Fast Multipole Method

MAT 280: Laplacian Eigenfunctions

Xiaodong Xue

Department of Mathematics
University of California, Davis

May 25, 2007

Outline

Outline

Motivations

Why to Use Fast Multipole Method?

- The integral kernel which commute with the Laplacian operator is

$$k(\boldsymbol{x},\boldsymbol{y}) = -\frac{1}{2\pi}\log\|\boldsymbol{x}-\boldsymbol{y}\|_2, \quad \boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^2.$$

Motivations

Why to Use Fast Multipole Method?

- The integral kernel which commute with the Laplacian operator is

$$k(\boldsymbol{x},\boldsymbol{y}) = -\frac{1}{2\pi}\log\|\boldsymbol{x}-\boldsymbol{y}\|_2, \quad \boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^2.$$

- The eigenvalue problem

$$\int_\Omega k(\boldsymbol{x},\boldsymbol{y})\phi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \mu\phi(\boldsymbol{x}), \quad \boldsymbol{x}\in\Omega\subset\mathbb{R}^2.$$

Motivations

Why to Use Fast Multipole Method?

- The integral kernel which commute with the Laplacian operator is

$$k(\boldsymbol{x},\boldsymbol{y}) = -\frac{1}{2\pi}\log\|\boldsymbol{x}-\boldsymbol{y}\|_2, \quad \boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^2.$$

- The eigenvalue problem

$$\int_\Omega k(\boldsymbol{x},\boldsymbol{y})\phi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \mu\phi(\boldsymbol{x}), \quad \boldsymbol{x}\in\Omega\subset\mathbb{R}^2.$$

- In terms of matrix,

$$K\phi = \mu\phi,$$

where $K_{i,j} = -\frac{1}{2\pi}\log\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2$, and ϕ can be considered as a vector of charge strengths at points $\boldsymbol{x}_i$, $i = 1, 2, \ldots$.

Motivations . . .

Why to Use Fast Multipole Method? . . .

- Eigenvalue problem $K\phi = \mu\phi$ needs a fast routine to compute matrix vector product.

Why to Use Fast Multipole Method? . . .

- Eigenvalue problem $K\phi = \mu\phi$ needs a fast routine to compute matrix vector product.
- FMM supplies a fast approximation algorithm. Its accuracy is guaranteed by analytic consideration.

Motivations ...

Why to Use Fast Multipole Method? ...

- Eigenvalue problem $K\phi = \mu\phi$ needs a fast routine to compute matrix vector product.
- FMM supplies a fast approximation algorithm. Its accuracy is guaranteed by analytic consideration.
- FMM is insensitive to the distribution of the sampling data.

Outline

$\log \|\boldsymbol{x} - \boldsymbol{y}\|_2$ and Potential

Definition (Potential)

Suppose that a point charge of unit strength is located at point $(x_0, y_0) = \boldsymbol{x}_0 \in \mathbb{R}^2$. Then, for any $\boldsymbol{x} = (x, y) \in \mathbb{R}^2$ with $\boldsymbol{x} \neq \boldsymbol{x}_0$, the potential due to this charge is described by

$$\phi_{\boldsymbol{x}_0}(x, y) = -\log(\|\boldsymbol{x} - \boldsymbol{x}_0\|_2). \tag{1}$$

$\log \|\boldsymbol{x} - \boldsymbol{y}\|_2$ and Potential

Definition (Potential)

Suppose that a point charge of unit strength is located at point $(x_0, y_0) = \boldsymbol{x}_0 \in \mathbb{R}^2$. Then, for any $\boldsymbol{x} = (x, y) \in \mathbb{R}^2$ with $\boldsymbol{x} \neq \boldsymbol{x}_0$, the potential due to this charge is described by

$$\phi_{\boldsymbol{x}_0}(x, y) = -\log(\|\boldsymbol{x} - \boldsymbol{x}_0\|_2). \qquad (1)$$

Fact 1

Let $z = x + \mathrm{i}y,\ z_0 = x_0 + \mathrm{i}y_0\ \in \mathbb{C}$. We have $\phi_{\boldsymbol{x}_0}(\boldsymbol{x}) = \mathrm{Re}(-\log(z - z_0))$.

$\log \|\boldsymbol{x} - \boldsymbol{y}\|_2$ and Potential

Definition (Potential)

Suppose that a point charge of unit strength is located at point $(x_0, y_0) = \boldsymbol{x}_0 \in \mathbb{R}^2$. Then, for any $\boldsymbol{x} = (x, y) \in \mathbb{R}^2$ with $\boldsymbol{x} \neq \boldsymbol{x}_0$, the potential due to this charge is described by

$$\phi_{\boldsymbol{x}_0}(x, y) = -\log(\|\boldsymbol{x} - \boldsymbol{x}_0\|_2). \tag{1}$$

Fact 1

Let $z = x + \mathrm{i}y,\ z_0 = x_0 + \mathrm{i}y_0 \ \in \mathbb{C}$. We have $\phi_{\boldsymbol{x}_0}(\boldsymbol{x}) = \mathrm{Re}(-\log(z - z_0))$.

Fact 2

$$\log(1 - w) = -\sum_{k=1}^{\infty} \frac{w^k}{k},$$

which is valid for any $w \in \mathbb{C}$ with $|w| < 1$.

Lemma

Let a point charge of strength q be located at z_0. Then for any z such that $|z| > |z_0|$,

$$\phi_{z_0}(z) = q \log(z - z_0) = q \left(\log z - \sum_{k=1}^{\infty} \frac{1}{k} \left(\frac{z_0}{z} \right)^k \right). \tag{2}$$

$\log \|x - y\|_2$ and Potential ...

Lemma

Let a point charge of strength q be located at z_0. Then for any z such that $|z| > |z_0|$,

$$\phi_{z_0}(z) = q \log(z - z_0) = q \left(\log z - \sum_{k=1}^{\infty} \frac{1}{k} \left(\frac{z_0}{z} \right)^k \right). \tag{2}$$

Notice:

Given a set of particles $\mathcal{S} = \{z_1, z_2, \ldots, z_m\}$ and their strengths $\{q_1, q_2, \cdots, q_m\}$, then the potential at z due to the set $\mathcal{S}$ will be

$$\phi(z) = \sum_{i=1}^{m} \phi_{z_i}(z) = \sum_{i=1}^{m} q_i \log(z - z_i).$$

Outline

Multipole Expansion

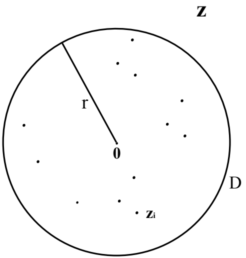
Theorem (Multipole Expansion)

Suppose that m *charges of strengths* $\{q_i,\ i=1,\ldots,m\}$ *are located at points* $\{z_i,\ i=1,\ldots,m\}$, *with* $|z_i|<r$. *Then for any* z *with* $|z|>r$, *the potential* $\phi(z)$ *induced by the charges is given by*

$$\phi(z) = Q\log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k}, \tag{3}$$

where

$Q = \sum_{i=1}^{m} q_i$ *and* $a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k}$.



Multipole Expansion . . .

Error Bound of Multipole Expansion

For any $p \geq 1$,

$$\left| \phi(z) - Q\log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \text{const} \cdot \left| \frac{r}{z} \right|^p, \tag{4}$$

Multipole Expansion ...

Error Bound of Multipole Expansion

For any $p \geq 1$,

$$\left| \phi(z) - Q\log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \text{const} \cdot \left| \frac{r}{z} \right|^p, \tag{4}$$

Distant Parameter c

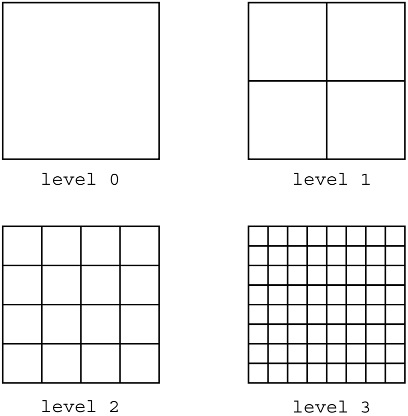
Let $c \triangleq \left| \frac{z}{r} \right| = 2$, then the error bound will be

$$\left| \phi(z) - Q\log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \text{const} \cdot \left(\frac{1}{2} \right)^p, \tag{5}$$

and if we want to obtain the a relative precision ε, p must be of the order $-\log_2(\varepsilon)$.

