FMM CMSC 878R/AMSC 698R

Lecture 10

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Progression

- Direct ($O(N^2)$)
  - No data structures
- Middleman: Degenerate Factorizations ($O(N)$)
  - Factorization needed, no data-structure
  - Factorization not always available
- Pre-FMM: S-expansions and R-expansions ($O(N^{3/2})$)
  - Factorizations in terms of near or far-field functions
  - $O(N^{3/2})$ for optimal number of boxes
  - Need boxes to organize source or target sets, and manage those pairs that require direct summation
- SLFMM: S and R-expansions, S|R translation ($O(N^{4/3})$)
- MLFMM: S and R-expansions, S|S, S|R and R|R translations ($O(N \log N)$)

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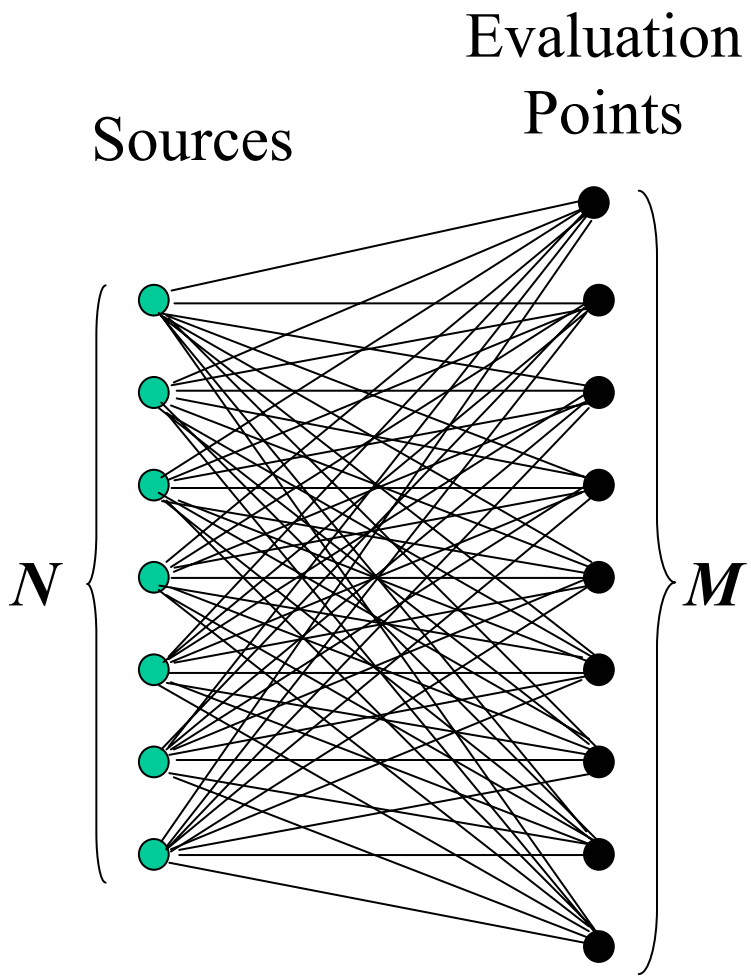
Middleman Algorithm

Standard algorithm



Total number of operations: ***O(NM)***

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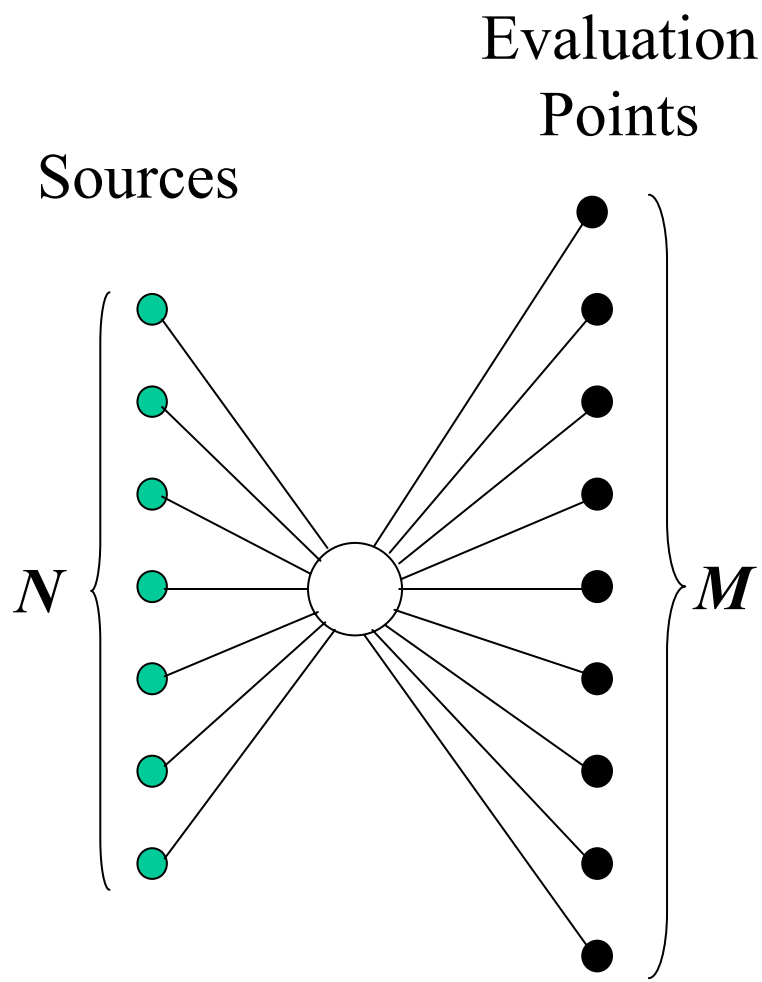
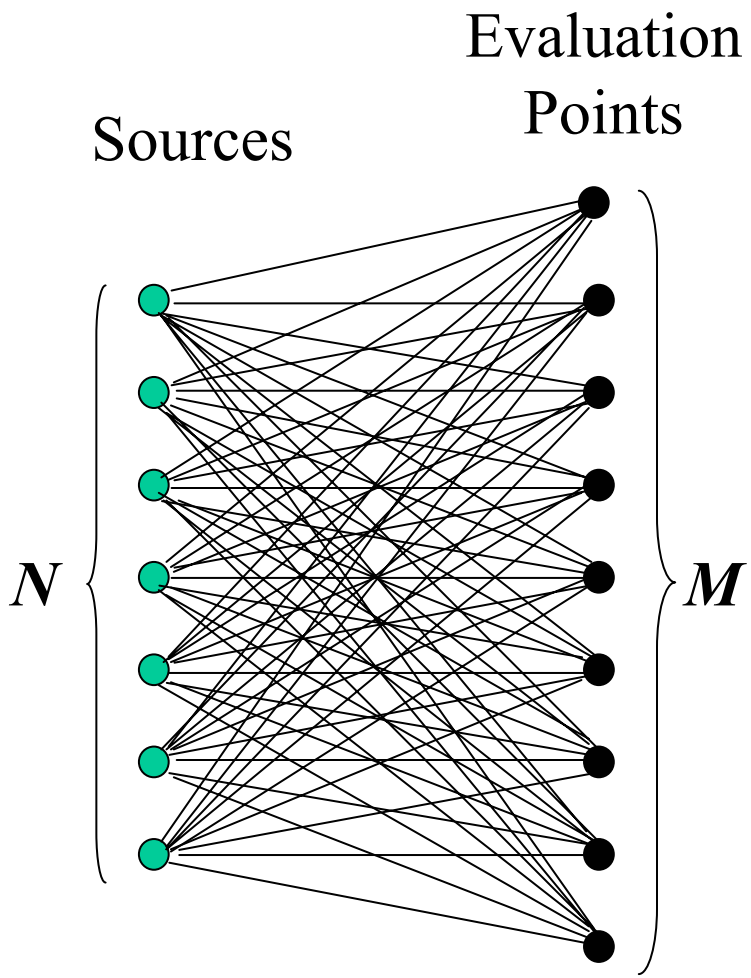
Middleman algorithm



Total number of operations: ***O(N+M)***

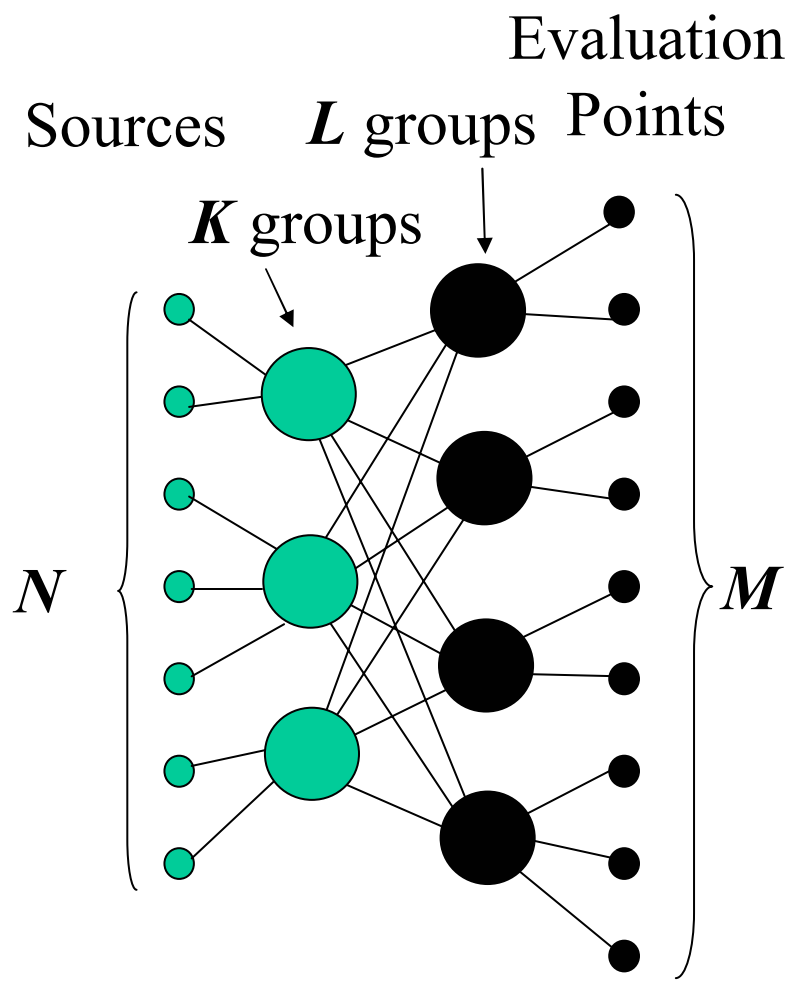
Idea of a Single Level FMM

Standard algorithm



Total number of operations: ***O(NM)***

SLFMM



Total number of operations: ***O(N+M+KL)***

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Why do we need SLFMM if Middleman has smaller complexity?

