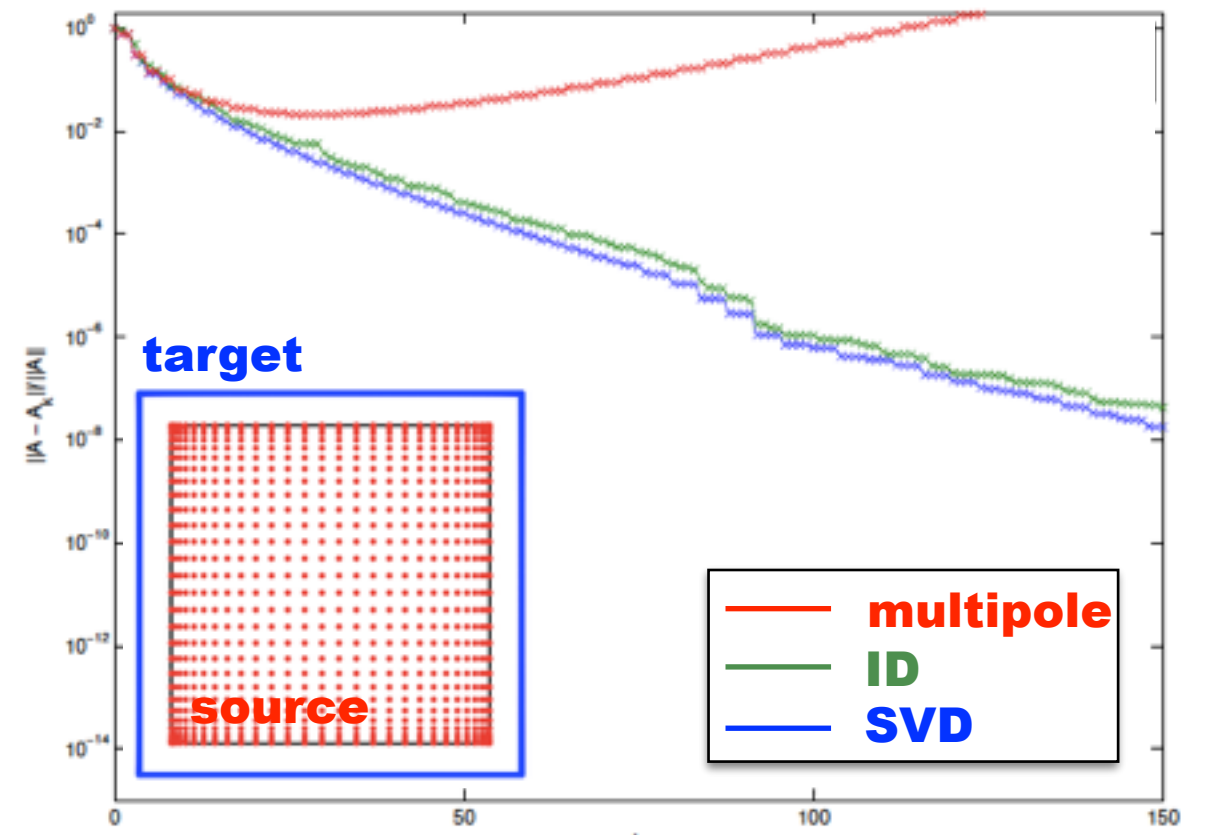
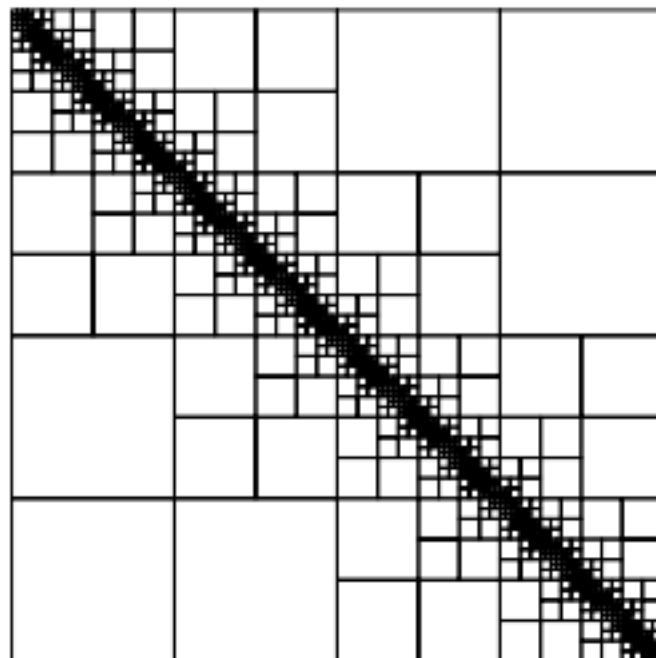
Requires:
analytical form
(doesn't have to be a Green's function)
e.g. kernel-independent/black-box FMM

