Outline

• One Theorem (inspired by Homework 4)
• Basic Idea of Multilevel FMM (MLFMM);
• Formal Requirements for Functions (Potentials) in MLFMM;
• Setting Hierarchical Data Structure;
  – Hierarchical Domains and Associated Potentials (Functions);
  – Dimensionality Limits;
• MLFMM Algorithm;
  – Structure of the Algorithm;
  – Upward Pass;
  – Downward Pass;
  – Final Summation.
Truncated Translation Theorem (2)

Let \( \{F_n(y)\} \) and \( \{G_n(y)\} \) be two expansion bases in \( \Omega \), and the reexpansion series converges everywhere in \( \Omega \):

\[
\forall y \in \Omega, \quad F_n(y) = \sum_{m=0}^{\infty} (F|G)_{mn} G_m(y), \quad n = 0, 1, 2, \ldots
\]

Let also \( \{A_n\} \) be a set of coefficients, such that the double sum converges absolutely and uniformly in \( \Omega \):

\[
\forall y \in \Omega, \quad \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A_n (F|G)_{mn} G_m(y) = \Phi(y),
\]

\[
\forall \epsilon, \exists p(\epsilon), \quad \sum_{n=0}^{\infty} \sum_{m=p}^{\infty} |A_n (F|G)_{mn} G_m(y)| < \epsilon, \quad \sum_{n=p}^{\infty} \sum_{m=0}^{\infty} |A_n (F|G)_{mn} G_m(y)| < \epsilon.
\]

Then

\[
\left| \Phi(y) - \sum_{n=0}^{p-1} \sum_{m=0}^{p-1} A_n (F|G)_{mn} G_m(y) \right| < 2\epsilon.
\]
Proof

Let us denote

\[ c_{mn} = (F|G)_{mn} a_n g_m(y) \]

\[
\left| \Phi(y) - \sum_{n=0}^{p-1} \sum_{m=0}^{p-1} c_{mn} \right| = \left| \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} c_{mn} - \sum_{n=0}^{p-1} \sum_{m=0}^{p-1} c_{mn} \right |
\]

\[
= \left| \sum_{m=0}^{p-1} \sum_{n=0}^{\infty} c_{mn} + \sum_{m=p}^{\infty} \sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1} \sum_{n=0}^{p-1} c_{mn} \right |
\]

\[
= \left| \sum_{m=0}^{p-1} \sum_{n=0}^{p-1} c_{mn} + \sum_{m=0}^{p-1} \sum_{n=p}^{\infty} c_{mn} + \sum_{m=p}^{\infty} \sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1} \sum_{n=0}^{p-1} c_{mn} \right |
\]

\[
\leq \sum_{m=0}^{p-1} \sum_{n=p}^{\infty} |c_{mn}| + \sum_{m=p}^{\infty} \sum_{n=0}^{\infty} |c_{mn}| < \epsilon + \epsilon = 2\epsilon.
\]
Middleman Algorithm

Standard algorithm

Sources

Evaluation
Points

Total number of operations: $O(NM)$

Middleman algorithm

Sources

Evaluation
Points

Total number of operations: $O(N+M)$
Single Level FMM

Middleman algorithm

Sources

Evaluation Points

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

SLFMM

Sources

$L$ groups

Evaluation Points

$K$ groups

Total number of operations: $O(N+M+KL)$
Two Level FMM

SLFMM=1LFMM

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

Evaluation Points

(2LFMM)

Total number of operations: $O(N+M+K+L+K_1L_1)$
**KxL**-interaction of two groups can be reduced by further grouping to \( K+L+K_1L_1 \)

Indeed, if \( K=nK_1, L=mL_1 \), then

\[
K+L+K_1L_1 = nK_1 + mL_1 + K_1L_1,
\]

while \( KL = nmK_1L_1 \).

**Problem for Thinking:** What are conditions for \( n,m,K_1,L_1 \) to have

\[
zmK_1L_1 > nK_1 + mL_1 + K_1L_1
\]
Example of Multi Level Structure (Post Offices)

Source Hierarchy (Area)  ↓  Mail Transfer

- People (sources, Level 5)
- Mail Box, Post Master (Level 4)
- Local Post Offices (Level 3)
- City Post Office (Level 2)

Receiver Hierarchy (Area)  ↑  Mail Transfer

- City Post Office (Level 2)
- Local Post Offices (Level 3)
- Post Master (Level 4)
- People (receivers, Level 5)

AIRCRAFT
Example of MLFMM
(Computation of Gravity Field)

Source Hierarchy
(Mass, Distance)

• Planets (Level 5)
• Solar Systems (Level 4)
• Galaxies (Level 3)
• Metagalaxies (Level 2)

Receiver Hierarchy
(Mass, Distance)

• Metagalaxies (Level 2)
• Galaxies (Level 3)
• Solar Systems (Level 4)
• Planets (Level 5)

Far Field to Local Field

Influence

Influence
Exercise:

Create your own example!
Complexity of MLFMM

Definitions:

Upward Pass: Going Up on SOURCE Hierarchy
Downward Pass: Going Down on EVALUATION Hierarchy