Outline

A 2D domain and Quadtree

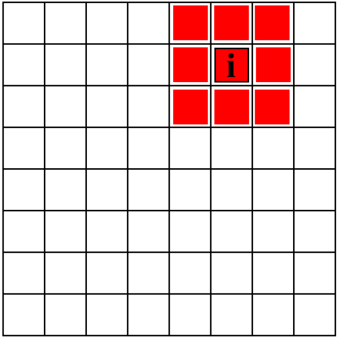


Quadtree structure induced by a uniform subdivision of a square domain.

A 2D Domain and Quadtree . . .

Definition (Near Neighbors)

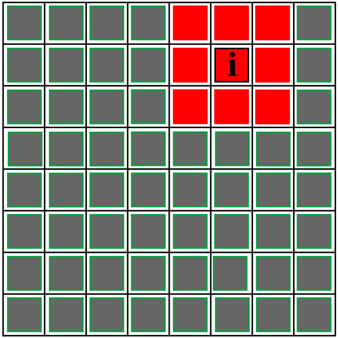
Two boxes are said to be **near neighbors** if they are at the same refinement level and share a boundary point. A box is a near neighbor of itself.



A 2D Domain and Quadtree . . .

Definition (Well Separated)

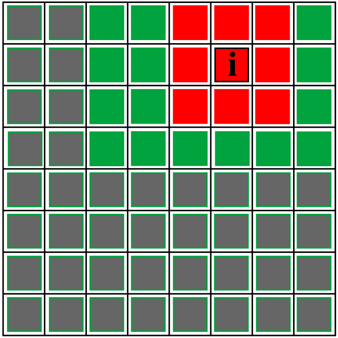
Two boxes are said to be **well separated** if they are at the same refinement level and are not near neighbors.



A 2D Domain and Quadtree . . .

Definition (Interaction List)

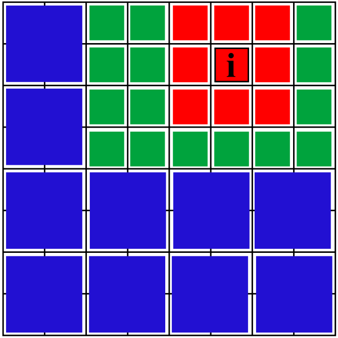
Each box i has its own **interaction list**, consisting of the children of the near neighbors of i's parent which are well separated from box i.



A 2D Domain and Quadtree . . .

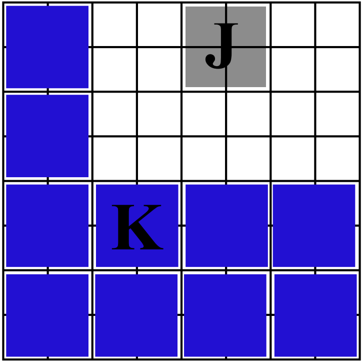
Hierarchical Structure

Notice that the blue boxes in are the interaction list of i's parent.



Outline

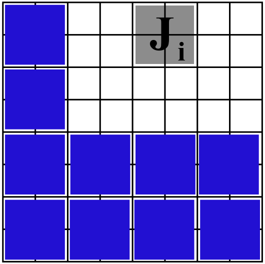
Interaction List and Multipole Expansion



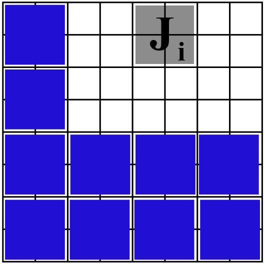
Application of the Theorem of Multipole Expansion

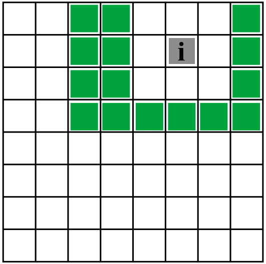
For two boxes J and K, they are well separated and the **distance parameter** $c > 2$, which allows us to use truncated multipole expansion.

Hierarchical Algorithm

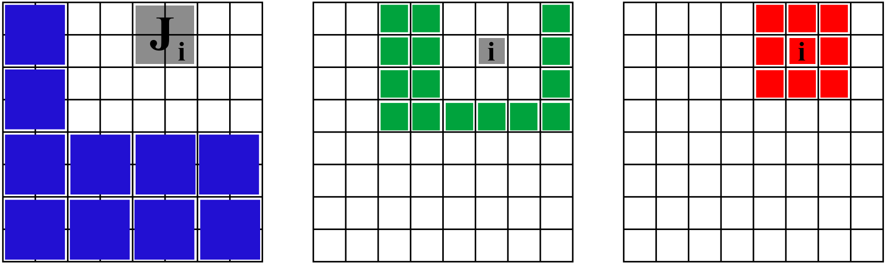


Hierarchical Algorithm

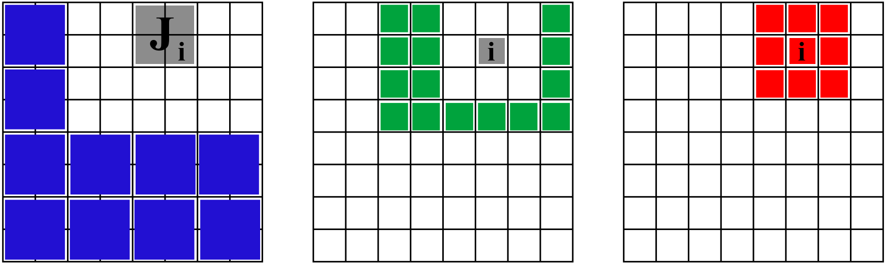




Hierarchical Algorithm



Hierarchical Algorithm



Computation Cost: $O(N \log N)$

$$\left| \phi(z) - Q \log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \text{const} \cdot \left(\frac{1}{2} \right)^p ,$$

To prepare the coefficients $\{a_k\}_{k=1}^{p}$, each particle will be used p times. Therefore, for each level, the computation cost is about $O(Np)$. And the total number of levels will be approximately $\log N$.

Outline

Translation of Multipole Expansion

Theorem (Translation of a multipole expansion)

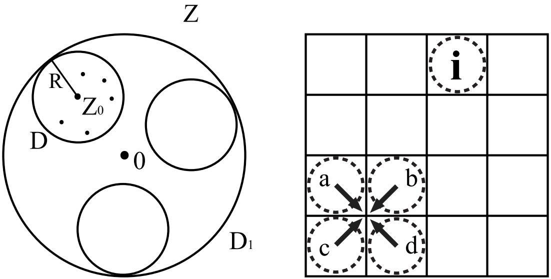
Suppose that

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k} \tag{6}$$

is a multipole expansion of the potential due to a set of m charges of strength $q_1, q_2, \ldots, q_m$, all of which are located inside the circle D of radius R with center at z_0. Then for z outside the circle D_1 of radius $(R + |z_0|)$ and center at the origin,

$$\phi(z) = a_0 \log(z) + \sum_{l=1}^{\infty} \frac{b_l}{z^l}, \tag{7}$$

Translation of Multipole Expansion . . .



(a) (b)

Translation from the Children to the Parent

Fig.(a) shows that the multipole expansion about child disk D can be translated to the multipole expansion about the parent disk D_1. Fig.(b) shows the similar behavior of the quadtree structure.

Error Bound for Translation of Multipole Expansion

The translation of the multipole expansion

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k} \Rightarrow \phi(z) = a_0 \log(z) + \sum_{l=1}^{\infty} \frac{b_l}{z^l},$$

where $b_l = -\frac{a_0 z_0^l}{l} + \sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1}$. Furthermore, for any $p \geq 1$,

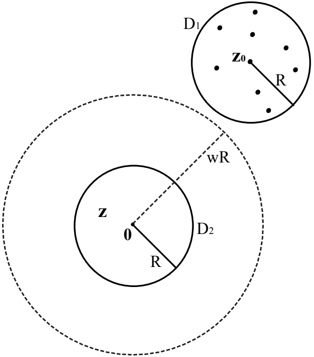
$$\left| \phi(z) - a_0 \log(z) - \sum_{l=1}^{p} \frac{b_l}{z^l} \right| \leq \left(\frac{A}{1 - \left| \frac{|z_0| + R}{z} \right|} \right) \left| \frac{|z_0| + R}{z} \right|^{p+1} \quad (8)$$

Conversion of a Multipole Expansion (MP) into a Local Expansion (LP)

Theorem (Multipole expansion $\Rightarrow$ local expansion)

Suppose that m charges are located inside the circle D_1 with radius R and center at z_0, and that $|z_0| > (w+1)R$ with $w > 1$. Then the corresponding multipole expansion (6) *converges inside the circle D_2 of radius R center at origin. Inside D_2,*

$$\phi(z) = \sum_{l=0}^{\infty} b_l \cdot z^l, \qquad (9)$$



Conversion of a MP into a LP ...