Admissibility condition

Weak admissibility

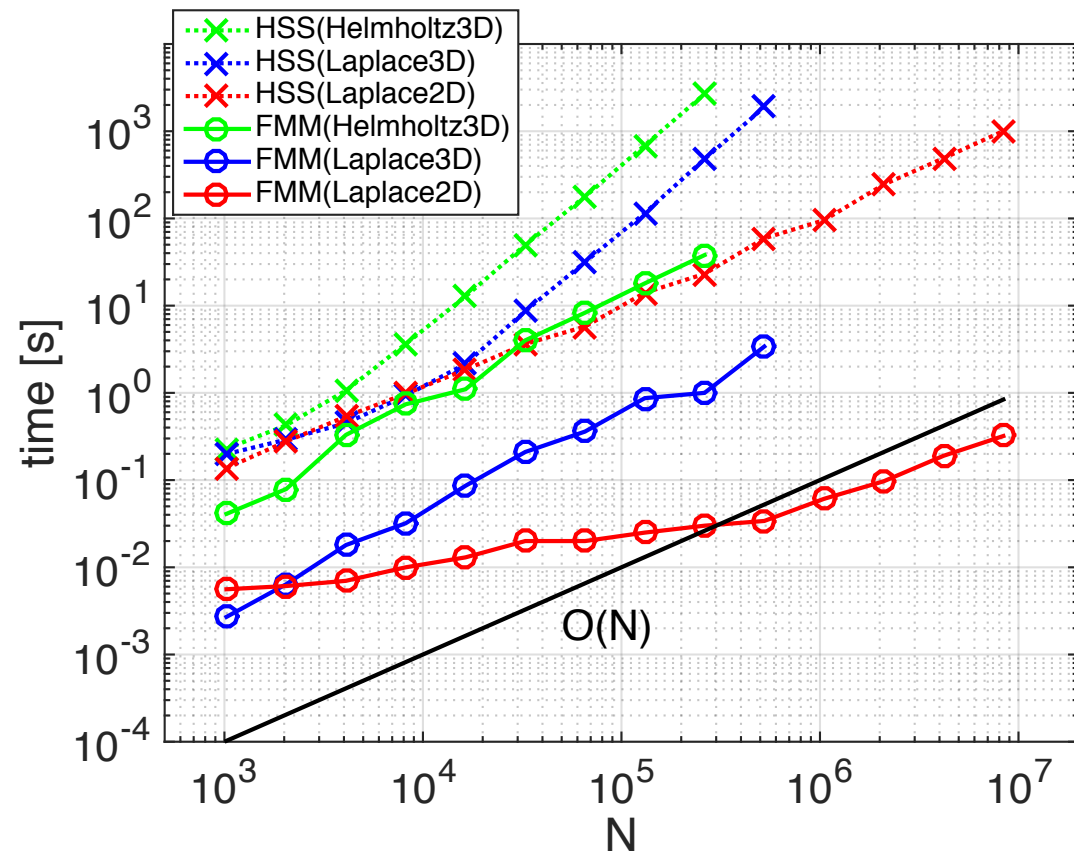


Standard admissibility

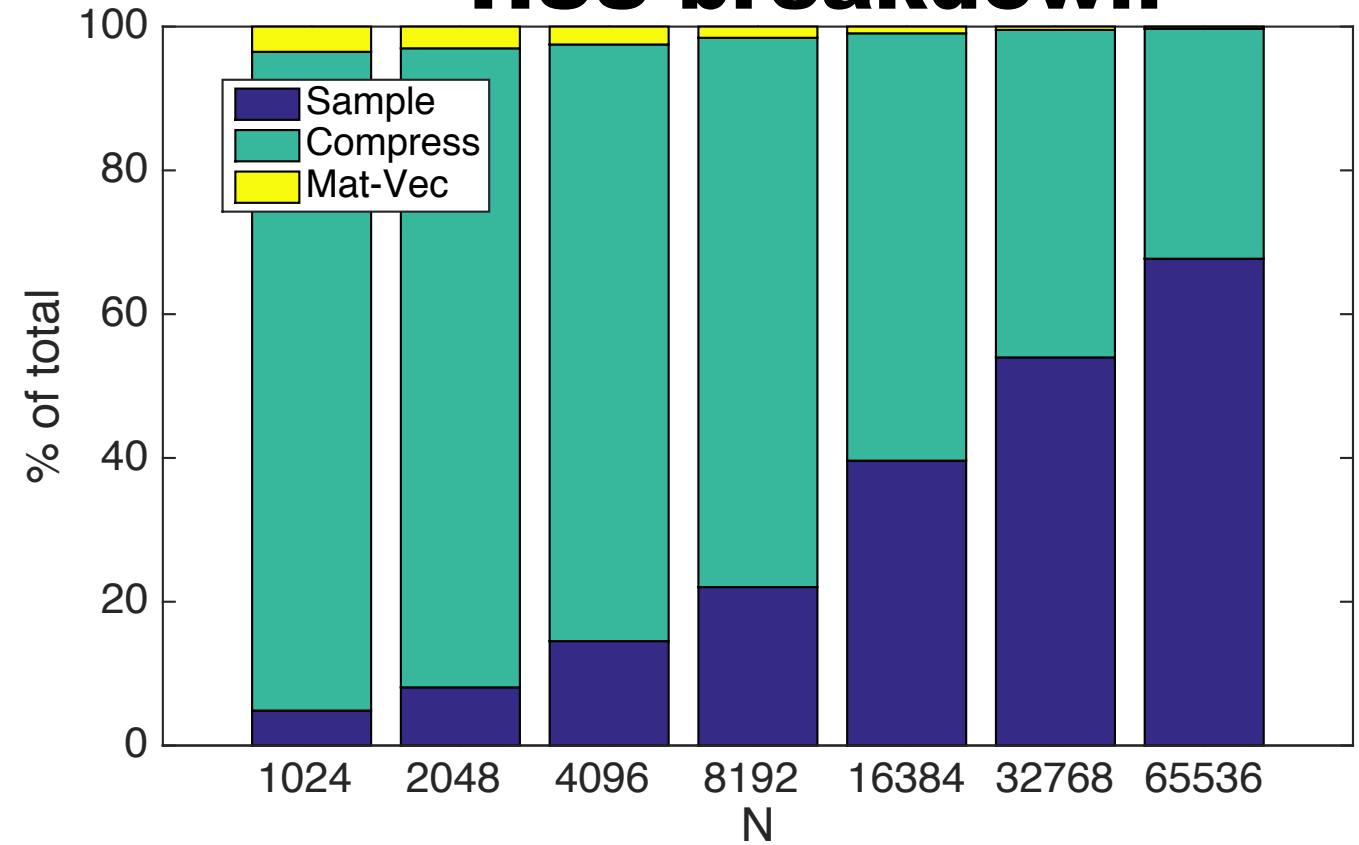


