
Lecture 9

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Fast Multipole Method (FMM)

We consider the problem of efficiently compute integrals of the form

\[ u(\mathbf{x}) = \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) q(\mathbf{y}) \, ds_\mathbf{y}, \]

or its discrete counterpart

\[ u_i = \sum_j G(\mathbf{x}_i, \mathbf{y}_j) q_j, \quad i = 1, \ldots, N. \]

We start by considering the simplified problem of evaluating

\[ u_i = \sum_{y_j \in B} G(\mathbf{x}_i, \mathbf{y}_j) q_j, \quad \mathbf{x}_i \in A \]

where \( A \) and \( B \) are “well-separated” boxes.

\( B \) contains \( N_B \) charges or sources \( q_j \) at \( \mathbf{y}_j \in B \)
\( A \) contains \( N_A \) evaluation points at \( \mathbf{x}_i \in A \)
Examples of projection/interpolation

1. Polynomial interpolation
2. Collocation
3. Multipole expansions
2. Collocation: Projection

We construct a projection rule by matching the potentials produced by the true sources with the potential produced by the equivalent sources, at a set of test points $\mathbf{x}_i^t$:

\[
\sum_m G(\mathbf{x}_i^t, \mathbf{y}_m^B)q_m^B \approx \sum_{\mathbf{y}_j \in B} G(\mathbf{x}_i^t, \mathbf{y}_j)q_j.
\]

The projection matrix is given by

\[
Q_m^B(\mathbf{y}_j) = \sum_i [G(\mathbf{x}_i^t, \mathbf{y}_m^B)]^+_{m,i} G(\mathbf{x}_i^t, \mathbf{y}_j)
\]

where $[G(\mathbf{x}_i^t, \mathbf{y}_m^B)]^+_{m,i}$ denote the entries of the pseudo-inverse of the matrix $G(\mathbf{x}_i^t, \mathbf{y}_m^B)$. 
2. Collocation: Selection of test points

- The test points are chosen such that the linear system
  \[
  \sum_m G(x^t_i, y^B_m) q^B_m \approx \sum_{y_j \in B} G(x^t_i, y_j) q_j
  \]
  is “well-posed”.

- A good choice is to pick the test points \( x^t_i \) on a test surface enclosing the source box \( B \).

- The source points on the test surface should be equispaced or near-equispaced and the number of test points \( x^t_i \) should be greater than the number of \( y^B_m \).

- Using uniformly distributed test points on a test circle enclosing the box \( B \), the error can be bounded as
  \[
  \left| \sum_m G(x, y^B_m) q^B_m - \sum_{y_j \in B} G(x, y_j) q_j \right| \leq C \left( \frac{a}{r_c} \right)^M, \quad |x| > r_c
  \]

where \( a > 0 \) is the radius of the circle that circumscribes \( B \), \( r_c > a \) is the radius of the test circle and \( M \) is the number of test points.
2. Collocation: Interpolation

The interpolation function \( P^A_n(x_i) \) is determined by requiring that the potential generated by unit charges at test points \( y_j^t \) is reproduced by interpolation from samples at \( x_n^A \):

\[
G(x_i, y_j^t) = \sum_n P^A_n(x_i) G(x_n^A, y_j^t).
\]

The interpolation matrix is determined by “solving” this linear system, which leads to:

\[
P^A_n(x_i) = \sum_j [G(x_n^A, y_j^t)]^+_{j,n} G(x_i, y_j^t),
\]

where \([G(x_n^A, y_j^t)]^+_{j,n}\) denote the entries of the pseudo-inverse of the matrix \(G(x_n^A, y_j^t)\).

Note that relabeling \( B \rightarrow A, y_j \rightarrow x_i, y_j^t \rightarrow x_i^t \) and \( y_m^B \rightarrow x_n^A \) and using the fact that \( G(x, y) = G(y, x) \), we have

\[
P^A_n(x_i) = Q^A_n(y_i).
\]
Examples of projection/interpolation

1. Polynomial interpolation

2. Collocation

3. Multipole expansions
Multipole Expansions

We consider $x, y \in \mathbb{R}^2$ and

$$G(x, y) = \log |x - y|,$$

with $x \in A$ and $y \in B$, where $A$ and $B$ are well-separated boxes.

We let $r > 0$ be the radius of the circumscribed circle of $B$ and $d > 2r$ be the distance from the center of $B$ to the box $A$.