- Expansions can be valid in domains smaller than the computational domain.
- Even though expansion can be valid everywhere, the truncation number can be huge for large domains to provide accuracy.
- Sources and evaluation points can be spatially close, and there is a problem to evaluate singular potentials.
- Important theoretical question: determining optimal number of groups automatically

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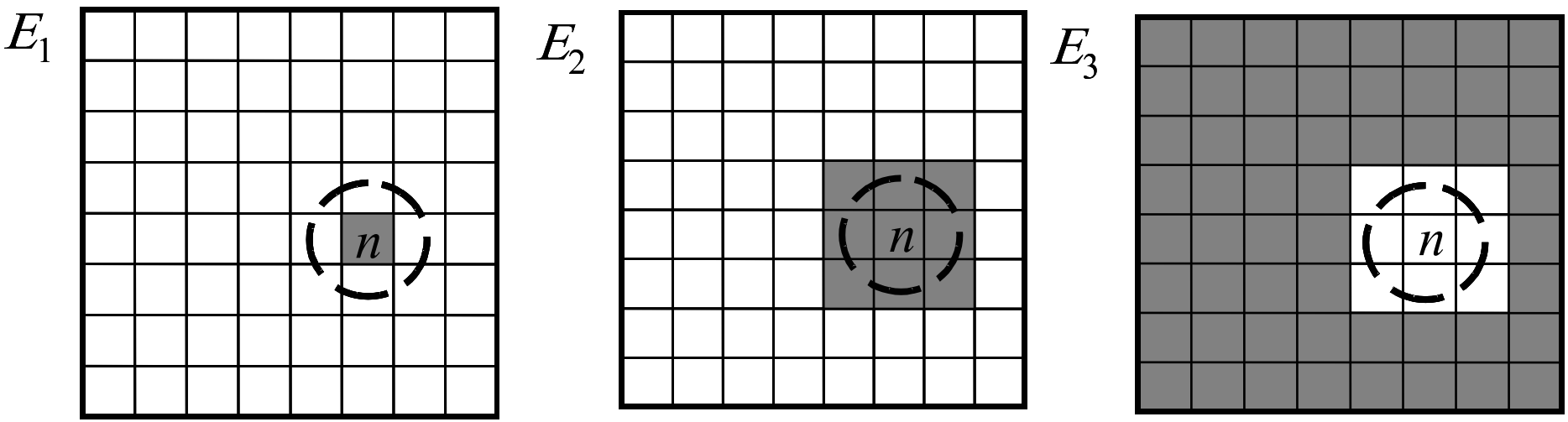
Spatial Domains

Potentials due to sources in these spatial domains

$\Phi_1^{(n)}(\mathbf{y})$ $\Phi_2^{(n)}(\mathbf{y})$ $\Phi_3^{(n)}(\mathbf{y})$



$I_1(n) = n$ $I_2(n) = \{Neighbors(n)\} \cup n$

$I_3(n) = \{All\ boxes\} \setminus I_2(n)$

Boxes with these numbers belong to these spatial domains

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Definition of potentials

$$\Phi_1^{(n)}(\mathbf{y}) = \sum_{\mathbf{x}_i \in E_1(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i),$$

$$\Phi_2^{(n)}(\mathbf{y}) = \sum_{\mathbf{x}_i \in E_2(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i),$$

$$\Phi_3^{(n)}(\mathbf{y}) = \sum_{\mathbf{x}_i \in E_3(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i),$$

Since domains $E_2(n)$ and $E_3(n)$ are complimentary:

$$\Phi(\mathbf{y}) = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}, \mathbf{x}_i) = \sum_{\mathbf{x}_i \in E_2(n) \cup E_3(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i) = \Phi_2^{(n)}(\mathbf{y}) + \Phi_3^{(n)}(\mathbf{y})$$

for arbitrary n.

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SLFMM Algorithm

Step 1. Generate S-expansion coefficients for each box

$$\Phi_1^{(n)}(\mathbf{x}) = \mathbf{C}^{(n)} \circ \mathbf{S}(\mathbf{x} - \mathbf{x}_c^{(n)}),$$
$$\mathbf{C}^{(n)} = \sum_{\mathbf{x}_i \in E_1(n,L)} u_i \mathbf{B}\left(\mathbf{x}_i, \mathbf{x}_c^{(n)}\right).$$

loop over all non-empty source boxes

For $n \in NonEmptySource$

Get $\mathbf{x}_c^{(n)}$, the center of the box;

$\mathbf{C}^{(n)} = \mathbf{0}$;

loop over all sources in the box

For $\mathbf{x}_i \in E_1(n)$

Get $\mathbf{B}\ (\mathbf{x}_i, \mathbf{x}_c^{(n)})$, the S-expansion coefficients near the center of the box;

$\mathbf{C}^{(n)} = \mathbf{C}^{(n)} + u_i \mathbf{B}\ (\mathbf{x}_i, \mathbf{x}_c^{(n)})$;

End;

End;

Implementation can be different!
All we need is to get $\mathbf{C}^{(n)}$.

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SLFMM Algorithm

Step 2. (S|R)-translate expansion coefficients

$$\Phi_3^{(n)}(\mathbf{y}) = \mathbf{D}^{(n)} \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_c^{(n)}),$$
$$\mathbf{D}^{(n)} = \sum_{m \in I_3(n)} (\mathbf{S}|\mathbf{R})\left(\mathbf{x}_c^{(n)} - \mathbf{x}_c^{(m)}\right)\mathbf{C}^{(m)}.$$

loop over all non-empty evaluation boxes

For $n \in NonEmptyEvaluation$

Get $\mathbf{x}_c^{(n)}$, the center of the box;

$\mathbf{D}^{(n)} = \mathbf{0}$;

loop over all non-empty source boxes outside the neighborhood of the n-th box

For $m \in I_3(n)$

Get $\mathbf{x}_c^{(m)}$, the center of the box;

$\mathbf{D}^{(n)} = \mathbf{D}^{(n)} + (\mathbf{S}|\mathbf{R})(\mathbf{x}_c^{(n)} - \mathbf{x}_c^{(m)})\ \mathbf{C}^{(m)}$;

End;

End;

Implementation can be different!
All we need is to get $\mathbf{D}^{(n)}$.

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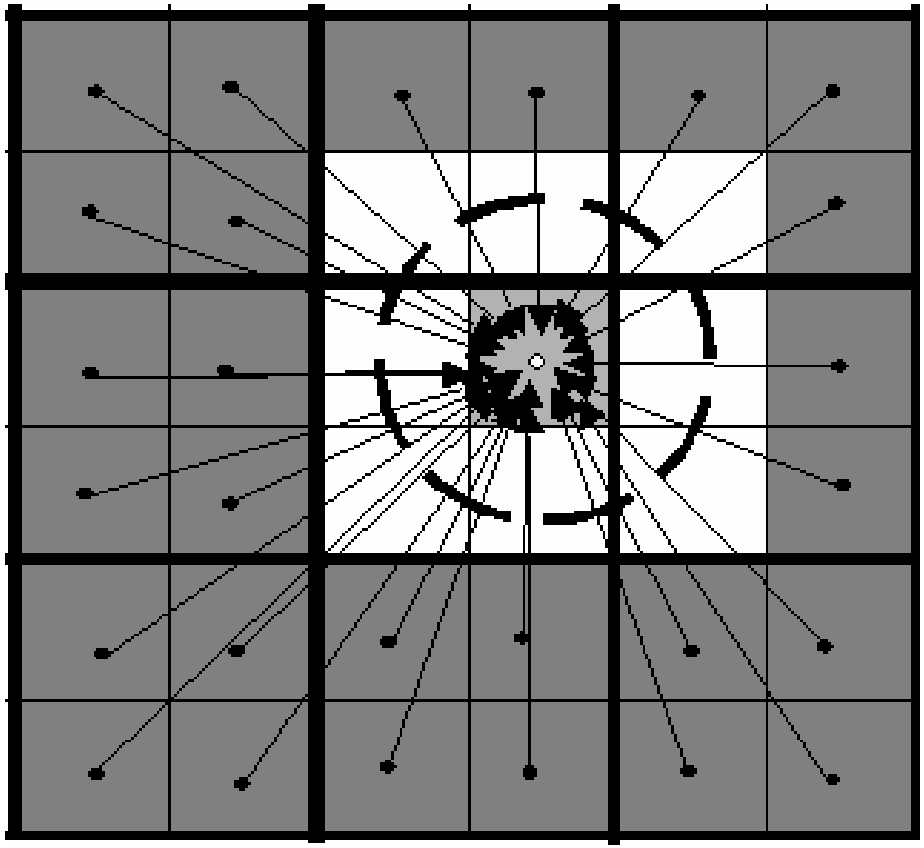
S|R-translation



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SLFMM Algorithm

Step 3. Final Summation

$$v_j = \Phi(\mathbf{y}_j) = \sum_{\mathbf{x}_i \in E_2(n)} u_i \Phi(\mathbf{y}_j, \mathbf{x}_i) + \mathbf{D}^{(n)} \circ \mathbf{R}(\mathbf{y}_j - \mathbf{x}_c^{(n)}), \quad \mathbf{y}_j \in E_1(n).$$

For $n \in$ *NonEmptyEvaluation* ← loop over all boxes containing evaluation points

Get $\mathbf{x}_c^{(n)}$, the center of the box;

For $\mathbf{y}_j \in E_1(n)$ ← loop over all evaluation points in the box

$v_j = \mathbf{D}^{(n)} \circ \mathbf{R}(\mathbf{y}_j - \mathbf{x}_c^{(n)})$;

For $\mathbf{x}_i \in E_2(n)$ ← loop over all sources in the neighborhood of the n-th box

$v_j = v_j + \Phi(\mathbf{y}_j , \mathbf{x}_i)$;

End;

End;

End;

Implementation can be different!
All we need is to get v_j

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Asymptotic Complexity of SLFMM

- By some magic we can easily find neighbors, and lists of points in each box.
  - Assume that cost of finding these is less than the most expensive operation
  - Magic will come from data-structures
- Translation is performed by straightforward $P \times P$ matrix-vector multiplication, where $P(p)$ is the total length of the translation vector. So the complexity of a single translation is $O(P^2)$.
- The source and evaluation points are distributed uniformly, and there are K boxes, with s source points in each box ($s=N/K$). We call s the *grouping* (or *clustering*) parameter.
- The number of neighbors for each box is $O(1)$.