Theorem Continued ...

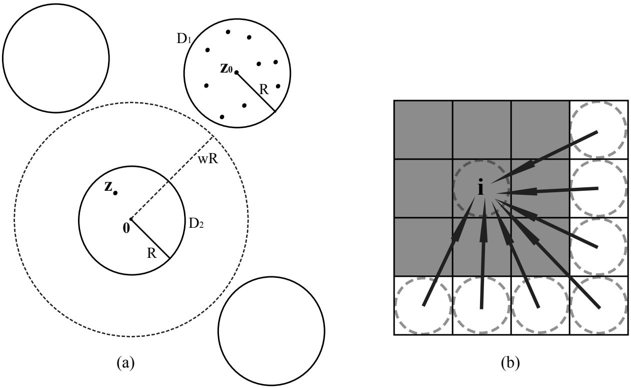
The conversion of the MP into a LP:

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z-z_0)^k} \;\Rightarrow\; \phi(z) = \sum_{l=0}^{\infty} b_l \cdot z^l,$$

Furthermore, an error bound for the truncated series is given by

$$\left| \phi(z) - \sum_{l=0}^{p} b_l \cdot z^l \right| \leq \text{const} \cdot \left(\frac{1}{w} \right)^{p+1}, \tag{10}$$

Conversion of a MP into a LP ...



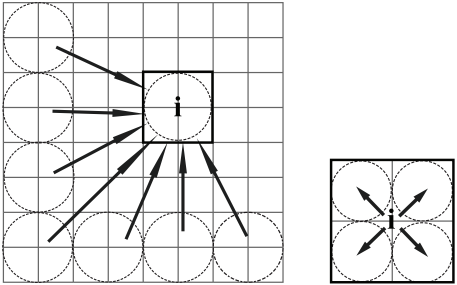
(a)

(b)

Conversion of Several MPs to a LP

Fig.(a) shows that the multipole expansion about disk D_1 can be converted to a local expansion about the disk D_2. Fig.(b) shows the similar behavior of the quadtree structure.

Translation of Local Expansion



(a) (b)

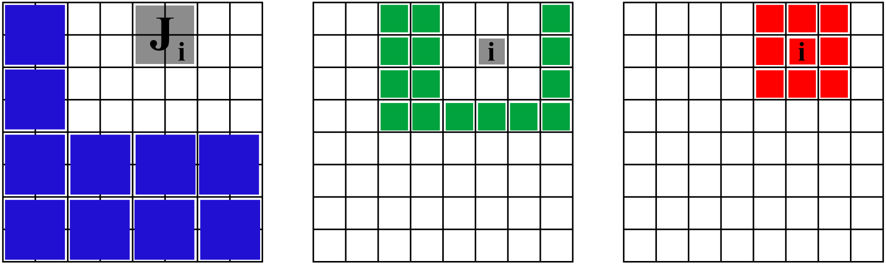
Theorem (**Translation of a local expansion**)

For any complex z_0, z, *and* $\{a_k\}$, $k = 0, 1, 2, \ldots, n$,

$$\sum_{k=0}^{n} a_k (z - z_0)^k = \sum_{l=0}^{n} \left(\sum_{k=l}^{n} a_k \binom{k}{l} (-z_0)^{k-l} \right) z^l. \qquad (11)$$

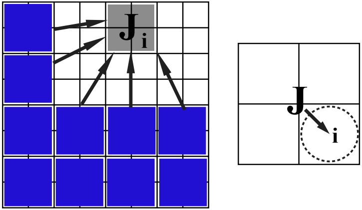
FMM V.S. $N \log N$ Algorithm

$N \log N$ Algorithm



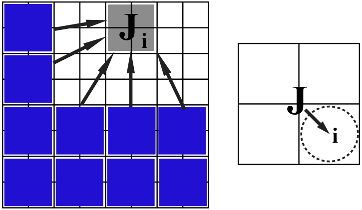
FMM Can Improve $N \log N$ Algorithm

- Conversion of the multipole expansions to a local expansion.
- Translation of a local expansion from parent box to children boxes.



FMM Can Improve $N \log N$ Algorithm

- Conversion of the multipole expansions to a local expansion.
- Translation of a local expansion from parent box to children boxes.

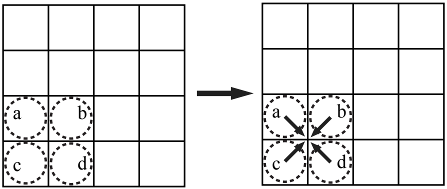


AND FMM CAN SAVE MORE!!!

FMM V.S. $N \log N$ Algorithm

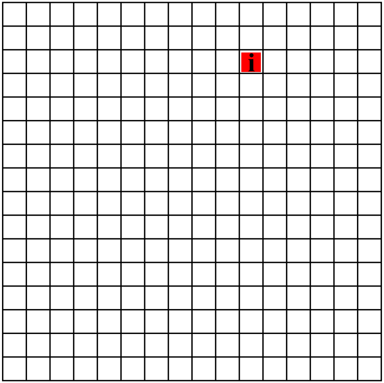
Save More by Using Translation of Multipole Expansion

- Start with finest level, translate the multipole expansion centered at a child box into a multipole expansion centered at its parent box in the coarser level.
- Add the four translated expansions together to get the multipole expansion for the parent box.



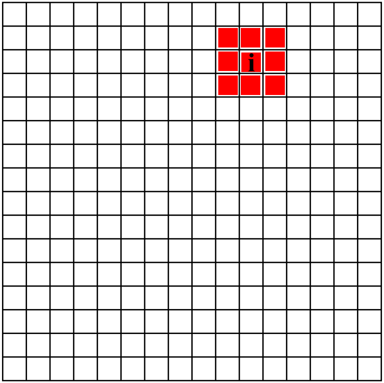
Decomposition of the Domain

Notice: $P^{\ell}_{x,S}$ is the potential (Local Expansion) centered around x, due to the particles set S.



Decomposition of the Domain

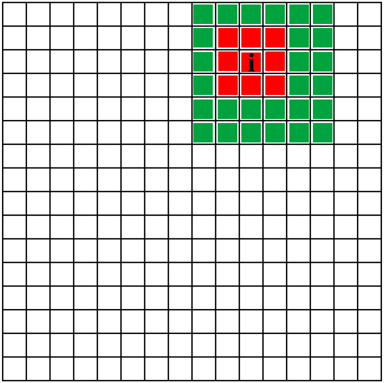
Notice: $P^{\ell}_{x,S}$ is the potential (Local Expansion) centered around x, due to the particles set S.



- $P^{\ell}_{i,\ nnb}$: the potential due to the particles inside of i's near neighbors.

Decomposition of the Domain

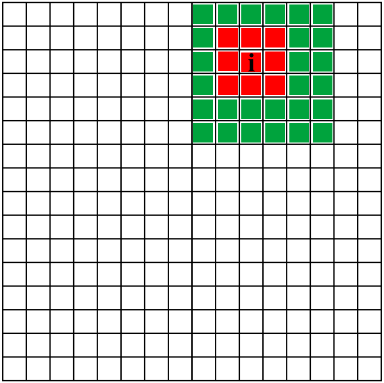
Notice: $P^{\ell}_{x,S}$ is the potential (Local Expansion) centered around x, due to the particles set S.



- $P^{\ell}_{i,\ nnb}$: the potential due to the particles inside of i's near neighbors.
- $P^{\ell}_{i,\ list}$: the potential due to the particles inside of i's interaction list.