**Theorem.** Consider $A$ and $B$ as described above. For all $p > 0$ there exist functions $f_k(x)$ and $g_k(y)$ for $1 \leq k \leq 2p + 1$, and a constant $C_p$ such that

$$\max_{(x, y) \in A \times B} \left| \log |x - y| - \sum_{k=1}^{2p+1} f_k(x)g_k(y) \right| \leq C_p \left( \frac{r}{d} \right)^p.$$
Why is it called multipole expansion?

Note that $1/z_x$ decomposes into a sum of two functions of $\mathbf{x} = (x_1, x_2)$:

$$\frac{\cos \theta_x}{|\mathbf{x}|} = \frac{x_1}{x_1^2 + x_2^2} = \frac{\partial}{\partial x_1} \log |\mathbf{x}|$$

and

$$\frac{\sin \theta_x}{|\mathbf{x}|} = \frac{x_2}{x_1^2 + x_2^2} = \frac{\partial}{\partial x_2} \log |\mathbf{x}|.$$

These are the expressions of two dipoles oriented horizontally and vertically, respectively.

At higher order, there are again two multipoles

$$\frac{\cos(k\theta_x)}{|\mathbf{x}|^k} \quad \text{and} \quad \frac{\sin(k\theta_x)}{|\mathbf{x}|^k}$$

corresponding to the non-mixed higher partials derivatives of log.
Multipole Expansions: Moments

The multipole expansion can be used to compute interactions from charges in box $B$ to potentials in box $A$ in an efficient way.

$$u(x_i) = \text{Re} \{u(z_{x_i})\} = \text{Re} \left\{ \sum_{y_j \in B} \log(z_{x_i} - z_{y_j})q_j \right\}$$

where $z_{x_i} = x_{i1} + i x_{i2}$ and $z_{y_j} = y_{j1} + i y_{j2}$. Then

$$u(z_{x_i}) = \log z_{x_i} \sum_{y_j \in B} q_j - \sum_{k=1}^{\infty} \frac{(k - 1)!}{z_{x_i}^k} \sum_{y_j \in B} \frac{z_{y_j}^k}{k!} q_j$$

We then define the moments associated with the charges $q_j$ at $y_j \in B$ as

$$\mu_0 = \sum_{y_j \in B} q_j \quad \text{and} \quad \mu_k = \sum_{y_j \in B} \frac{z_{y_j}^k}{k!} q_j, \quad k \geq 0,$$
Fast algorithm based on the multipole expansion

Here is a simple algorithm to evaluate

\[ u_i = \sum_{y_j \in B} G(x_i, y_j)q_j, \quad x_i \in A \]

\( A \) and \( B \) are “well-separated” boxes.

1. Compute \( r > 0 \) moments \( \mu_k \) requiring \( O(rN_B) \) operations.

2. Assign the moments to multipole components \( \log z_{x_i} \) and \( (k - 1)!/z_{x_i}^k \)
   evaluated at \( z_{x_i} \) requiring \( O(rN_A) \) operations.

The total cost amounts to \( O(r(N_A + N_B)) \) operations, instead of \( O(N_AN_B) \).
In order to see that the multipole expansion provides a projection rule, we interpret 

\( \frac{(k - 1)!}{z^k_x} \) as the following partial derivative of \( \log(z_x - z_y) \) with respect to \( z_y \):

\[
\frac{(k - 1)!}{z^k_x} = (-1)^k \left( \frac{\partial}{\partial z_y} \right)^k \log(z_x - z_y) \bigg|_{z_y=0}, \quad k \geq 0,
\]

which is approximated by a finite difference formula:

\[
\left( \frac{\partial}{\partial z_y} \right)^k \log(z_x - z_y) \bigg|_{z_y=0} \approx \sum_m T_{m,k} \log(z_x - z_{y_m}^B), \quad \mathbf{x} \in A, \ k \geq 1,
\]

where \( y_m^B = (\text{Re} \ z_{y_m}^B, \text{Im} \ z_{y_m}^B) \in B \).
Multipole expansion as a projection rule