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Then Complexity is:

- For Step 1: $O(PN)$
- For Step 2: $O(P^2K^2)$
- For Step 3: $O(PM+Ms)$
- Total: $O(PN+ P^2K^2 +PM+Ms) =$
  $O(PN+ P^2K^2 +PM+MN/K)$

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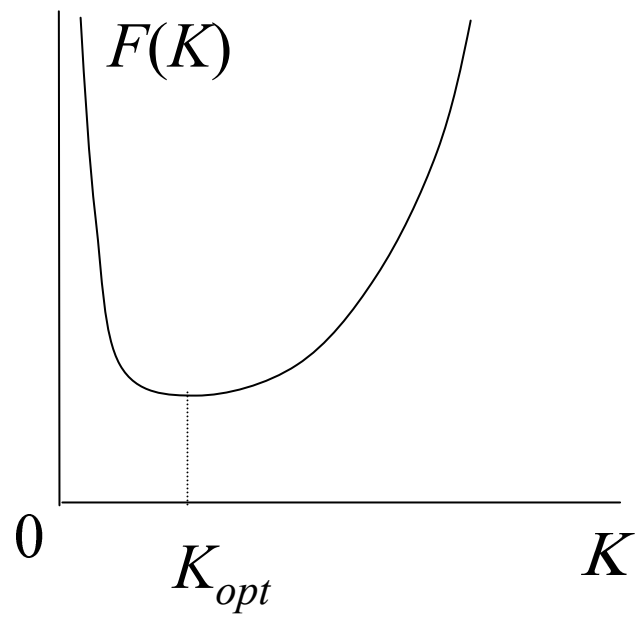
Selection of Optimal K (or s)

$$F(K) = PN + P^2K^2 + PM + PMN/K.$$

$$F'(K) = 2P^2K - PMN/K^2 = 0.$$

$$K_{opt} = \left(\frac{MN}{2P}\right)^{1/3} = O\left(\left(\frac{MN}{P}\right)^{1/3}\right).$$

$$s_{opt} = \frac{N}{K_{opt}} = \left(\frac{2PN^2}{M}\right)^{1/3} = O\left(\frac{PN^2}{M}\right)^{1/3}.$$



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Complexity of Optimized SLFMM

$$F(K_{opt}) = PN + P^2\left(\frac{MN}{2P}\right)^{2/3} + PM + PMN\left(\frac{MN}{2P}\right)^{-1/3}$$
$$= P(M+N) + (MN)^{2/3}O(P^{4/3}).$$

At $K = K_{opt}$, and $M = O(N)$, the complexity of SLFMM is:

$$O(PN + P^{4/3}N^{4/3}) = O(P^{4/3}N^{4/3}).$$

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SLFMM Characteristics

- Group source points into clusters
  - Group evaluation points into clusters
- Find the cluster center ($\mathbf{x}_*$) for each cluster
- Find distances from cluster center to points in cluster
- Find distances between clusters
- Build a S representation for points in each source cluster

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \sum_{m=1}^{p} b_m(\mathbf{x}_i, \mathbf{x}_*)\, S_m\, (\mathbf{y}-\mathbf{x}_*)$$

  - Consolidate S series from all $\mathbf{x}_i$ in the cluster
  - For each evaluation box find clusters that are outside min. radius at which S expansion converges. Translate S series to R series
  - Evaluate R series at the evaluation points
  - Clean-up by evaluating at points which are inside min. radius

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Algorithms needed

- Space division and grouping of points
- Center finding for groups
- Distance between points (group centers)
- Neighbor finding
- Hierarchical division in FMM adds
  - Hierarchical grouping, center finding
  - Finding parents, children, siblings
  - Finding neighbors
- Spatial data-structures
- Also, the structures used to store these relationships require memory
- Determine optimal parameters and “break-even” point

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Spatial Data Structures

- Spatial data structures have developed since late 1980s,
  - Aside: one of the founders of the field (Hanan Samet) is local
- FMM developed over the same period
  - So don't use the latest spatial data structure algorithms
- For effective "generalization" we need to use state-of-the-art spatial data structures
- Optimal data structures for FMM is an open research area
- In this course we will mostly use hierarchical division into boxes using 2^d trees
  - Use asymptotically optimal algorithms for performing operations on them
- Next class …

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- Constant time methods to
  - number the boxes in a way that can be generated from the coordinate
  - assign points to boxes using their binary coordinates
  - find box centers
  - Find neighboring boxes
- Use bit interleaving and bit shift
- Apply to the general *d*- dimensional case
- Storage is also minimized as most necessary relations are directly generated from point coordinates

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Summary of formal requirements for functions that can be used in FMM

- We have two sets of points:

$$\mathsf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}, \quad \mathbf{x}_i \in \mathsf{R}^d, \quad i = 1, \ldots, N,$$
$$\mathsf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_M\}, \quad \mathbf{y}_j \in \mathsf{R}^d, \quad j = 1, \ldots, M.$$

- We have functions (potentials):

$$\Phi(\mathbf{x}_i, \mathbf{y}) : \mathsf{R}^d \to \mathsf{R}, \quad \mathbf{y} \in \mathsf{R}^d, \quad i = 1, \ldots, N.$$

- These functions can be factorized as (local expansion):

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \mathbf{A}(\mathbf{x}_i, \mathbf{x}_*) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*), \quad |\mathbf{y} - \mathbf{x}_*| < r < |\mathbf{x}_i - \mathbf{x}_*|, \quad i = 1, \ldots, N$$

- These functions can be factorized as (far field expansion):

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \mathbf{B}(\mathbf{x}_i, \mathbf{x}_*) \circ \mathbf{S}(\mathbf{x} - \mathbf{x}_*), \quad |\mathbf{y} - \mathbf{x}_*| > R > |\mathbf{x}_i - \mathbf{x}_*|, \quad i = 1, \ldots, N$$

- The product is distributive operation with respect to addition

$$(u_1 \mathbf{A}_1 + u_2 \mathbf{A}_2) \circ \mathbf{F} = u_1 \mathbf{A}_1 \circ \mathbf{F} + u_2 \mathbf{A}_2 \circ \mathbf{F}, \quad \mathbf{F} = \mathbf{S}, \mathbf{R}$$

Summary of formal requirements for functions that can be used in FMM (2)

- R-expansion coefficients can be $R|R$-translated:

$$|\mathbf{x} - \mathbf{x}_{*2}| < |\mathbf{x}_i - \mathbf{x}_{*1}| - |\mathbf{x}_{*1} - \mathbf{x}_{*2}| :$$

$$\mathbf{A}(\mathbf{x}_i, \mathbf{x}_{*2}) = (\mathbf{R}|\mathbf{R})(\mathbf{x}_{*2} - \mathbf{x}_{*1})\mathbf{A}(\mathbf{x}_i, \mathbf{x}_{*1})$$

- S-expansion coefficients can be $S|S$-translated:

$$|\mathbf{x} - \mathbf{x}_{*2}| > |\mathbf{x}_{*1} - \mathbf{x}_{*2}| + |\mathbf{x}_i - \mathbf{x}_{*1}|,$$

$$\mathbf{B}(\mathbf{x}_i, \mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{S})(\mathbf{x}_{*2} - \mathbf{x}_{*1})\mathbf{B}(\mathbf{x}_i, \mathbf{x}_{*1})$$

- S-expansion coefficients can be $S|R$-translated (converted to R-expansion coefficients)

$$|\mathbf{x} - \mathbf{x}_{*2}| < |\mathbf{x}_{*1} - \mathbf{x}_{*2}| + |\mathbf{x}_i - \mathbf{x}_{*1}|,$$

$$\mathbf{A}(\mathbf{x}_i, \mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{R})(\mathbf{x}_{*2} - \mathbf{x}_{*1})\mathbf{B}(\mathbf{x}_i, \mathbf{x}_{*1})$$

- And we are looking for sums:

$$v_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j, \mathbf{x}_i), \quad j = 1, \ldots, M.$$