HSS vs FMM

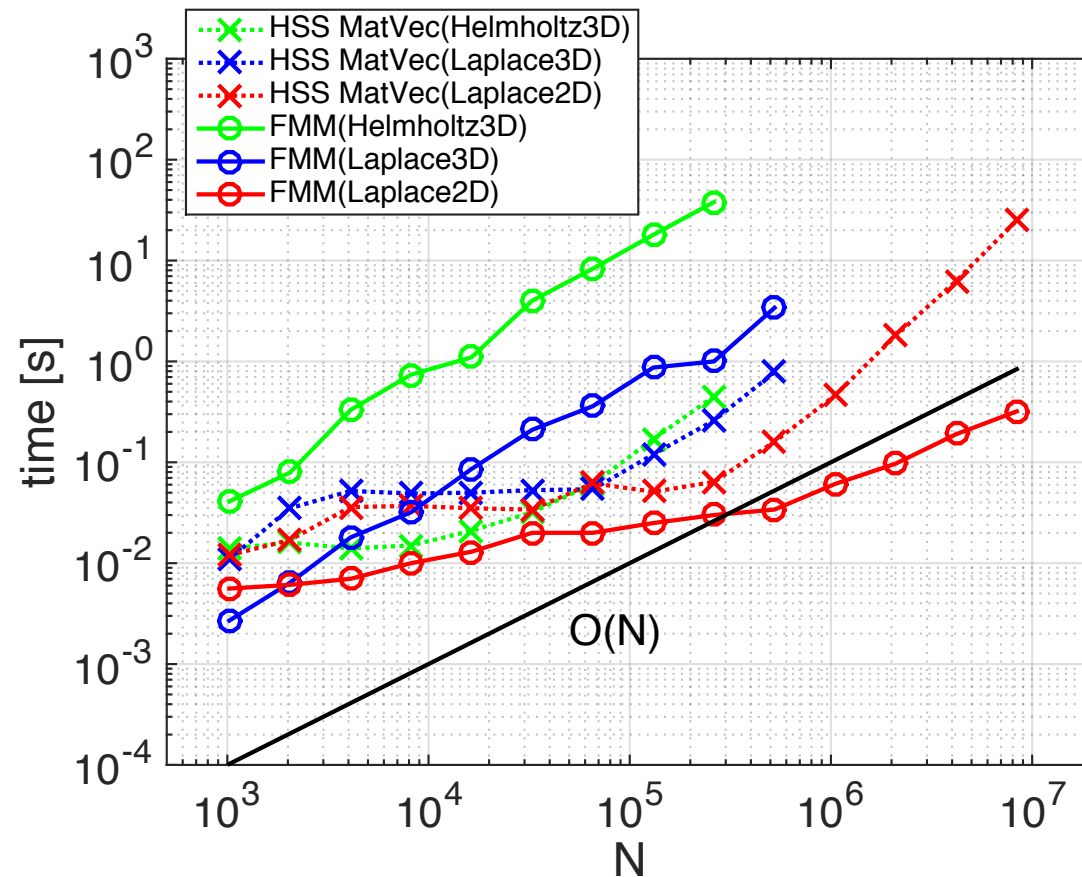
total time



HSS breakdown



Mat-Vec only



1000 Mat-Vecs