Decomposition of the Domain

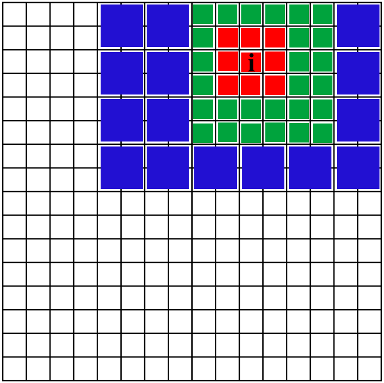
Notice: $P^{\ell}_{x,S}$ is the potential (Local Expansion) centered around x, due to the particles set S.



- $P^{\ell}_{i,\ nnb}$: the potential due to the particles inside of i's near neighbors.
- $P^{\ell}_{i,\ list}$: the potential due to the particles inside of i's interaction list.
- $P^{\ell}_{i,\ out}$: the potential due to the particles outside of i's parent's near neighbors, which can be computed recursively.

Decomposition of the Domain

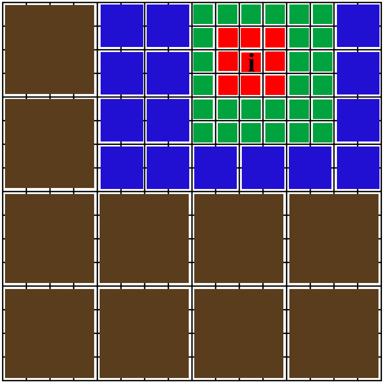
Notice: $P^{\ell}_{x,S}$ is the potential (Local Expansion) centered around x, due to the particles set S.



- $P^{\ell}_{i,\ nnb}$: the potential due to the particles inside of i's near neighbors.
- $P^{\ell}_{i,\ list}$: the potential due to the particles inside of i's interaction list.
- $P^{\ell}_{i,\ out}$: the potential due to the particles outside of i's parent's near neighbors, which can be computed recursively.
- $P^{\ell-1}_{j,\ list}$: j is the parent box of box i.

Decomposition of the Domain

Notice: $P^{\ell}_{x,S}$ is the potential (Local Expansion) centered around x, due to the particles set S.



- $P^{\ell}_{i,\ nnb}$: the potential due to the particles inside of i's near neighbors.
- $P^{\ell}_{i,\ list}$: the potential due to the particles inside of i's interaction list.
- $P^{\ell}_{i,\ out}$: the potential due to the particles outside of i's parent's near neighbors, which can be computed recursively.
- $P^{\ell-1}_{j,\ list}$: j is the parent box of box i.
- $P^{\ell-2}_{k,\ list}$: k is the grandparent box of box i.

FMM Algorithm

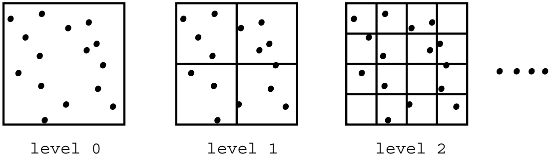
Initialization

- Given N particles distributed in a square domain.

FMM Algorithm

Initialization

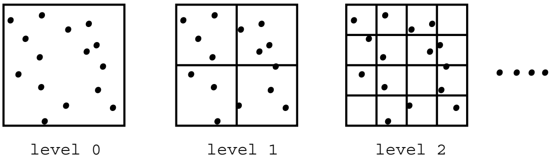
- Given N particles distributed in a square domain.
- Construct a quadtree with $L + 1$ levels.



FMM Algorithm

Initialization

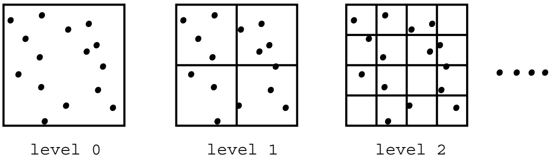
- Given N particles distributed in a square domain.
- Construct a quadtree with $L + 1$ levels.
- The indices of levels will be $0, 1, 2, \dots, L - 1, L$.



FMM Algorithm

Initialization

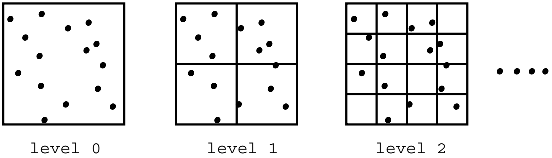
- Given N particles distributed in a square domain.
- Construct a quadtree with $L + 1$ levels.
- The indices of levels will be $0, 1, 2, \ldots, L-1, L$.
- Assume that, on average, s particles per box in the finest level.



FMM Algorithm

Initialization

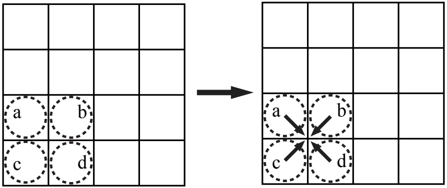
- Given N particles distributed in a square domain.
- Construct a quadtree with $L+1$ levels.
- The indices of levels will be $0, 1, 2, \ldots, L-1, L$.
- Assume that, on average, s particles per box in the finest level.
- $4^L \cdot s = N$, or equivalently, $L = \log_4(N/s)$.



FMM algorithm . . .

Upward Pass

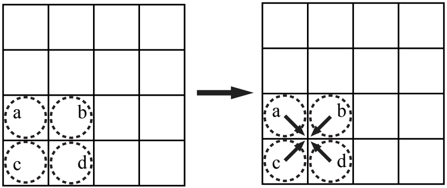
- Start with the finest level, construct multipole expansions for each box.



FMM algorithm . . .

Upward Pass

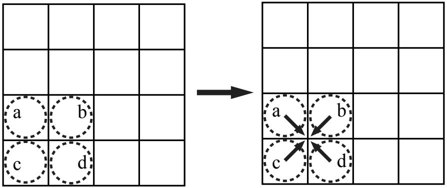
- Start with the finest level, construct multipole expansions for each box.
- Translate the multipole expansion to coarser levels.



FMM algorithm . . .

Upward Pass

- Start with the finest level, construct multipole expansions for each box.
- Translate the multipole expansion to coarser levels.
- The multipole expansion about every box in the coarser levels will be constructed by the merging procedure.



FMM Algorithm . . .

Downward Pass

- Start with the coarsest level, in fact, level 2, where each box k has its interaction list. Construct the local expansion $P^2_{k,list}$.

FMM Algorithm . . .

Downward Pass

- Start with the coarsest level, in fact, level 2, where each box k has its interaction list. Construct the local expansion $P^2_{k,list}$.
- Repeat this for every finer level. For simplicity, assume finest level $L = 4$.

FMM Algorithm . . .

Downward Pass

- Start with the coarsest level, in fact, level 2, where each box k has its interaction list. Construct the local expansion $P^2_{k,list}$.
- Repeat this for every finer level. For simplicity, assume finest level $L = 4$.
- Let box i at level 4 be the target. We already have $P^4_{i,list}$, $P^3_{j,list}$, $P^2_{k,list}$, where j is the parent of i, and k is the parent of j.

FMM Algorithm . . .

Downward Pass

- Start with the coarsest level, in fact, level 2, where each box k has its interaction list. Construct the local expansion $P^2_{k,list}$.
- Repeat this for every finer level. For simplicity, assume finest level $L = 4$.
- Let box i at level 4 be the target. We already have $P^4_{i,list}$, $P^3_{j,list}$, $P^2_{k,list}$, where j is the parent of i, and k is the parent of j.
- Start with the coarsest level again, translate the local expansion from the parent to its children.

FMM Algorithm . . .

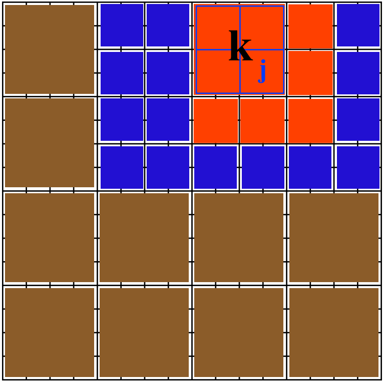
Downward Pass

- Start with the coarsest level, in fact, level 2, where each box k has its interaction list. Construct the local expansion $P^2_{k,list}$.
- Repeat this for every finer level. For simplicity, assume finest level $L = 4$.
- Let box i at level 4 be the target. We already have $P^4_{i,list}$, $P^3_{j,list}$, $P^2_{k,list}$, where j is the parent of i, and k is the parent of j.
- Start with the coarsest level again, translate the local expansion from the parent to its children.
- $$\begin{aligned} P^2_{k,list} &\Rightarrow P^3_{j,out} \\ P^3_{j,out} + P^3_{j,list} &\Rightarrow P^4_{i,out} \end{aligned}$$

FMM Algorithm . . .