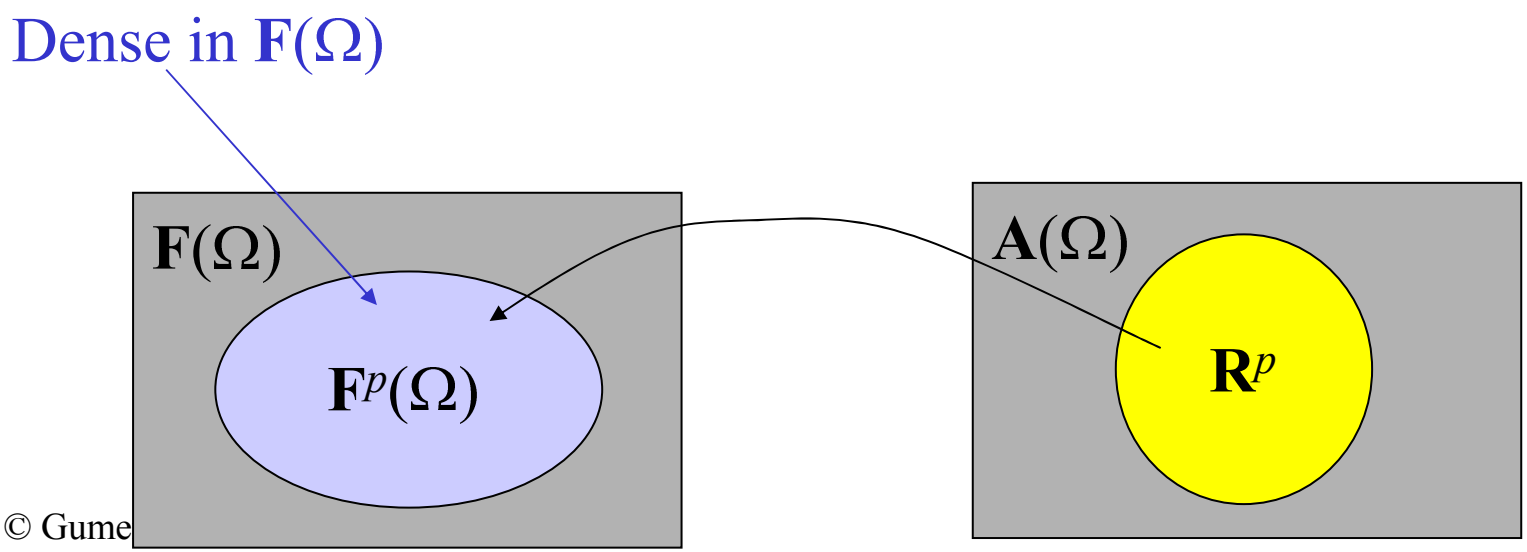
- Some generalization are possible, say instead of $\Phi(\mathbf{y}_j, \mathbf{x}_i)$ we can consider $\Phi_i(\mathbf{y}_j)$, etc.

p-Truncated Vectors

$$\forall \mathbf{A} \in \mathbb{R}^p, \quad \exists \Phi^p(\mathbf{y}) = \sum_{n=0}^{p-1} A_n F_n(\mathbf{y}) \in \mathbb{F}^p(\Omega) \subset \mathbb{F}(\Omega).$$

$\mathbb{F}^p(\Omega)$ is dense in $\mathbb{F}(\Omega)$:

$$\forall \Phi(\mathbf{y}) \in \mathbb{F}(\Omega), \quad \exists p, \Phi^p(\mathbf{y}) \in \mathbb{F}^p(\Omega), \quad \|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| = \underset{\mathbf{r} \in \Omega}{} |\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})| < \epsilon.$$



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Matrix Representation of Linear Operators

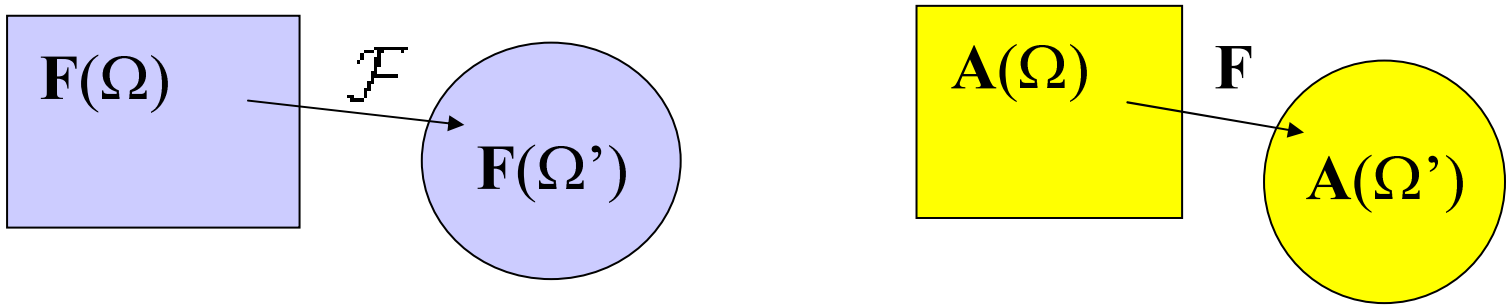
Let $\Omega' \subset \Omega$ and $\mathcal{F}$ is a mapping of $\mathbb{F}(\Omega)$ to $\mathbb{F}(\Omega')$. Such mapping can be considered as action of operator $\mathcal{F}$ on Φ :

$$\mathcal{F}[\Phi(\mathbf{y})] = \widetilde{\Phi(\mathbf{y})}, \quad \Phi(\mathbf{y}) \in \mathbb{F}(\Omega), \quad \widetilde{\Phi(\mathbf{y})} \in \mathbb{F}(\Omega') \subset \mathbb{F}(\Omega)$$

Respectively, operator $\mathcal{F}$ generates operator $\mathbf{F}$ that maps the space of expansion coefficients $\mathbb{A}(\Omega) \to \mathbb{A}(\Omega')$, which can be considered as *representation* of the operator $\mathcal{F}$ in the space of expansion coefficients:

$$\mathbf{FA} = \widetilde{\mathbf{A}}, \quad \mathbf{A} \in \mathbb{A}(\Omega), \quad \widetilde{\mathbf{A}} \in \mathbb{A}(\Omega') \subset \mathbb{A}(\Omega).$$

Inversly, if we introduce any transform of expansion coefficients $\mathbf{FA} = \widetilde{\mathbf{A}}$ which provides uniform convergence of function $\widetilde{\Phi(\mathbf{y})}$ corresponding to these coefficients in $\Omega' \subset \Omega$ then such transform can be treated as operator $\mathcal{F}$ that convert one function from $\mathbb{F}(\Omega)$ to another.



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Representation of a Linear Operator

p-Truncation (Projection) Operator

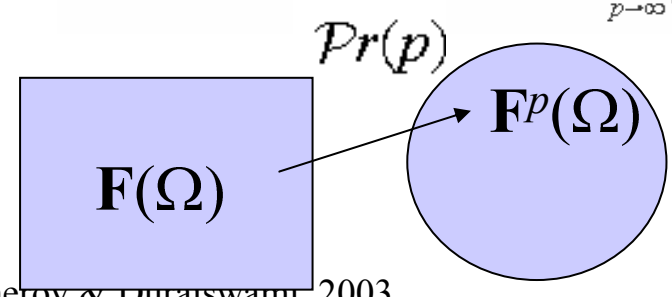
$$\mathbf{Pr}(p)\mathbf{A} = \widetilde{\mathbf{A}}, \quad \mathbf{A} \in \mathbb{A}(\Omega), \quad \widetilde{\mathbf{A}} \in \mathbb{A}^p(\Omega).$$

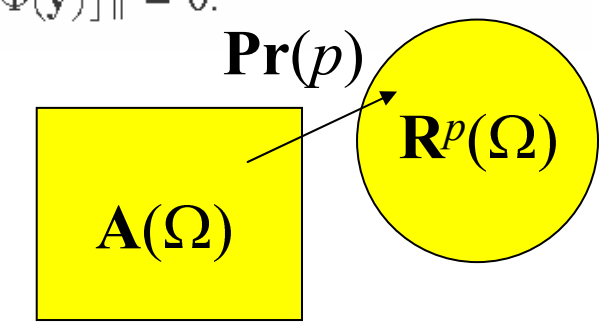
$$\mathbf{A} = \begin{pmatrix} A_0 \\ A_1 \\ \dots \\ A_{p-1} \\ A_p \\ A_{p+1} \\ \dots \end{pmatrix} \rightarrow \widetilde{\mathbf{A}} = \begin{pmatrix} A_0 \\ A_1 \\ \dots \\ A_{p-1} \\ 0 \\ 0 \\ \dots \end{pmatrix}, \qquad \widetilde{\mathbf{A}} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 & \dots \\ 0 & 1 & \dots & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 & 0 & 0 & \dots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \mathbf{A}$$

In space $\mathbb{F}(\Omega)$:

$$\mathcal{P}r(p)[\Phi(\mathbf{y})] = \Phi^p(\mathbf{y}), \quad \Phi(\mathbf{y}) \in \mathbb{F}(\Omega), \quad \Phi^p(\mathbf{y}) \in \mathbb{F}^p(\Omega),$$

$$\lim_{p\to\infty} \| \Phi(\mathbf{y}) - \mathcal{P}r(p)[\Phi(\mathbf{y})] \| = 0.$$





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Norm of p-Truncation Operator (important for error bounds)

Norm:

$$\|\mathsf{P}r(p)\| = \frac{\sup_{\mathbf{y}\in\Omega}\|\mathsf{P}r(p)[\Phi(\mathbf{y})]\|}{\sup_{\mathbf{y}\in\Omega}\|\Phi(\mathbf{y})\|}.$$

Triangle unequality:

$$\|\mathbf{I}\| - \|\mathbf{I} - \mathsf{P}r(p)\| \leqslant \|\mathsf{P}r(p)\| \leqslant \|\mathbf{I}\| + \|\mathbf{I} - \mathsf{P}r(p)\| = 1 + \|\mathbf{I} - \mathsf{P}r(p)\|$$

$$\forall\epsilon > 0, \quad \exists p, \quad \|\mathbf{I} - \mathsf{P}r(p)\| < \epsilon,$$

so

$$\forall\epsilon > 0, \quad \exists p, \quad 1 - \epsilon < \|\mathsf{P}r(p)\| < 1 + \epsilon,$$

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p-Truncated Operator

Let $\mathsf{H} : \mathsf{F}(\Omega) \to \mathsf{F}(\Omega)$ be an operator, that is represented by infinite matrix

$$\mathbf{H} = \begin{pmatrix} h_{00} & h_{01} & \dots & h_{0,p-1} & h_{0p} & \dots \\ h_{10} & h_{11} & \dots & h_{1,p-1} & h_{1p} & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ h_{p-1,0} & h_{p-1,1} & \dots & h_{p-1,p-1} & h_{p-1,p} & \dots \\ h_{p0} & h_{p1} & \dots & h_{p-1,p} & h_{pp} & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix},.$$

We call operator $\mathsf{H}^{(p)} : \mathsf{F}(\Omega) \to \mathsf{F}(\Omega)$, $p - \textit{truncated}$ if it is represented by matrix

$$\mathbf{H}^{(p)} = \begin{pmatrix} h_{00} & h_{01} & \dots & h_{0,p-1} & 0 & \dots \\ h_{10} & h_{11} & \dots & h_{1,p-1} & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ h_{p-1,0} & h_{p-1,1} & \dots & h_{p-1,p-1} & 0 & \dots \\ 0 & 0 & \dots & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

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Norm of p-Truncated Operator (important for error bounds)

Theorem: Let $\mathsf{H} : \mathsf{F}(\Omega) \to \mathsf{F}(\Omega)$, such that $0 < \|\mathsf{H}\| < \infty$, and $\mathsf{H}^{(p)}: \mathsf{F}(\Omega) \to \mathsf{F}(\Omega)$ is the -truncated operator H. Let also $p(\epsilon)$ be such that $1 - \epsilon < \|\mathsf{P}r(p)\| < 1 + \epsilon$. Then

$$(1-\epsilon)^2 < \|\mathsf{P}r(p)\|^2 = \frac{\|\mathsf{H}^{(p)}\|}{\|\mathsf{H}\|} = \|\mathsf{P}r(p)\|^2 < (1+\epsilon)^2,$$

$$\lim_{p\to\infty} \frac{\|\mathsf{H}^{(p)}\|}{\|\mathsf{H}\|} = 1.$$

Proof.