Replacing the finite difference formula in the multipole expansion we recognize the projection rule

\[ u(z_{x_i}) \approx \log(z_{x_i}) \sum_j Q_{0,j} q_j + \sum_m \log(z_{x_i} - z_{y_m}) \sum_j Q_{B_m} Q_{B_m}(z_{y_j}) q_j \]

with projection functions

\[ Q_{0,j} = 1, \quad Q_{B_m}(z_{y_j}) = -\sum_k \frac{T_{mk}}{k!} z_{y_j}^k. \]
Multipole expansion as an interpolation rule

Let \( x^A \) be the center of the evaluation box. We then perform a Taylor expansion of \( \log(z_x - z_y) \) around \( z_x = z_x^A \) to obtain

\[
\log(z_{x_i} - z_y) = \log(z_x^A - z_y) + \sum_{k \geq 1} \frac{(z_{x_i} - z_x^A)^k}{k!} \left( \frac{\partial}{\partial z_x} \right)^k |_{z_x = z_x^A} \log(z_x - z_y).
\]

Approximating the derivatives by the finite difference formula

\[
\left( \frac{\partial}{\partial z_x} \right)^k |_{z_x = z_x^A} \log(z_x - z_y) \approx -\sum_n T_{nk} \log(z_x^A - z_y)
\]

and replacing it in the multipole expansion we recognize the interpolation rule

\[
\log(z_{x_i} - z_y) \approx P_{0,i} \log(z_x^A - z_y) + \sum_n P_n^A(z_{x_i}) \log(z_x^A, z_y)
\]

with interpolation functions

\[
P_{0,i} = 1, \quad P_n^A(z_{x_i}) = -\sum_k \frac{T_{nk}}{k!} (z_{x_i} - z_x^A)^k.
\]
• We present a fast multipole method (FMM) based on interpolation.

• The FMM presented here applies to potentials given in terms of kernels $G$ that exhibit smoothness properties similar to those of $1/|\mathbf{x} - \mathbf{y}|$ or $\log |\mathbf{x} - \mathbf{y}|$.

• We continue assuming that $G$ is symmetric and we consider the two-dimensional case only.
We consider the problem of efficiently compute integrals of the form

$$u(x) = \int_{\Gamma} G(x, y) q(y) \, ds_y, \quad x \in [0, 1]^2, \quad \Gamma \subset [0, 1]^2.$$ 

- We consider a dyadic tree partitioning of the domain $[0, 1]^2$ into target boxes $A$ and source boxes $B$ of side length $2^{-\ell}$ with $\ell = 0, \ldots, L$.

- The collection of boxes has associated a quadtree structure: call $A_p$ the parent of a box $A$, and call $B_c$ the four children of a box $B$.

- The highest level of the tree ($\ell = 0$) is called root, while the lowest-level boxes are called leafs.

- The tree may not be “perfect”, in the sense that not all leaf boxes occur at the same level.
FMM setup
FMM setup
**Definition (adjacent boxes).** Two boxes at the same level \( \ell \) are said to be adjacent cells at level \( \ell \) if they have at least one common vertex.

**Definition (well-separated boxes).** Two boxes at the same scale \( \ell \) are said to be well-separated if they are not adjacent to one another, i.e., if \( B \) is neither \( A \) nor any of its eight nearest neighbors. In that case we say that the boxes are in the far-field of one another: \( B \in \text{far}(A) \), or equivalently \( A \in \text{far}(B) \).

**Definition (interaction list).** The interaction list of a box \( A \) is defined as the set of boxes \( B \), at the same scale as \( A \), in the far-field of \( A \), and such that \( B_p \) is not in the far field of \( A_p \). We denote the interactions list of box \( A \) as \( \text{IL}(A) \).

**Definition (neighbor list).** The neighbor list of a box \( A \) is defined as the box \( A \) itself and its 8 nearest neighbors at the same scale. The neighbor list of \( A \) is denoted as \( \text{NL}(A) \).
FMM setup: far(A)
FMM setup: interaction list
FMM setup: interaction list

$A_p$
FMM setup: interaction list
FMM setup: interaction list

$B_p$
FMM setup: neighbor list
In what follows we will make use of the following notation:

- For a source box $B$ we let the partial potentials from $B$ be denoted by
  \[ u^B(x) = \int_{B \cap \Gamma} G(x, y)q(y) \, ds_y, \quad x \in \text{far}(B). \]

- For each evaluation box $A$, we let the partial potential to $A$ be denoted by
  \[ u^{\text{far}(A)}(x) = \int_{\text{far}(A) \cap \Gamma} G(x, y)q(y) \, ds_y, \quad x \in A. \]

- Finally, we use a projection rule
  \[ G(x, y) = \sum_m G(x, y_m^B)P_m^B(y), \quad x \in \text{far}(B), \, y \in B, \]
  and an interpolation rule
  \[ G(x, y) = \sum_n P_n^A(x)G(x_n^A, y), \quad x \in A, \, y \in \text{far}(A). \]
The three main steps of the fast multipole method (FMM) are:

1. The projection rule is successively applied from finer to coarser scales to create canonical charges in sources boxes at all the levels of the tree.