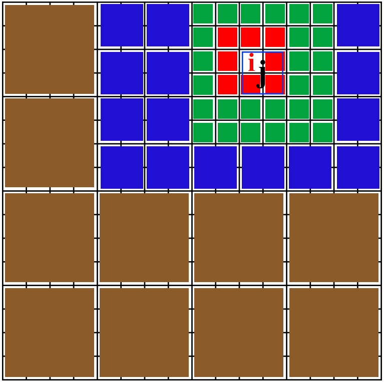
Downward Pass

- Start with the coarsest level, in fact, level 2, where each box k has its interaction list. Construct the local expansion $P^2_{k,list}$.
- Repeat this for every finer level. For simplicity, assume finest level $L = 4$.
- Let box i at level 4 be the target. We already have $P^4_{i,list}$, $P^3_{j,list}$, $P^2_{k,list}$, where j is the parent of i, and k is the parent of j.
- Start with the coarsest level again, translate the local expansion from the parent to its children.
- $$\begin{aligned} P^2_{k,list} &\Rightarrow P^3_{j,out} \\ P^3_{j,out} + P^3_{j,list} &\Rightarrow P^4_{i,out} \end{aligned}$$
- Finally, $P^4_{i,out} + P^4_{i,list} + P^4_{i,nnb}$ will be the total potential centered at i due to all the other particles.



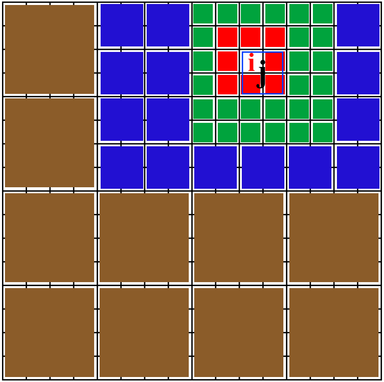
- $P^2_{k,list} \Rightarrow P^3_{j,out}$.

FMM Algorithm : Downward Pass . . .



- $P^2_{k,list} \Rightarrow P^3_{j,out}$.
- $P^3_{j,out} + P^3_{j,list} \Rightarrow P^4_{i,out}$.

FMM Algorithm : Downward Pass . . .



- $P^2_{k,list} \Rightarrow P^3_{j,out}$.
- $P^3_{j,out} + P^3_{j,list} \Rightarrow P^4_{i,out}$.
- $P^4_{i,out} + P^4_{i,list} + P^4_{i,nnb}$.

Computation Cost of FMM

Cost of Upward Pass

- In the finest level, to form the multipole expansion centered at each box, we need about Np operations, where p is the number of terms in the multipole expansion.
- Then for the translations for the higher levels, we need about $(\frac{N}{s})p^2$ operations, where s is the average number of particles in each box of the finest level.
- Totally, cost of upward pass is $Np + (\frac{N}{s})p^2$.

Computation Cost of FMM

Cost of Downward Pass

- To convert the multipole expansions about all boxes in the interaction list of each box in an arbitrary level, we need about $27(\frac{N}{s})p^2$ operations.
- Then for the translations from the parent to its children, we need about $(\frac{N}{s})p^2$ operations.
- For the evaluation of a local expansion in the finest level and computing potential directly from the near neighbor, we need about Np and $9Ns$ respectively.
- Totally, cost of downward pass is $27(\frac{N}{s})p^2 + (\frac{N}{s})p^2 + Np + 9Ns$.

Computation Cost of FMM

Cost of Downward Pass

- To convert the multipole expansions about all boxes in the interaction list of each box in an arbitrary level, we need about $27(\frac{N}{s})p^2$ operations.
- Then for the translations from the parent to its children, we need about $(\frac{N}{s})p^2$ operations.
- For the evaluation of a local expansion in the finest level and computing potential directly from the near neighbor, we need about Np and $9Ns$ respectively.
- Totally, cost of downward pass is $27(\frac{N}{s})p^2 + (\frac{N}{s})p^2 + Np + 9Ns$.

Cost of FMM

Cost $= 2Np + 29\left(\frac{N}{s}\right)p^2 + 9Ns$, where if $s = p$, the cost will be $40Np$.

Outline

Matrix Vector Product

Given a set of N particles located at N distinct points, i.e., $\mathrm{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\} \subset \mathbb{R}^2$. and a set of reals $\{q_1, q_2, \ldots, q_N\}$, where q_i is the charge strength of the particle located at $\boldsymbol{x}_i$.

Matrix Vector Product

Given a set of N particles located at N distinct points, i.e., $\mathrm{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\} \subset \mathbb{R}^2$. and a set of reals $\{q_1, q_2, \ldots, q_N\}$, where q_i is the charge strength of the particle located at $\boldsymbol{x}_i$.

We want to compute the potential for each particle at $\boldsymbol{x}_i$ due to the rest of particles located at $\{\boldsymbol{x}_j\}_{j=1, j\neq i}^{N}$.

$$\phi(\boldsymbol{x}_i) = \sum_{j=1, j\neq i}^{N} q_j \log ||\boldsymbol{x}_j - \boldsymbol{x}_i||.$$

Matrix Vector Product

Given a set of N particles located at N distinct points, i.e., $\mathrm{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\} \subset \mathbb{R}^2$. and a set of reals $\{q_1, q_2, \ldots, q_N\}$, where q_i is the charge strength of the particle located at $\boldsymbol{x}_i$.

We want to compute the potential for each particle at $\boldsymbol{x}_i$ due to the rest of particles located at $\{\boldsymbol{x}_j\}_{j=1, j\neq i}^{N}$.

$$\phi(\boldsymbol{x}_i) = \sum_{j=1, j\neq i}^{N} q_j \log ||\boldsymbol{x}_j - \boldsymbol{x}_i||.$$

$$\begin{pmatrix} \phi(\boldsymbol{x}_1) \\ \phi(\boldsymbol{x}_2) \\ \vdots \\ \phi(\boldsymbol{x}_N) \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \log ||\boldsymbol{x}_1 - \boldsymbol{x}_2|| & \cdots & \log ||\boldsymbol{x}_1 - \boldsymbol{x}_N|| \\ \log ||\boldsymbol{x}_1 - \boldsymbol{x}_2|| & 0 & \cdots & \log ||\boldsymbol{x}_2 - \boldsymbol{x}_N|| \\ \vdots & \vdots & \vdots & \vdots \\ \log ||\boldsymbol{x}_1 - \boldsymbol{x}_N|| & \log ||\boldsymbol{x}_2 - \boldsymbol{x}_N|| & \cdots & 0 \end{pmatrix}}_{\mathbf{P}} \cdot \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_N \end{pmatrix}$$

Structure of matrix $\mathbf{P}$

- The sequence of $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ determine the structure of $\mathbf{P}$.

Structure of matrix $\mathbf{P}$

- The sequence of $\{x_1, x_2, \ldots, x_N\}$ determine the structure of $\mathbf{P}$.
- The well separated groups of points are the key to the FMM.

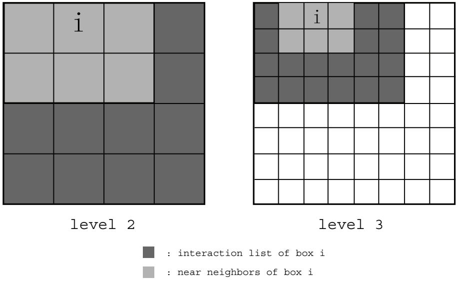


Figure: Quadtree structure induced by a uniform subdivision of a square domain.

Structure of matrix $\mathbf{P}$

- The sequence of $\{x_1, x_2, \ldots, x_N\}$ determine the structure of $\mathbf{P}$.
- The well separated groups of points are the key to the FMM.
- An indexing scheme for the hierarchical refinement structure is needed.