We have $N$ sources. Let us we group them hierarchically. At level $i$ we have $N_i$ source groups. Each group at level $i+1$ contains $N_iS$ sources, so

$$N_{i+1} = N_iS, \quad i = 2, 3, ..., L,$$

and

$$N_L = N.$$

Then the number of operations for the Upward Pass is of order

$$N_L + N_{L-1} + ... + N_2 = N + \frac{N}{S} + \frac{N}{S^2} + ... + \frac{N}{S^{L-2}}$$

$$= N\left(1 + \frac{1}{S} + ... + \frac{1}{S^{L-2}}\right) = N \frac{1 - 1/S^{L-1}}{1 - 1/S} = O(N).$$

Similarly, the number of operations for the Downward Pass is of order $O(M)$.

$$MLFMM\_Complexity = O(M + N)!$$
Summary of requirements for functions that can be used in FMM

- We have two sets of points:
  \[ X = \{x_1, x_2, \ldots, x_N\}, \quad x_i \in \mathbb{R}^d, \quad i = 1, \ldots, N, \]
  \[ Y = \{y_1, y_2, \ldots, y_M\}, \quad y_j \in \mathbb{R}^d, \quad j = 1, \ldots, M. \]

- We have functions (potentials):
  \[ \Phi(x_i, y) : \mathbb{R}^d \rightarrow \mathbb{R}, \quad y \in \mathbb{R}^d, \quad i = 1, \ldots, N. \]

- These functions can be factorized as (local expansion):
  \[ \Phi(x_i, y) = A(x_i, x_*) \cdot R(y - x_*), \quad |y - x_*| < r < |x_i - x_*|, \quad i = 1, \ldots, N \]

- These functions can be factorized as (far field expansion):
  \[ \Phi(x_i, y) = B(x_i, x_*) \cdot S(x - x_*), \quad |y - x_*| > R > |x_i - x_*|, \quad i = 1, \ldots, N \]

- The product is distributive operation with respect to addition
  \[ (u_1A_1 + u_2A_2) \circ F = u_1A_1 \circ F + u_2A_2 \circ F, \quad F = S, R \]
Summary of requirements for functions that can be used in FMM (2)

- **R-expansion coefficients** can be $R|R$-translated:
  \[ |x - x_{*2}| < |x_i - x_{*1}| - |x_{*1} - x_{*2}| : \]
  \[ A(x_i, x_{*2}) = (R|R)(x_{*2} - x_{*1})A(x_i, x_{*1}) \]

- **S-expansion coefficients** can be $S|S$-translated:
  \[ |x - x_{*2}| > |x_{*1} - x_{*2}| + |x_i - x_{*1}|, \]
  \[ B(x_i, x_{*2}) = (S|S)(x_{*2} - x_{*1})B(x_i, x_{*1}) \]

- **S-expansion coefficients** can be $S|R$-translated (converted to $R$-expansion coefficients)
  \[ |x - x_{*2}| < |x_{*1} - x_{*2}| + |x_i - x_{*1}|, \]
  \[ A(x_i, x_{*2}) = (S|R)(x_{*2} - x_{*1})B(x_i, x_{*1}) \]

- And we are looking for sums:
  \[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i), \quad j = 1, \ldots, M. \]

- Some generalization are possible, say instead of $\Phi(y_j, x_i)$ we can consider $\Phi_i(y_j)$, etc.
Two Parts of the MLFMM

- Setting Hierarchical Data Structure
  (MLFMM Constructor) \(O(N \log N + M \log M)\)

- MLFMM Solver \(O(N + M)\) or \(O(N \log^q N + M \log^q M)\),
  *Will evaluate the complexity in more details later.*

- In iterative and multiple solutions of the same system
  the MLFMM Constructor should be called only once.
Setting Hierarchical Data Structure

- Scale source and evaluation data to have the computational domain of size of a unit box.
- Sort data using interleaving technique.
- Determine the level of space subdivision with $2^d$-tree to have $s$ sources at the finest subdivision level, $L_{max}$.
- If you choose to spend memory for trees, neighbor lists, and so on, compute and store information that does not change in the process of execution of the MLFMM solver.
Hierarchical Spatial Domains

$E_1$ $E_2$

$E_3$ $E_4$
Hierarchical Spatial Domains

We accept the hierarchical numbering system described above and define four elements (domains) of fractal structure for each box with number $n = \text{Number} = 0, \ldots, 2^{id} - 1$ at level $l = 0, \ldots, L$.

$E_1(n, l) \subset \mathbb{R}^d$ denotes spatial points inside the box $(n, l)$;

$E_2(n, l) \subset \mathbb{R}^d$ denotes spatial points inside the box $(n, l)$ and its neighbors, $\{(\text{Neighbor}(n, l), l)\}$;

$E_3(n, l) = E_1(0, 0) \setminus E_2(n, l)$ denotes spatial points outside the box $(n, l)$ and its neighbors, $\{(\text{Neighbor}(n, l), l)\}$.