2. The kernel $G$ is used to compute potentials, at selected locations, from these canonical charges.

3. The interpolation rule is successively applied from coarser to finer scales to compute canonical potentials in evaluation boxes at all levels of the tree.
FMM basic architecture: multipole-to-multipole

Upward pass

Consider canonical charges $q^B_m$ at nodes $y^B_m$, expected to obey

$$u^B(x) = \sum_m G(x, y^B_m) q^B_m, \quad x \in \text{far}(B),$$

where

$$q^B_m = \int_{B \cap \Gamma} P^B_m(y) q(y) \, ds_y.$$  

Then observe that the canonical charge $q^B_m$ at $y^B_m$ can be expressed as the projection of the canonical charges $q^{B_c}_{m'}$ of the child boxes $B_c$:

$$q^B_m = \sum_c \sum_{m'} P^B_m(y^{B_c}_{m'}) q^{B_c}_{m'}.$$  

This relation is called a multipole-to-multipole (M2M) operation, or M2M translation, or moment-to-moment (M2M) translation. The first step of the FMM is the cascade of M2M translations in an upward step of the quad tree.
FMM basic architecture: multipole-to-multipole

Upward pass

projection rule at level $\ell_0 - 1$

$\ell = \ell_0$

$\ell = \ell_0 - 1$

$B$

$B_p$

...using bilinear interpolation
FMM basic architecture: multipole-to-local

Downward pass: NL contribution

At every scale, for every box $A$, and every box $B$ in the interaction list of $A$, the canonical charges are converted into potentials via the so-called multipole-to-local (or moment-to-local) (M2L) conversion rule:

$$ u_{n,M2L}^{A} = \sum_{B \in \text{IL}(A)} \sum_{m} G(x_n^A, y_m^B) q_m^B. $$
Consider canonical potentials $u_n^A$ at the nodes $x_n^A$ which are expected to obey

$$u_n^A = \int_{\text{far}(A) \cap \Gamma} G(x_n^A, y) q(y) \, ds_y,$$

The interpolation rule gives a relation between the potentials in $A$ and the canonical potentials $u_n^A$:

$$u^{\text{far}(A)}(x) = \sum_n P_n^A(x) u_n^A, \quad x \in A.$$

Apply this rule in the case when the canonical potentials are those of the parent box $A_p$:

$$u_n^{A,\text{L2L}} = \sum_{n'} P_{n'}^{A_p}(x_{n'}^A) u_{n'}^{A_p}.$$

This relation is called a local-to-local (L2L) operation, or L2L translation.
**FMM basic architecture: local-to-local**

**Downward pass: far-field contribution**

Interpolation rule at level $\ell_0 - 1$

\[ \ell = \ell_0 - 1 \]

...using bilinear interpolation
FMM basic architecture: upward pass

Downward pass: far-field contribution

Since

$$\text{far}(A) = \text{far}(A_p) \cup \text{IL}(A),$$

it remains to add the M2L and L2L potentials to obtain the canonical potentials for box $A$:

$$u^A_n = u^{A,M2L}_n + u^{A,L2L}_n.$$

The last step of the FMM is the cascade of L2L translations, added to the M2L conversions, in a downward pass of the quad tree.
FMM basic architecture: upward pass

Downward pass: far-field contribution

\[ \ell = 0 \]

there is no parent box and no interaction list, therefore:

\[ u_n^A = 0 \]

...using bilinear interpolation
FMM basic architecture: upward pass

Downward pass: far-field contribution

Let's denote the interaction list as follows:

\[ u_{00}^A, u_{10}^A, u_{11}^A \]

The parent box at \( l=0 \) but no boxes in the interaction list, therefore:

\[ u_n^A = u_{n,L2L}^A = 0 \]