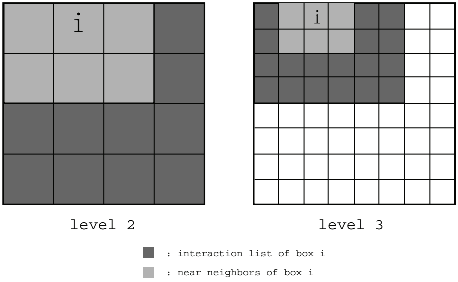


Figure: Quadtree structure induced by a uniform subdivision of a square domain.

Quadtree and Indexing

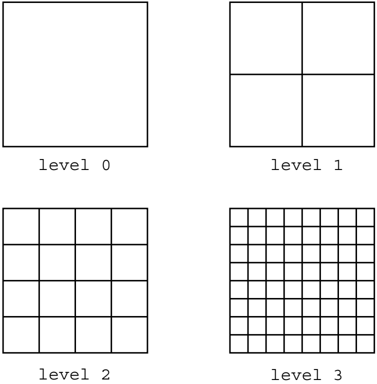
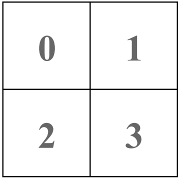
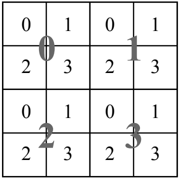


Figure: Quadtree structure induced by a uniform subdivision of a square domain.

Quadtree and Indexing

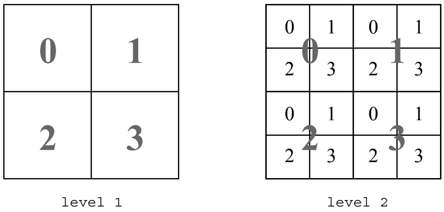


level 1



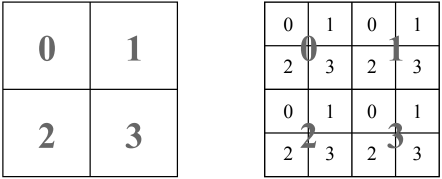
level 2

Quadtree and Indexing



Indexing

- $\mathcal{I} = (I_1, I_2, \ldots, I_\ell)$, where $I_j = 0, 1, 2, 3$, with $j = 1, 2, \ldots, \ell$.



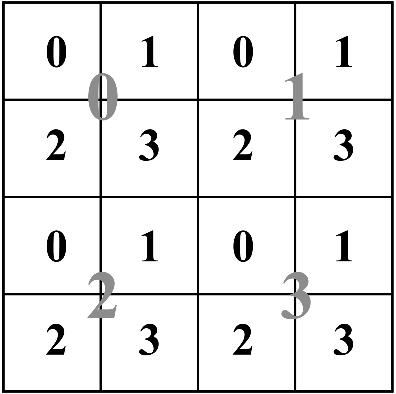
level 1 level 2

Indexing

- $\mathcal{I} = (I_1, I_2, \ldots, I_\ell)$, where $I_j = 0, 1, 2, 3$, with $j = 1, 2, \ldots, \ell$.
- Introduce a new index: $D = \sum_{j=1}^{\ell} 4^{\ell - j} \cdot I_j$.

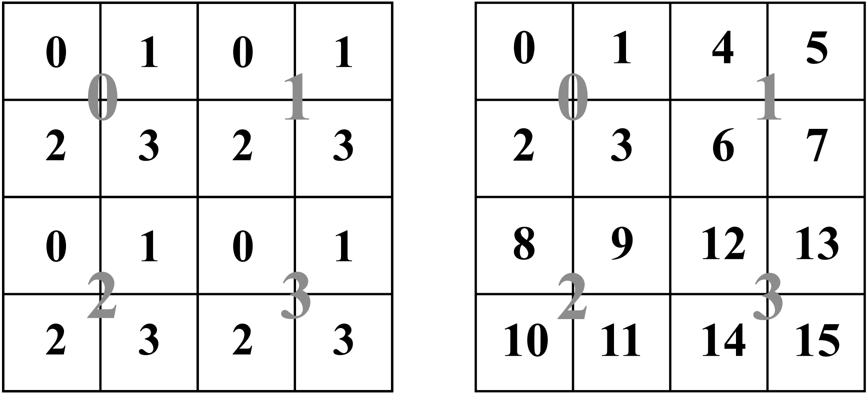
Indexing

- $\mathcal{I} = (I_1, I_2, \ldots, I_\ell)$, where $I_j = 0, 1, 2, 3$, with $j = 1, 2, \ldots, \ell$.

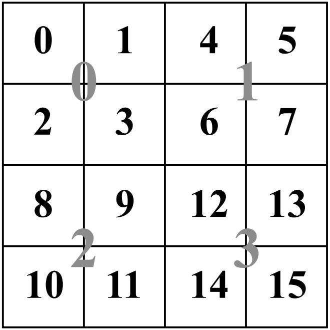


Indexing

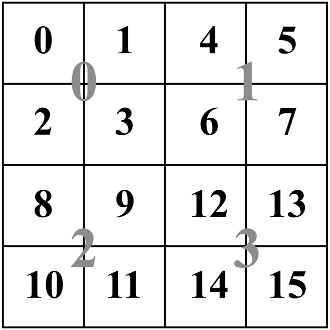
- $\mathcal{I} = (I_1, I_2, \ldots, I_\ell)$, where $I_j = 0, 1, 2, 3$, with $j = 1, 2, \ldots, \ell$.
- Introduce a new index: $D = \sum_{j=1}^{\ell} 4^{\ell - j} \cdot I_j$.



Low Rank Sub Matrices of P

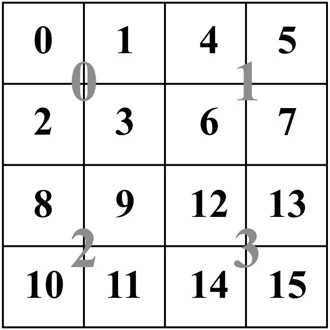


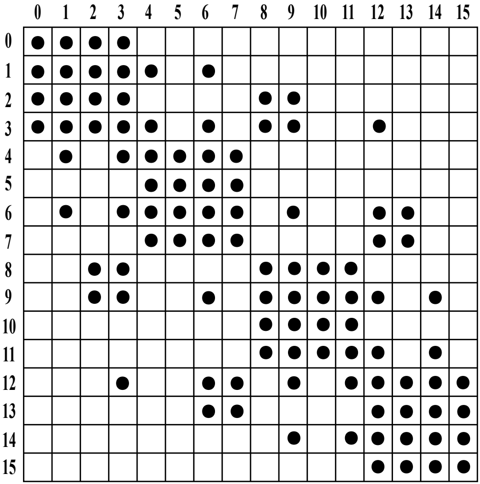
Low Rank Sub Matrices of $\mathbf{P}$



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

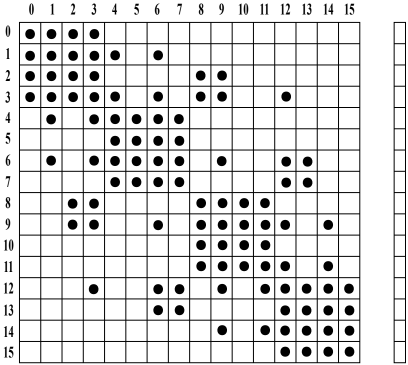
Low Rank Sub Matrices of $\mathbf{P}$



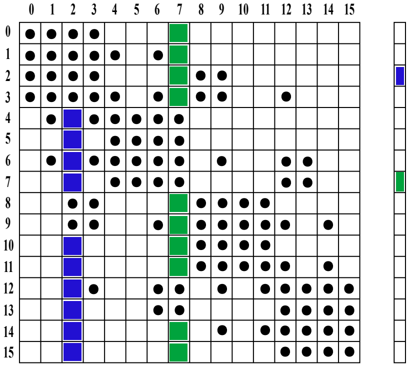


The blank blocks are low rank matrices!