A p-truncated operator can be represented in the form

$$\mathsf{H}^{(p)} = \mathsf{P}r(p)\mathsf{H}\mathsf{P}r(p)$$

(check!)

So the norm of $\mathbf{H}^{(p)}$ is

$$\|\mathsf{H}^{(p)}\| = \|\mathsf{P}r(p)\|\|\mathsf{H}\|\|\mathsf{P}r(p)\| = \|\mathsf{H}\|\|\mathsf{P}r(p)\|^2.$$

End of Proof.

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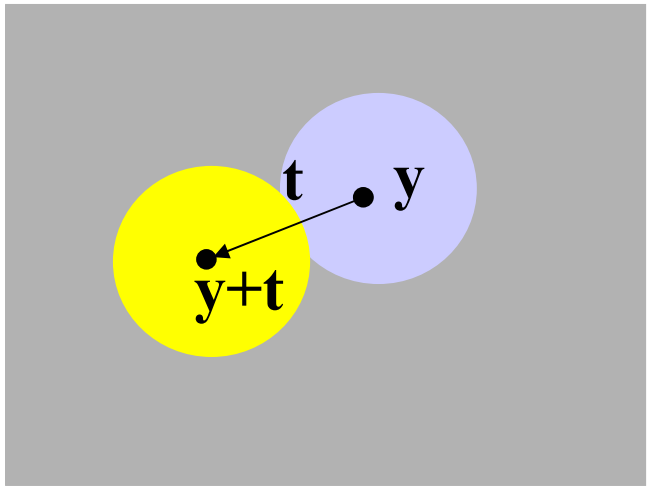
Translation Operator

Operator $\mathcal{T}(\mathbf{t}) : \mathbb{F}(\Omega) \to \mathbb{F}(\Omega'), \Omega' \subset \mathbb{R}^d, \quad \Omega \subset \mathbb{R}^d$ is called *translation* operator corresponding to *translation* vector $\mathbf{t}$, if

$$\mathcal{T}(\mathbf{t})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t}), \quad (\mathbf{y} \in \Omega, \quad \mathbf{y}+\mathbf{t} \in \Omega').$$



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Translation (Passive view point)

- Take a function or equivalently a function expressed as a series expansion and express it in another coordinate system (reference frame)
- Function is the same on the common parts of domains of definition
- but is represented in different forms
  - $\Phi(\mathbf{x}_i,\mathbf{y})$
  - $\sum_m b_m(\mathbf{x}_i,\mathbf{x}_{*1})\, S_m(\mathbf{y}-\mathbf{x}_*)$
  - $\sum_m a_m(\mathbf{x}_i,\mathbf{x}_{*2})\, R_m(\mathbf{y}-\mathbf{x}_{*2})$ with $a_m = \mathcal{T} b_m$

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Translation (Active view point)

- In a fixed coordinate system move the vector (or function), and evaluate it at the same point
- $\Phi(\mathbf{x}_i,\mathbf{y}) \rightarrow \Phi(\mathbf{x}_i+\mathbf{t},\mathbf{y})$
- Functions evaluated at the same point are not the same
- Operator transforms the reference frame

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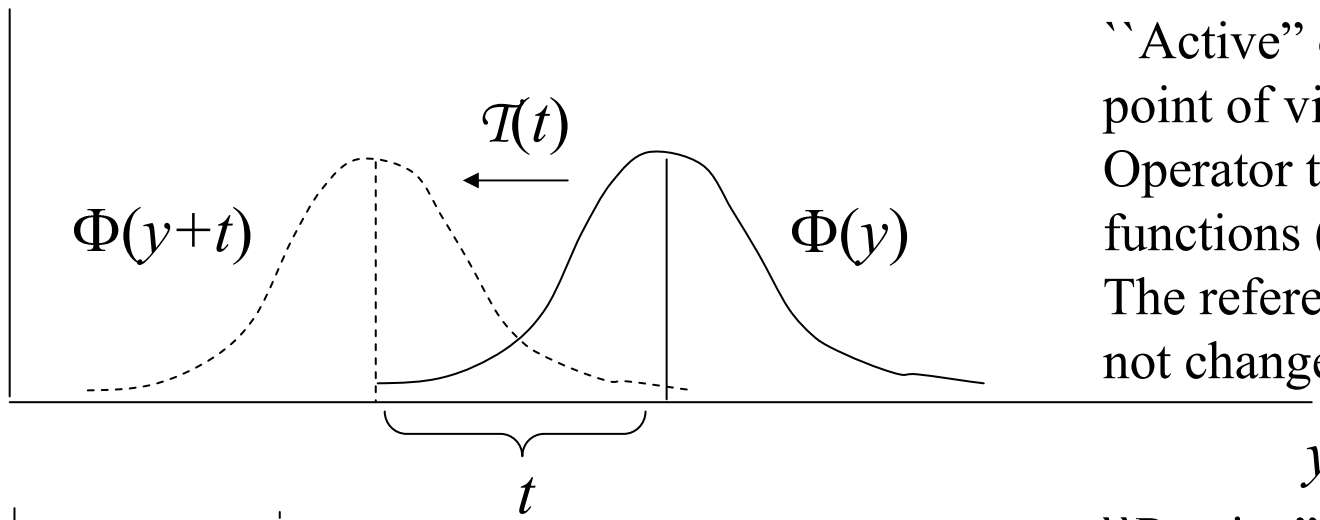
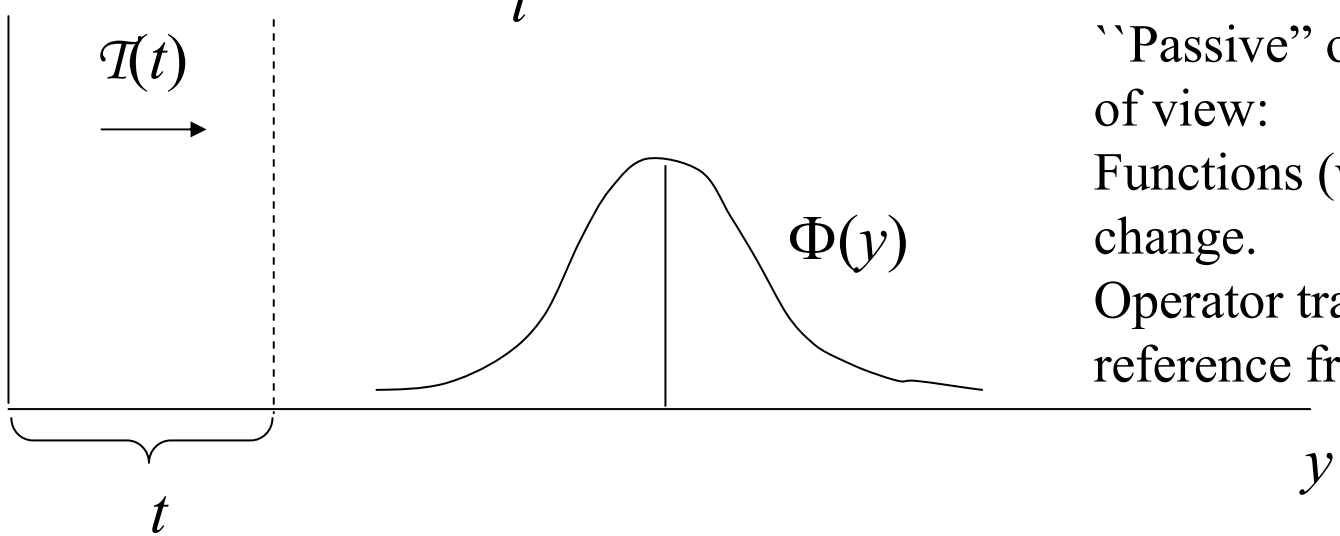
Alibi and Alias points of view on translation operator



``Active" or ``Alibi" point of view:
Operator transforms functions (vectors).
The reference frame does not change.



``Passive" or ``Alias" point of view:
Functions (vectors) do not change.
Operator transforms the reference frame.

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- Translation operators of the two view-points are related to each other (transposes)
  - Active view point transforms the vectors (functions)
  - Passive view point transforms the coordinate frame (basis functions)
- What we want in the FMM is a way to express a vector with “coordinates” at one center to represent vector at another “center” and basis
- We use duality of view points to construct matrix version of our translation operators
- Express the basis function in new basis in terms of a series of old basis functions

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R|R-reexpansion

Let $\mathbf{y}-\mathbf{x}_* \in \Omega_r(\mathbf{x}_*) \subset \mathbb{R}^d$, $\Omega_r(\mathbf{x}_*) : |\mathbf{y}-\mathbf{x}_*| < r$, and $\{R_n(\mathbf{y}-\mathbf{x}_*)\}$ be a regular basis in $C(\Omega)$. Let $\mathbf{y}-\mathbf{x}_*+\mathbf{t} \in \Omega_r(\mathbf{x}_*)$ and

$$R_n(\mathbf{y}-\mathbf{x}_*+\mathbf{t}) = \sum_{l=0}^{\infty}(R|R)_{ln}(\mathbf{t})R_l(\mathbf{y}-\mathbf{x}_*).$$

Coefficients $(R|R)_{ln}(\mathbf{t})$ are called $R|R$ – *reexpansion coefficients* (regular-to-regular) , and infinite matrix

$$(\mathbf{R}|\mathbf{R})(\mathbf{t}) = \begin{pmatrix} (R|R)_{00} & (R|R)_{01} & \dots \\ (R|R)_{10} & (R|R)_{11} & \dots \\ \dots & \dots & \dots \end{pmatrix}$$

is called $R|R$ – *reexpansion matrix*.