$E_4(n, l) = E_2(\text{Parent}(n), l - 1) \setminus E_2(n, l)$ denotes spatial points inside the parent box $(\text{Parent}(n), l - 1)$ and its neighbors, $\{(\text{Neighbor}(\text{Parent}(n), l - 1), l - 1)\}$, from which the domain $E_2(n, l)$ is excluded.

Accordingly we associate sets of boxes of level $l$ which constitute each domain $E_m(n, l)$. Their numbers we denote as $I_m(n, l)$. So we have:

$I_1(n, l) = (n, l)$,

$I_2(n, l) = \{(n, l), (\text{Neighbor}(n, l), l)\}$,

$I_3(n, l) = \{0, 1, \ldots, 2^{id} - 1\} \setminus I_2(n, l)$,

$I_4(n, l) = \{(\text{Children}(\text{Neighbor}(\text{Parent}(n), l - 1), l - 1))\} \setminus \{(n, l), (\text{Neighbor}(n, l), l)\}$. 
With Such Neighborhood
the dimensionality of space
in FMM cannot exceed $d=9$.

$$0.5a\sqrt{d} < 1.5a,$$
$$\sqrt{d} < 3,$$
$$d < 9.$$  

For larger dimensions larger
neighborhoods should be
considered (but seems it is
not practical to use $2^d$-trees
in this case and something
better should be invented).
Hierarchical Potentials (Functions)

Based on these domains for each box the following functions (potentials) are defined:

\[
\Phi_1^{(n,l)}(y) = \sum_{x_i \in E_1(n,l)} u_i \Phi(y, x_i),
\]

\[
\Phi_2^{(n,l)}(y) = \sum_{x_i \in E_2(n,l)} u_i \Phi(y, x_i),
\]

\[
\Phi_3^{(n,l)}(y) = \sum_{x_i \in E_3(n,l)} u_i \Phi(y, x_i),
\]

\[
\Phi_4^{(n,l)}(y) = \sum_{x_i \in E_4(n,l)} u_i \Phi(y, x_i),
\]

Note that since domains \( E_2(n,l) \) and \( E_3(n,l) \) are complimentary, and

\[
\Phi(y) = \Phi_2^{(n,l)}(y) + \Phi_3^{(n,l)}(y)
\]

for arbitrary \( l \) and \( n \).
The MLFMM Algorithm (Solver)

- "Build Function" or "Build Potential" means find its expansion coefficients over some basis;
- The MLFMM Algorithm (we also call it sometimes "Regular FMM") consists of
  - Upward Pass;
  - Downward Pass;
  - Final Summation;
Step 1. At the finest level of space subdivision, build far-field expansion for sources inside each non-empty box of set $\mathbb{X}$ near the center of that box $x_c^{(n,L)}$:

$$\Phi_1^{(n,L)}(y) = C^{(n,L)} \circ S(y - x_c^{(n,L)}),$$

$$C^{(n,L)} = \sum_{x_i \in B_1^{(n,L)}} u_i B(x_i, x_c^{(n,L)}).$$

In the algorithm this means generation of the expansion coefficients $B(x_i, x_c^{(n,L)})$ and determination of $C^{(n,L)}$ for each box. If at the finest level each non-empty box contains only one source $x_i$, then for such box $C^{(n,L)} = u_i B(x_i, x_c^{(n,L)})$. Note that this expansion for $n$th box is valid in domain $E_3(n, L)$. If the $n$th box is empty $\Phi_1^{(n,L)}(y) = 0$ (or $C^{(n,L)} = 0$) for such a box. There is no need to keep zero $C^{(n,L)}$ in the memory, since the empty boxes can be skipped in the procedure.
Upward Pass. Step 1.

S-expansion valid in $\bar{\Omega}$

$E_3$

S-expansion valid in $E_3(n,L)$
Upward Pass. Step 2.

**Step 2.** For $l = L - 1, ..., 2$ recursively form $\Phi_1^{(n,l)}(y)$ (in other words determine expansion coefficients of this function) by reexpansion of $\Phi_1^{(\text{Children}(n),l+1)}(y)$ near the center of the parent box and summing up of contribution of all children boxes:

\[
\Phi_1^{(n,l)}(y) = C^{(n,l)} \circ S(y - x_c^{(n,l)}),
\]

\[
C^{(n,l)} = \sum_{n' \in \text{Children}(n)} (S|S)(x_c^{(n',l+1)} - x_c^{(n,l)}) C^{(n',l+1)}.
\]

For the $n$th box this expansion is valid in domain $E_3(n,l)$ which is a subdomain, where far-to-far translation is applicable. The set $\text{Children}(n)$ has $2^d$ entries, and summation over empty boxes of set $\mathbb{X}$ can be skipped (anyway for such boxes $C^{(n',l+1)} = 0$).
Upward Pass. Step 2.

S|S-translation.
Build potential for the parent box (find its S-expansion).
Result of the Upward Pass

In the entire hierarchy of boxes containing sources S-expansion coefficients for potentials due to sources in each box (domains $E_1$) are found. Expansions are valid in $E_3$ domains.
Downward Pass. Step 1.