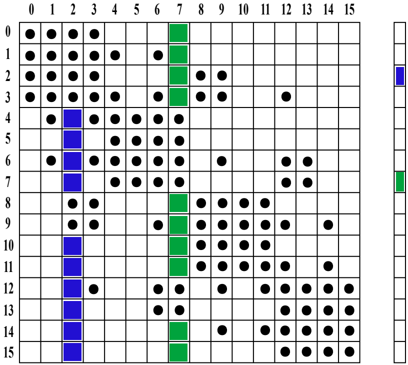
Matrix Vector Product



Matrix Vector Product



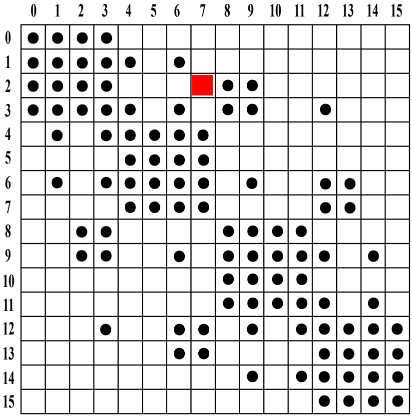
Matrix Vector Product



Computation Cost

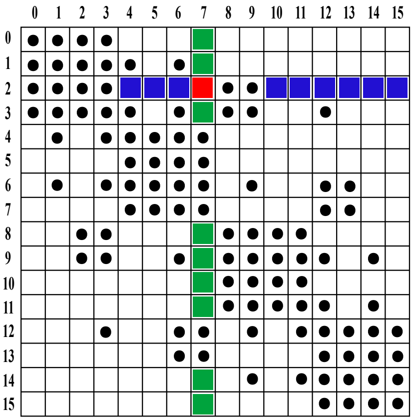
- Given A: $m \times n$. The cost of $A \cdot v$ is mn.
- If $A = U \cdot S \cdot V$, where S is of size $p \times p$, then the computation cost of $U \cdot S \cdot V \cdot v$ is $p(m + n + p)$.

Column Bases and Row Bases



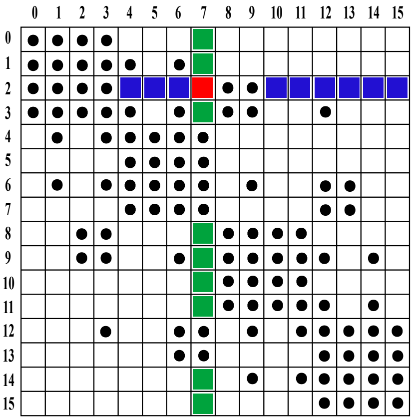
- $B_{2,7}$ is the block matrix in red.

Column Bases and Row Bases



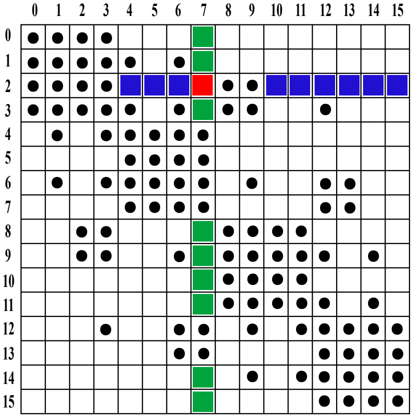
- $B_{2,7}$ is the block matrix in red.
- We want $B_{2,7} = U_2 \cdot S_{2,7} \cdot V_7^T$.

Column Bases and Row Bases



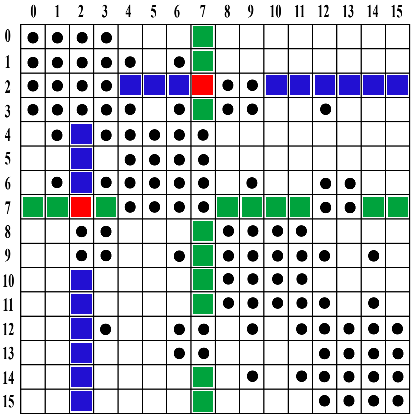
- $B_{2,7}$ is the block matrix in red.
- We want $B_{2,7} = U_2 \cdot S_{2,7} \cdot V_7^T$.
- U_2 will capture the column bases of the blue blocks.

Column Bases and Row Bases



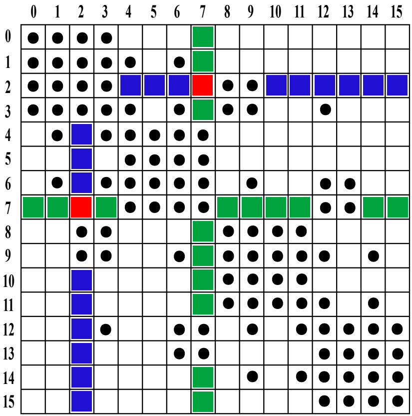
- $B_{2,7}$ is the block matrix in red.
- We want $B_{2,7} = U_2 \cdot S_{2,7} \cdot V_7^T$.
- U_2 will capture the column bases of the blue blocks.
- V_7 will capture the row bases of the green blocks.

Column Bases and Row Bases



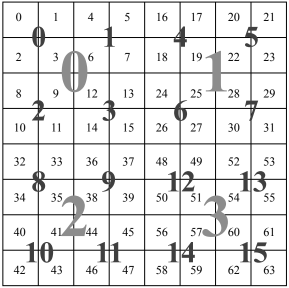
- $B_{2,7}$ is the block matrix in red.
- We want $B_{2,7} = U_2 \cdot S_{2,7} \cdot V_7^T$.
- U_2 will capture the column bases of the blue blocks.
- V_7 will capture the row bases of the green blocks.
- $B_{7,2} = U_7 \cdot S_{7,2} \cdot V_2^T$.

Column Bases and Row Bases

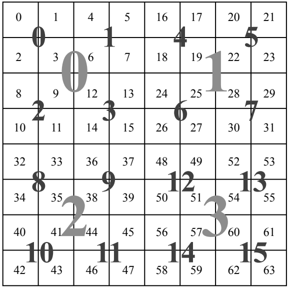


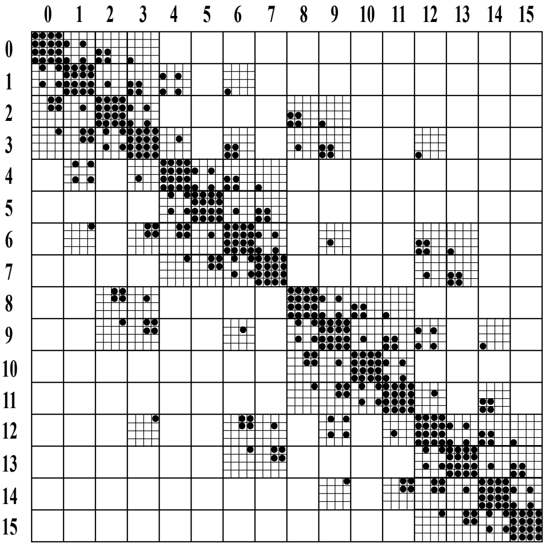
- $B_{2,7}$ is the block matrix in red.
- We want $B_{2,7} = U_2 \cdot S_{2,7} \cdot V_7^T$.
- U_2 will capture the column bases of the blue blocks.
- V_7 will capture the row bases of the green blocks.
- $B_{7,2} = U_7 \cdot S_{7,2} \cdot V_2^T$.
- $$B_{2,7} = U_2 \cdot S_{2,7} \cdot U_7^T$$
  $$B_{7,2} = U_7 \cdot S_{2,7}^T \cdot U_2^T$$

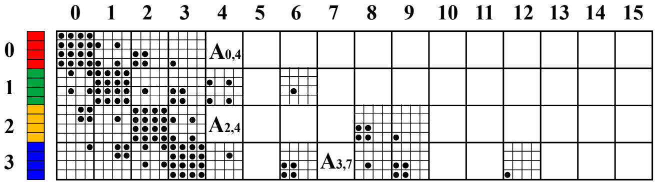
Low Rank Sub Matrices of $\mathbf{P}$ ......one more level