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Example of R|R-reexpansion

$$R_m(x) = x^m,$$

$$R_m(x+t) = (x+t)^m = x^m + \binom{m}{1} x^{m-1} t + \ldots + \binom{m}{m-1} x t^{m-1} + t^m$$

$$= \sum_{l=0}^{m} \binom{m}{l} t^l x^{m-l} = \sum_{l=0}^{m} \binom{m}{l} t^{m-l} x^l = \sum_{l=0}^{m} \binom{m}{l} t^{m-l} R_l(x),$$

$$(R|R)_{lm}(t) = \begin{cases} \binom{m}{l} t^{m-l}, & l \leqslant m, \\ 0, & l > m. \end{cases}$$

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R|R-translation operator

Translation operator $\mathcal{T}(\mathbf{t})$ which is represented in regular basis $\{R_n(\mathbf{y}-\mathbf{x}_*)\}$ by the $R|R$ – *reexpansion matrix* is called $\mathcal{R}|\mathcal{R}$-translation operator.

$$\mathcal{T}(\mathbf{t})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t})$$

$$(\mathcal{R}|\mathcal{R})(\mathbf{t}) = \mathcal{T}(\mathbf{t}).$$

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Different translation operators

$$\mathcal{T}(\mathbf{t})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t})$$

The first letter shows the basis for $\Phi(\mathbf{y})$

The second letter shows the basis for $\Phi(\mathbf{y}+\mathbf{t})$

$$\mathcal{T}(\mathbf{t}) = \begin{cases} (\mathcal{R}|\mathcal{R})(\mathbf{t}) \\ (\mathcal{S}|\mathcal{S})(\mathbf{t}) \\ (\mathcal{S}|\mathcal{R})(\mathbf{t}) \\ (\mathcal{R}|\mathcal{S})(\mathbf{t}) \end{cases}$$

Needed only to show the expansion basis (for operator representation)

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Matrix representation of R|R-translation operator

Consider $$\Phi(\mathbf{y}) = \sum_{n=0}^{\infty} A_n(\mathbf{x}_*) R_n(\mathbf{y} - \mathbf{x}_*).$$

$$\Phi(\mathbf{y}+\mathbf{t}) = (\mathcal{R}|\mathcal{R})(\mathbf{t})[\Phi(\mathbf{y})] = \sum_{n=0}^{\infty} A_n(\mathbf{x}_*)(\mathcal{R}|\mathcal{R})(\mathbf{t})[R_n(\mathbf{y} - \mathbf{x}_*)]$$

$$= \sum_{n=0}^{\infty} A_n(\mathbf{x}_*) R_n(\mathbf{y} - \mathbf{x}_* + \mathbf{t})$$

$$= \sum_{n=0}^{\infty} A_n(\mathbf{x}_*) \sum_{l=0}^{\infty} (R|R)_{ln}(\mathbf{t}) R_l(\mathbf{y} - \mathbf{x}_*)$$

$$= \sum_{l=0}^{\infty} \left[\sum_{n=0}^{\infty} (R|R)_{ln}(\mathbf{t}) A_n(\mathbf{x}_*) \right] R_l(\mathbf{y} - \mathbf{x}_*)$$

$$= \sum_{l=0}^{\infty} \widetilde{A}_l(\mathbf{x}_*, \mathbf{t}) R_l(\mathbf{y} - \mathbf{x}_*),$$

Coefficients of shifted function

Coefficients of original function

$$\widetilde{A}_l(\mathbf{x}_*, \mathbf{t}) = \sum_{n=0}^{\infty} (R|R)_{ln}(\mathbf{t}) A_n(\mathbf{x}_*), \quad \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) = (\mathbf{R}|\mathbf{R})(\mathbf{t}) \mathbf{A}(\mathbf{x}_*).$$

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Reexpansion of the same function over shifted basis

Compact notation:

$$\Phi(\mathbf{y}) = \sum_{n=0}^{\infty} A_n(\mathbf{x}_*) R_n(\mathbf{y} - \mathbf{x}_*) = \mathbf{A}(\mathbf{x}_*) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*),$$

$$\Phi(\mathbf{y} + \mathbf{t}) = \sum_{l=0}^{\infty} \widetilde{A}_l(\mathbf{x}_*, \mathbf{t}) R_l(\mathbf{y} - \mathbf{x}_*) = \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*)$$

We have:

$$\Phi(\mathbf{y}) = \Phi((\mathbf{y} - \mathbf{t}) + \mathbf{t}) = \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{R}((\mathbf{y} - \mathbf{t}) - \mathbf{x}_*)$$
$$= \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_* - \mathbf{t}).$$

Also

$$\Phi(\mathbf{y}) = \mathbf{A}(\mathbf{x}_*) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*) = \mathbf{A}(\mathbf{x}_* + \mathbf{t}) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_* - \mathbf{t}),$$

so

$$\mathbf{A}(\mathbf{x}_* + \mathbf{t}) = \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) = (\mathbf{R}|\mathbf{R})(\mathbf{t})\mathbf{A}(\mathbf{x}_*).$$

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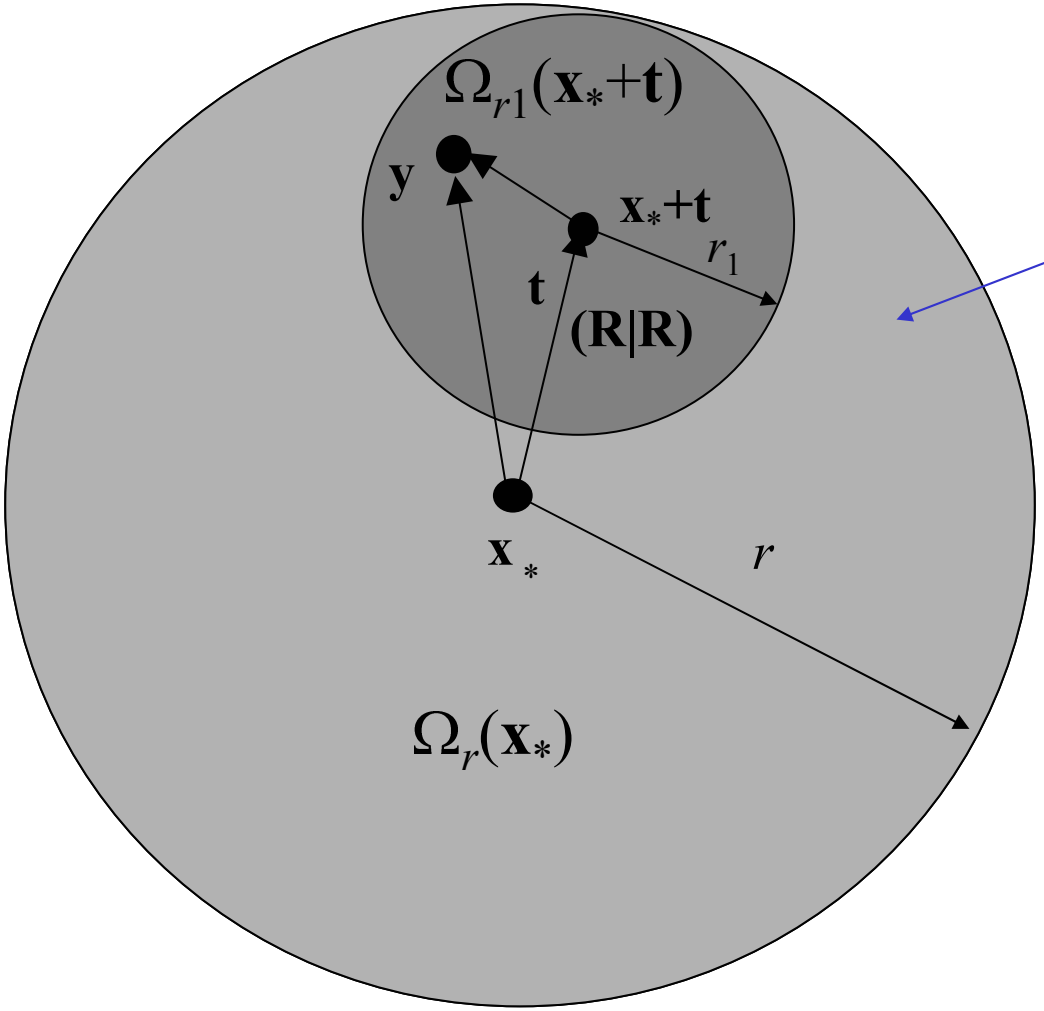
R|R-reexpansion of the same function over shifted basis (2)



Original expansion
Is valid only here!

$$|\mathbf{y} - \mathbf{x}_* - \mathbf{t}| < r_1 = r - |\mathbf{t}|$$

Since $\Omega_{r1}(\mathbf{x}_*+\mathbf{t}) \subset \Omega_r(\mathbf{t})$!