... using bilinear interpolation
FMM basic architecture: upward pass

Downward pass: far-field contribution

\[ \ell = 2 \]

\[ u_{00}^A \quad u_{10}^A \quad u_{11}^A \]

parent box at \( l=1 \) and 12 boxes in the interaction list, therefore:

\[ u_n^A = u_n^{A,L2L} + u_n^{A,M2L} = 0 \]

...using bilinear interpolation
FMM basic architecture: upward pass

Downward pass: far-field contribution

\[ \ell = 3 \]

parent box at \( l=2 \) and 12 boxes in the interaction list, therefore:

\[ u_n^A = u_{n}^{A,\ell 2L} + u_{n}^{A,\ell 2L} \]

... using bilinear interpolation
FMM: Algorithm

- Let $N$ be the maximum of the number of charges and number of evaluation points. We build the quad tree adaptively so that the leaf boxes contain no more than $s$ charges and evaluation points, with $s$ to be determined later.

- Assume that the projection and interpolation rule both involve (no more than) $p$ canonical charges and canonical potentials per box, i.e., both $m$ and $n$ run from 1 to $p$.

- Assume that the projection/interpolation rules, and the interaction lists, are precomputed (they do not depend on the particular charge distribution.)
**FMM: Algorithm**

**Initialization**

Collect the points source locations $y_j$ in boxes $B$ at all scales, and the observation locations $x_i$ in boxes $A$ at all scales.

Let $L$ be the level of the finest leaf box.

for all leaf boxes $B$:

Source-to-multipole: $q^B_m = \int_{B \cap \Gamma} P^B_m(y) q(y) \, ds_y$.

end

$u^A_n = 0$ for $A$ the root box
FMM: Algorithm

Upward pass

for $\ell = L - 1, \ldots, 1$

for $B$ in tree at at level $\ell$

M2M operation from $B_c$ to $B$:

$$q_m^B = \sum_c \sum_{m'} P_m^B(y_{m'}^B) q_m^{B_c}. $$

end

end

Downward pass

for $\ell = 2, \ldots, L$

for $A$ in tree at at level $\ell$

L2L operation from $A_p$ to $A$, and M2L conversion:

$$u_n^A = \sum_{n'} P_{n'}^{A_p}(x_n^A) u_{n'}^{A_p} + \sum_{B \in IL(A)} \sum_m G(x_n^A, y_m^B) q_m^B. $$

end

end
FMM: Algorithm

Termination

for all leaf boxes $A$

Local-to-evaluation and diagonal interactions:

$$u_i = \sum_{n} P_n^A(x_i) u_n^A + \sum_{B \in \text{NL}(A)} \int_{B \cap \Gamma} G(x_i, y) q(y) \, ds_y.$$
FMM: Complexity

Claim. If we take $s = p$, the complexity of the 2D FFM is $O(pN)$.

- $s$: maximum number of charges and evaluation points per leaf box.
- $p$: number of canonical charges and canonical potentials per box.

Proof.

- The number of leaf boxes is $O(N/s)$.
- The number of boxes is at most twice the number of leaf boxes, regardless of the tree, so it is also $O(N/s)$.
- The complexity of one M2M, or one M2L or one L2L operations is a small $p$-by-$p$ matrix vector multiplication, hence $O(p^2)$ operations.
- The construction of the quadtree structure requires $O(N)$ operations.
FMM: Complexity

Proof (cont.).

- The source-to-multipole step involves mapping every one of the $N$ charges to $p$ canonical charges, hence has complexity $O(pN)$.

- In the upward pass, every one of the $O(N/s)$ source boxes is visited once, with an M2M that costs $O(p^2)$ operations, for a total of $O(p^2N/s)$.

- In the downward pass, every one of the $O(N/s)$ evaluation boxes is visited once, with an M2L and an L2L that both cost $O(p^2)$ operations, for a total of $O(p^2N/s)$ as well.

- For the termination, the local-to-evaluation step involves mapping $p$ canonical potentials to every one of the $N$ evaluation points, hence has complexity $O(pN)$.

- The diagonal term is a sum over $O(s)$ sources for each of the $N$ evaluation points, hence has complexity $O(sN)$.

The overall operation count is $O(pN + p^2N/s + sN)$, and is minimized provided we take $s$ of order $p$. This shows that the complexity is $O(pN)$ in 2D.