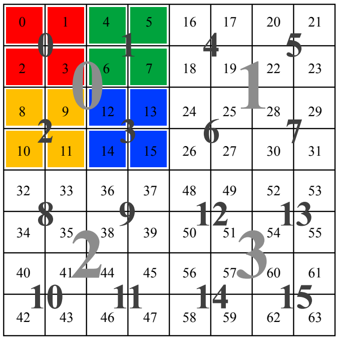


Low Rank Sub Matrices of P ......one more level

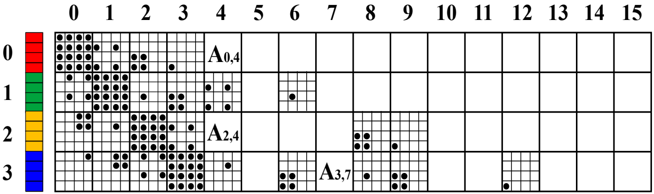




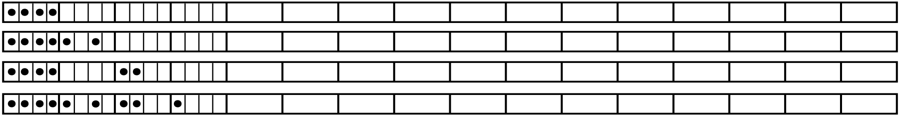




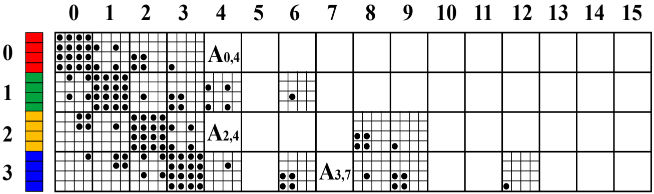
- $A_{0,4} = \widetilde{U}_0 \cdot \widetilde{Q}_{0,4} \cdot \widetilde{U}_4^T$.
- $\widetilde{U}_0 = \begin{pmatrix} U_0 \cdot R_{0,0} \\ U_1 \cdot R_{0,1} \\ U_2 \cdot R_{0,2} \\ U_3 \cdot R_{0,3} \end{pmatrix}$.
- $A_{3,7} = \widetilde{U}_3 \cdot \widetilde{Q}_{3,7} \cdot \widetilde{U}_7^T$.
- $\widetilde{U}_3 = \begin{pmatrix} U_{12} \cdot R_{3,0} \\ U_{13} \cdot R_{3,1} \\ U_{14} \cdot R_{3,2} \\ U_{15} \cdot R_{3,3} \end{pmatrix}$.



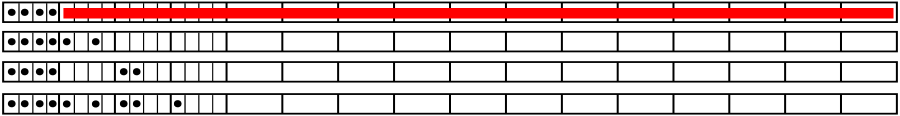
$$A_{0,4} = \widetilde{U}_0 \cdot \widetilde{Q}_{0,4} \cdot \widetilde{U}_4^T, \quad \text{where} \quad \widetilde{U}_0 = \begin{pmatrix} U_0 \cdot R_{0,0} \\ U_1 \cdot R_{0,1} \\ U_2 \cdot R_{0,2} \\ U_3 \cdot R_{0,3} \end{pmatrix}$$



What is U_0, U_1, U_2, U_3?

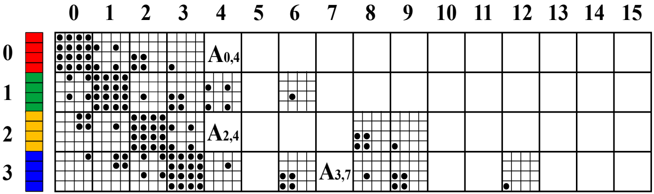


$$A_{0,4} = \widetilde{U}_0 \cdot \widetilde{Q}_{0,4} \cdot \widetilde{U}_4^T, \quad \text{where} \quad \widetilde{U}_0 = \begin{pmatrix} {\color{red}U_0} \cdot R_{0,0} \\ {\color{red}U_1} \cdot R_{0,1} \\ {\color{red}U_2} \cdot R_{0,2} \\ {\color{red}U_3} \cdot R_{0,3} \end{pmatrix}$$

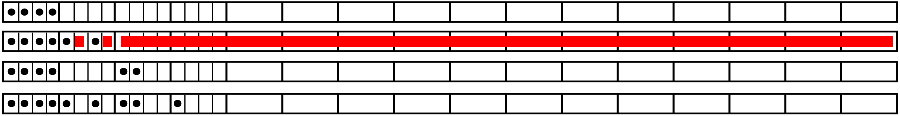


What is U_0, U_1, U_2, U_3?

Column Bases: ${\color{red}U_0}$.

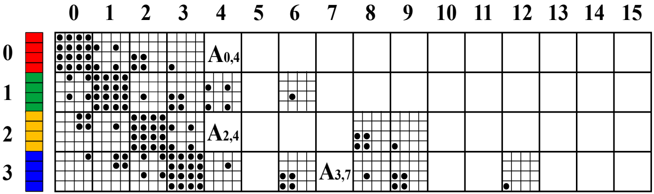


$$A_{0,4} = \widetilde{U}_0 \cdot \widetilde{Q}_{0,4} \cdot \widetilde{U}_4^T, \quad \text{where} \quad \widetilde{U}_0 = \begin{pmatrix} U_0 \cdot R_{0,0} \\ U_1 \cdot R_{0,1} \\ U_2 \cdot R_{0,2} \\ U_3 \cdot R_{0,3} \end{pmatrix}$$

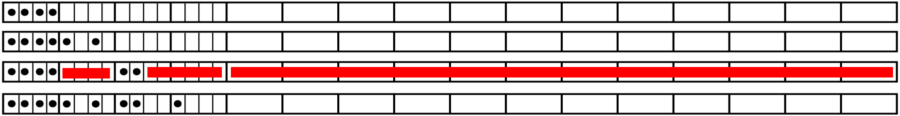


What is U_0, U_1, U_2, U_3?

Column Bases: U_1.

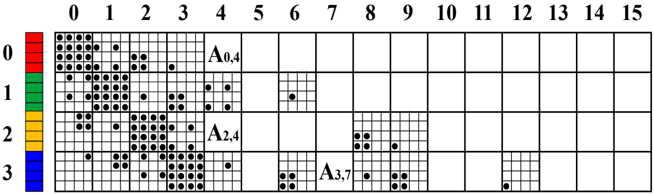


$$A_{0,4} = \widetilde{U}_0 \cdot \widetilde{Q}_{0,4} \cdot \widetilde{U}_4^T, \quad \text{where} \quad \widetilde{U}_0 = \begin{pmatrix} U_0 \cdot R_{0,0} \\ U_1 \cdot R_{0,1} \\ U_2 \cdot R_{0,2} \\ U_3 \cdot R_{0,3} \end{pmatrix}$$

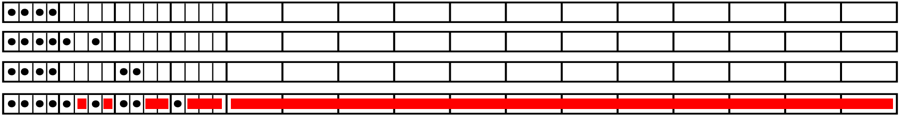


What is U_0, U_1, U_2, U_3?

Column Bases: U_2.



$$A_{0,4} = \widetilde{U}_0 \cdot \widetilde{Q}_{0,4} \cdot \widetilde{U}_4^T, \quad \text{where} \quad \widetilde{U}_0 = \begin{pmatrix} U_0 \cdot R_{0,0} \\ U_1 \cdot R_{0,1} \\ U_2 \cdot R_{0,2} \\ U_3 \cdot R_{0,3} \end{pmatrix}$$



What is U_0, U_1, U_2, U_3?

Column Bases: U_3.

- V. ROKHLIN, “Rapid solution of integral equations of classical potential theory”, *J. Comput. Phys.*, vol. 60, pp. 187-207, 1985.
- L. GREENGARD, *The Rapid Evaluation of Potential Fields in Particle Systems*, MIT Press, Cambridge, MA, 1988.
- L. GREENGARD, V. ROKHLIN, “A fast algorithm for particle simulations”, *J. Comput. Phys.*, vol. 73, pp. 325-348, 1987.
- S. CHANDRASEKARAN, M. GU, AND T. PALS, “A fast ULV decomposition solver for hierarchically semi-separable representations”, *SIAM J. MATRIX ANAL. APPL.*, vol. 28, No. 3, pp. 603C622, 2006.