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Example of power series reexpansion

$$R_m(x) = x^m.$$

$$\Phi(y,x_i) = \sum_{m=0}^{\infty} A_m(x_{*1},x_i)R_m(y-x_{*1}) = \sum_{m=0}^{\infty} A_m(x_{*2},x_i)R_m(y-x_{*2}),$$

$$\mathbf{A}(x_{*2},x_i) = (\mathbf{R}|\mathbf{R})(x_{*2}-x_{*1}) \bullet \mathbf{A}(x_{*1},x_i).$$

$$\begin{pmatrix} A_0(x_{*2},x_i) \\ A_1(x_{*2},x_i) \\ A_2(x_{*2},x_i) \\ \dots \end{pmatrix} = \begin{pmatrix} 1 & \begin{pmatrix} 1 \\ 0 \end{pmatrix}(x_{*2}-x_{*1}) & \begin{pmatrix} 2 \\ 0 \end{pmatrix}(x_{*2}-x_{*1})^2 & \dots \\ 0 & 1 & \begin{pmatrix} 2 \\ 1 \end{pmatrix}(x_{*2}-x_{*1}) & \dots \\ 0 & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} A_0(x_{*1},x_i) \\ A_1(x_{*1},x_i) \\ A_2(x_{*1},x_i) \\ \dots \end{pmatrix}$$

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Example of power series reexpansion (2). Relation to Taylor series.

Let's check this for Taylor series, when expansion coefficients are

$$A_m(x_{*1},x_i) = \frac{1}{m!}\frac{\partial^m \Phi(x_{*1},x_i)}{\partial x_{*1}^m}$$

For A_0 this yields Taylor series again!

Check for A_l

$$\Phi(x_{*2},x_i) = \sum_{m=0}^{\infty}\frac{1}{m!}\frac{\partial^m \Phi(x_{*1},x_i)}{\partial x_{*1}^m}(x_{*2}-x_{*1})^m,$$

$$\frac{1}{l!}\frac{\partial^l \Phi(x_{*2},x_i)}{\partial x_{*2}^l} = \sum_{m=l}^{\infty}\begin{pmatrix} m \\ l \end{pmatrix}\frac{1}{m!}\frac{\partial^m \Phi(x_{*1},x_i)}{\partial x_{*1}^m}(x_{*2}-x_{*1})^{m-l}$$

$$= \sum_{m=l}^{\infty}\frac{m!}{l!(m-l)!}\frac{1}{m!}\frac{\partial^m \Phi(x_{*1},x_i)}{\partial x_{*1}^m}(x_{*2}-x_{*1})^{m-l}$$

$$= \frac{1}{l!}\sum_{k=0}^{\infty}\frac{1}{k!}\frac{\partial^{k+l} \Phi(x_{*1},x_i)}{\partial x_{*1}^{k+l}}(x_{*2}-x_{*1})^k,$$

$$\frac{\partial^l \Phi(x_{*2},x_i)}{\partial x_{*2}^l} = \sum_{k=0}^{\infty}\frac{1}{k!}\frac{\partial^{k+l} \Phi(x_{*1},x_i)}{\partial x_{*1}^{k+l}}(x_{*2}-x_{*1})^k.$$

For A_l we obtained Taylor series for the l-th derivative! Wow!

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S|S-reexpansion

Let $\mathbf{y}-\mathbf{x}_* \in \Omega_r(\mathbf{x}_*) \subset \mathbb{R}^d$, $\Omega_r(\mathbf{x}_*) : |\mathbf{y}-\mathbf{x}_*| > r$, and $\{S_n(\mathbf{y}-\mathbf{x}_*)\}$ be a singular basis in $C(\Omega)$. Let $\mathbf{y}-\mathbf{x}_*+\mathbf{t} \in \Omega_r(\mathbf{x}_*)$ and

$$S_n(\mathbf{y}-\mathbf{x}_*+\mathbf{t}) = \sum_{l=0}^{\infty}(S|S)_{ln}(\mathbf{t})S_l(\mathbf{y}-\mathbf{x}_*).$$

Coefficients $(S|S)_{ln}(\mathbf{t})$ are called $S|S$ – *reexpansion coefficients* (singular-to-singular) , and infinite matrix

$$(\mathbf{S}|\mathbf{S})(\mathbf{t}) = \begin{pmatrix} (S|S)_{00} & (S|S)_{01} & \dots \\ (S|S)_{10} & (S|S)_{11} & \dots \\ \dots & \dots & \dots \end{pmatrix}$$

is called $S|S$ – *reexpansion matrix*.

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S|S-translation operator

Translation operator $\mathcal{T}(\mathbf{t})$ which is represented in singular basis $\{S_n(\mathbf{y}-\mathbf{x}_*)\}$ by the $S|S$ – *reexpansion matrix* is called $\mathcal{S}|\mathcal{S}$-translation operator.

$$\mathcal{T}(\mathbf{t})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t})$$

$$(\mathcal{S}|\mathcal{S})(\mathbf{t}) = \mathcal{T}(\mathbf{t}).$$

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S|R-translation operator

Translation operator $\mathcal{T}(\mathbf{t})$ which is represented in singular basis by the $S|R$ – *reexpansion matrix* is called $\mathcal{S}|\mathcal{R}$-translation operator if the basis of expansion is changed with the translation operation from singular $\{S_n(\mathbf{y}-\mathbf{x}_*)\}$ to regular $\{R_n(\mathbf{y}-\mathbf{x}_*+\mathbf{t})\}$

$$\mathcal{T}(\mathbf{t})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t})$$

$$(\mathcal{S}|\mathcal{R})(\mathbf{t}) = \mathcal{T}(\mathbf{t}).$$

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S|R-operator has almost the same properties as S|S and R|R

(**t** cannot be zero)

$$\Phi(\mathbf{y}) = \mathbf{B}(\mathbf{x}_*) \circ \mathbf{S}(\mathbf{y} - \mathbf{x}_*),$$

$$\Phi(\mathbf{y} + \mathbf{t}) = \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*)$$

$$\Phi(\mathbf{y}) = \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_* - \mathbf{t}).$$

$$\widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) = (\mathbf{S}|\mathbf{R})(\mathbf{t})\mathbf{B}(\mathbf{x}_*).$$

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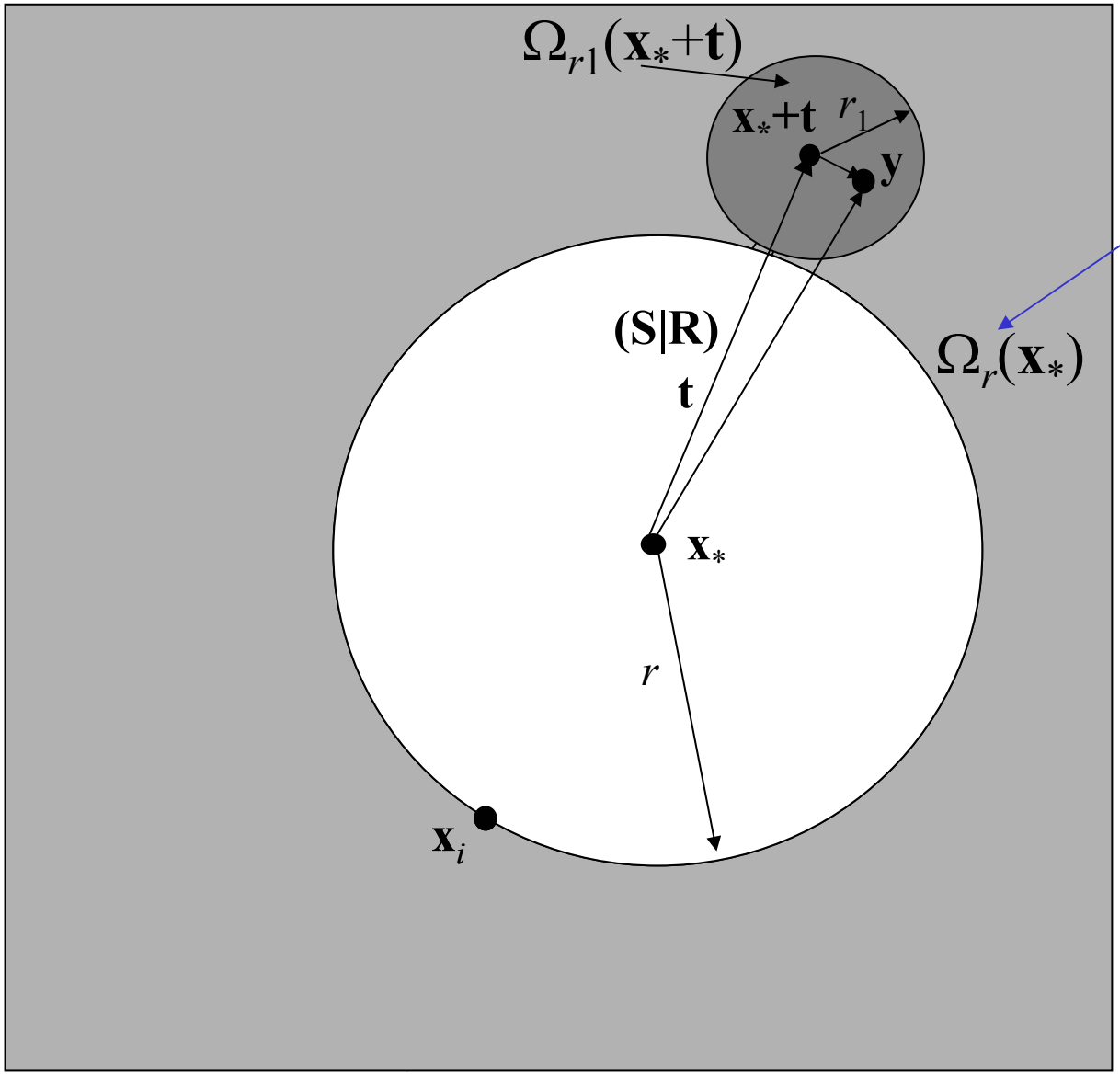
Picture is different…



Original expansion
Is valid only here!

$$|\mathbf{y} - \mathbf{x}_* - \mathbf{t}| < r_1 = |\mathbf{t}| - r$$

Since
$\Omega_{r1}(\mathbf{x}_*+\mathbf{t}) \subset \Omega_r(\mathbf{t})$!

Also

$$|\mathbf{x}_i - \mathbf{x}_*| < r$$

singular point !

Example from previous lectures

$$\Phi(y,x_i) = \frac{1}{y-x_i}.$$

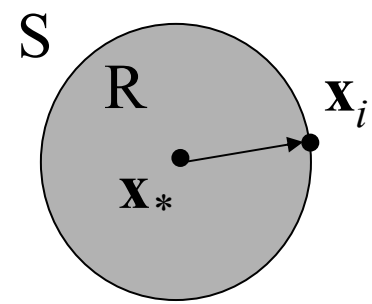
$|y-x_*| < |x_i - x_*|$:

R-expansion

$$\Phi(y,x_i) = \sum_{m=0}^{\infty} a_m(x_i,x_*) R_m(y-x_*),$$

$$a_m(x_i,x_*) = -(x_i - x_*)^{-m-1}, \quad m = 0,1,\ldots,$$

$$R_m(y-x_*) = (y-x_*)^m, \quad m = 0,1,\ldots$$



$|y-x_*| > |x_i - x_*|$:

S-expansion

$$\Phi(y,x_i) = \sum_{m=0}^{\infty} b_m(x_i,x_*) S_m(y-x_*),$$

$$b_m(x_i,x_*) = (x_i - x_*)^m, \quad m = 0,1,\ldots,$$

$$S_m(y-x_*) = (y-x_*)^{-m-1}, \quad m = 0,1,\ldots$$

In this case we have

$(|y - x_*| < |t|)$

$$S_n(y - x_* + t) = (t + y)^{-n-1} = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m S_n(t)}{dt^n} (y - x_*)^m$$

$$= \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m S_n(t)}{dt^n} R_m(y - x_*) = \sum_{m=0}^{\infty} (S|R)_{mn}(t) R_m(y - x_*).$$

So

$$(S|R)_{mn}(t) = \frac{1}{m!} \frac{d^m S_n(t)}{dt^n} = \frac{(-1)^m (m+n)!}{m! n! t^{n+m+1}}.$$

$$(\mathbf{S}|\mathbf{R})(t) = \begin{pmatrix} t^{-1} & t^{-2} & t^{-3} & \dots \\ -t^{-2} & -2t^{-3} & -3t^{-4} & \dots \\ t^{-3} & 3t^{-4} & 6t^{-5} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

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Norm of the Translation Operator

Theorem. Let $\mathbb{F}(\Omega)$ be a set of functions bounded in $\mathbb{R}^d$. Then $\|\mathcal{T}(\mathbf{t})\| = 1$.
Proof.

$$\|\mathcal{T}(\mathbf{t})\| = \frac{\|\mathcal{T}(\mathbf{t})\Phi(\mathbf{y})\|}{\|\Phi(\mathbf{y})\|} = \frac{\|\Phi(\mathbf{y}+\mathbf{t})\|}{\|\Phi(\mathbf{y})\|} = \frac{\sup_{\mathbf{y}\in\mathbb{R}^d}|\Phi(\mathbf{y}+\mathbf{t})|}{\sup_{\mathbf{y}\in\mathbb{R}^d}|\Phi(\mathbf{y})|} = 1.$$

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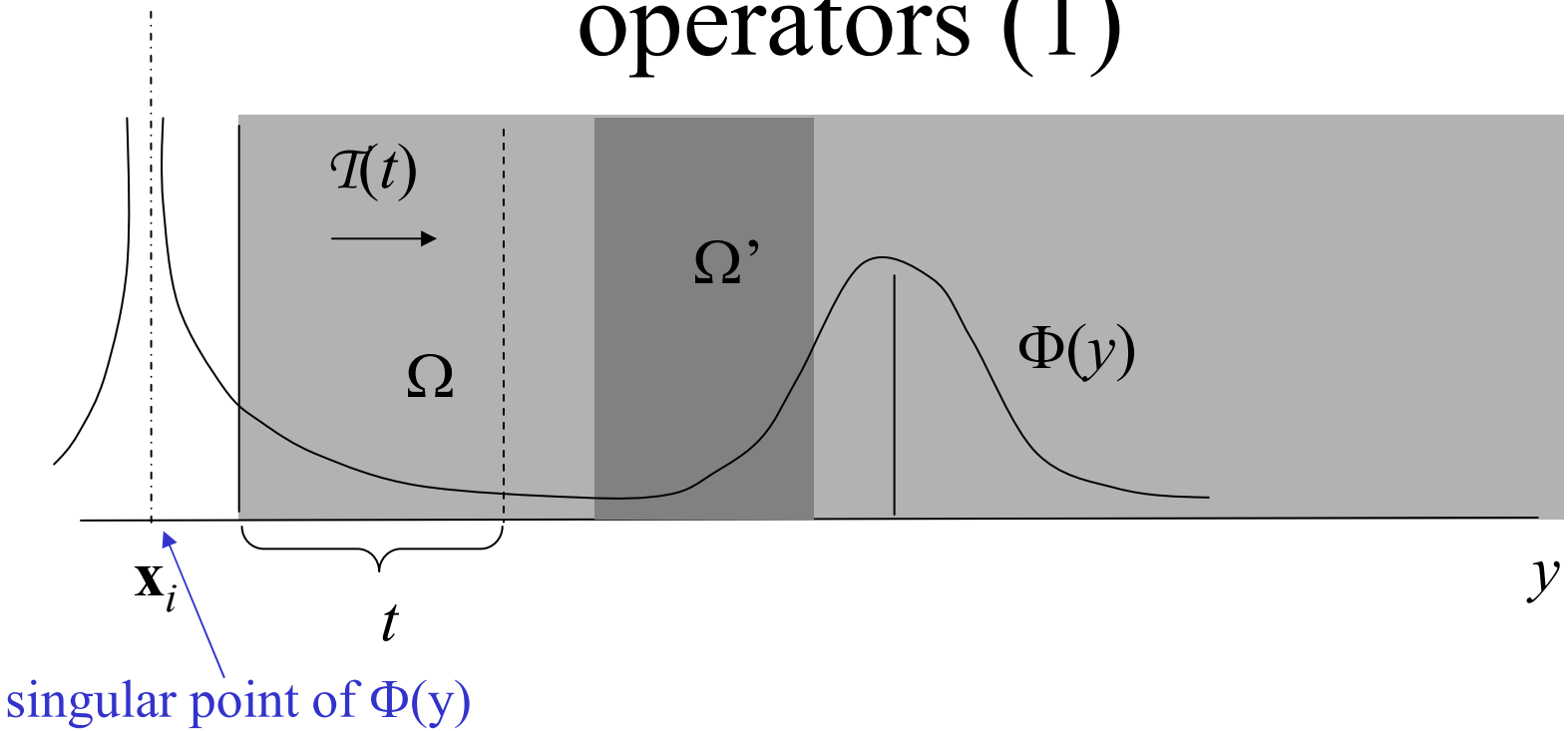
Norms of $R|R$, $S|S$, and $S|R$-operators (1)



$\Phi(\mathbf{y})$ is bounded in Ω.
$\Omega' \subset \Omega$.
Therefore $\Phi(\mathbf{y})$ is bounded in Ω', and

$$\|\Phi(\mathbf{y})\|_{\Omega'} = \sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})| \leqslant \sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})| = \|\Phi(\mathbf{y})\|_{\Omega}.$$

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Norms of $R|R$, $S|S$, and $S|R$-operators (2)

From the passive point of view, the translation operator does nothing, but just changes the reference frame. So if we consider that R|R, S|S, and S|R do just change of the reference frame **PLUS** *they shrink the domain, where the function is bounded, then their norms do not exceed* 1.

$$\Omega' \subset \Omega$$

$$\|(\mathcal{R}|\mathcal{R})(\mathbf{t})\| = \frac{\sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})|}{\sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})|} \leqslant 1,$$

$$\|(\mathcal{S}|\mathcal{S})(\mathbf{t})\| = \frac{\sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})|}{\sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})|} \leqslant 1,$$

$$\|(\mathcal{S}|\mathcal{R})(\mathbf{t})\| = \frac{\sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})|}{\sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})|} \leqslant 1.$$

This is the difference between general translation operator and $R|R$, $S|S$, and $S|R$ operators.

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Error of exact $R|R$, $S|S$, and $S|R$-translation

If

$$\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon,$$

then

$$\begin{aligned}
\|(\mathcal{R}|\mathcal{R})(\mathbf{t})(\Phi(\mathbf{y}) - \Phi^p(\mathbf{y}))\| &= \|(\mathcal{R}|\mathcal{R})(\mathbf{t})\|\,\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon, \\
\|(\mathcal{S}|\mathcal{S})(\mathbf{t})(\Phi(\mathbf{y}) - \Phi^p(\mathbf{y}))\| &= \|(\mathcal{S}|\mathcal{S})(\mathbf{t})\|\,\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon, \\
\|(\mathcal{S}|\mathcal{R})(\mathbf{t})(\Phi(\mathbf{y}) - \Phi^p(\mathbf{y}))\| &= \|(\mathcal{S}|\mathcal{R})(\mathbf{t})\|\,\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon.
\end{aligned}$$

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Five Key Stones of FMM

- Factorization
- Error
- Translation
- Grouping
- Data Structure

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Group Theory

- One of the key research areas in the FMM is reducing the cost of translations
- If one finds symmetries then computational costs are reduced
- Formal mathematics to study symmetry is Group Theory
- Interestingly FMM translational operators form a group
- Research: Use GT to improve efficiency

A set $\mathbb{G}$ of elements (objects) $a, b, c, \ldots$ is called *group* if there defined some binary operation $\odot$ called "group operation", which for any pair of elements $a, b \in \mathbb{G}$ correspond some object $a \odot b$, such that for any $a, b, c \in \mathbb{G}$ satisfies the following properties:

1). $a \odot b \in \mathbb{G}$, ($\mathbb{G}$ is closed with respect to $\odot$),

2). $a \odot (b \odot c) = (a \odot b) \odot c$, (associativity),

3). $\exists e \in \mathbb{G}$, $e \odot a = a$, $\left(\mathbb{G}\text{ contains the unity, } e\right)$,

4). $\exists a^{-1} \in \mathbb{G}$, $a^{-1} \odot a = e$, $\left(\mathbb{G}\text{ contains the inverse element for each } a \in \mathbb{G}\right)$.

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