
Lecture 10

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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: $q_m^B = \int_{B \cap \Gamma} P_m^B(y)q(y) \, ds_y.$

end

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

Upward pass

for \( \ell = L - 1, \ldots, 1 \)

for \( B \) in tree at level \( \ell \)

M2M operation from \( B_c \) to \( B \):

\[
q_m^B = \sum_{c} \sum_{m'} P_m^B(y_{m'}^{B_c}) q_{m'}^{B_c}.
\]

end

end

Downward pass

for \( \ell = 2, \ldots, L \)

for \( A \) in tree at level \( \ell \)

L2L operation from \( A_p \) to \( A \), and M2L conversion:

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

end

end
FMM: Algorithm

Termination

for all leaf boxes $A$

Local-to-evaluation and diagonal interactions:

$$u_i = \sum_n P_n^A(x_i)u_n^A + \sum_{B \in \text{NL}(A)} \int_{B \cap \Gamma} G(x_i, y)q(y) \, ds_y.$$
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 $O(N/s)$. \textbf{Important assumption!}
- 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.
Multipole expansions: Laplace equation in 2D

We proved that

\[ G(x, y) = -\frac{1}{2\pi} \log |x - y| = \frac{1}{2\pi} \text{Re} \left\{ \sum_{k=0}^{\infty} O_k(z_0 - z_c)I_k(z - z_c) \right\} \]

where \( z_0 = x_1 + ix_2, \ z = y_1 + iy_2 \) and \( |z - z_c| < |z_0 - z_c| \) and

\[ I_k(z) = \frac{z^k}{k!} \quad \text{for} \quad k \geq 0 \]

\[ O_k(z) = \frac{(k - 1)!}{z^k} \quad \text{for} \quad k \geq 1, \quad O_0(z) = -\log z. \]

Additionally we have the following identities:

\[ I_k(z_1 + z_2) = \sum_{l=0}^{k} I_{k-l}(z_1)I_l(z_2) = \sum_{l=0}^{k} I_l(z_1)I_{k-l}(z_2) \]

and

\[ O_k(z_1 + z_2) = \sum_{l=0}^{\infty} (-1)^l O_{k+l}(z_1)I_l(z_2), \quad |z_2| < |z_1|. \]
Multipole expansions: Laplace equation in 2D

We consider the problem of efficiently approximate the integral

\[
\int_{B \cap \Gamma} G(x, y)q(y) \, ds_y = \frac{1}{2\pi} \Re \left\{ \sum_{k=0}^{\infty} O_k(z_0 - z_c) \int_{\Gamma \cap B} I_k(z - z_c)q(z) \, ds_z \right\}
\]

for \( x = (\text{Re} \, z_0, \text{Im} \, z_0) \in A \) and \( y = (\text{Re} \, z, \text{Im} \, z) \in B \), where \( A \) and \( B \) are well-separated boxes, with \( y_c = (\text{Re} \, z_c, \text{Im} \, z_c) \) denoting the center of the source box \( B \).

We then define the moments associated with the source box \( B \) as

\[
\mu_k(z_c) = \int_{\Gamma \cap B} I_k(z - z_c)q(z) \, ds_z, \quad k \geq 0.
\]

**M2M translation.** If the expansion point \( z_c \) is moved to a new location \( z_c' \) the moments can be “translated” by using the following intensity:

\[
\mu_k(z_c') = \int_{\Gamma \cap B} I_k(z - z_c')q(z) \, ds_z
\]

\[
= \int_{\Gamma \cap B} I_k(z - z_c + z_c - z_c')q(z) \, ds_z
\]

\[
= \sum_{l=0}^{k} I_{k-l}(z_c - z_c') \mu_l(z_c) \quad \text{exact!}
\]
Multipole expansions: Laplace equation in 2D

**M2L conversion.** We introduce the so-called local expansion about the source point \( z_0 \) (\( x \)). Suppose \( z_L \) is a point close to the source point \( z_0 \), \( |z_0 - z_L| \ll |z_L - z_c| \), then:

\[
\int_{\Gamma \cap B} G(z_0, z) q(z) \, ds_z = \frac{1}{2\pi} \sum_{k=0}^{\infty} O_k(z_0 - z_c) \mu_k(z_c) \quad \text{Multipole expansion}
\]

\[
= \frac{1}{2\pi} \sum_{k=0}^{\infty} O_k(z_L - z_c) + O_k(z_0 - z_L) \mu_k(z_c)
\]

\[
= \frac{1}{2\pi} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} (-1)^l O_{k+l}(z_L - z_c) I_l(z_0 - z_L) \mu_k(z_c)
\]

\[
= \frac{1}{2\pi} \sum_{l=0}^{\infty} I_l(z_0 - z_L) (-1)^l \sum_{k=0}^{\infty} O_{k+l}(z_L - z_c) \mu_k(z_c)
\]

**Local expansion**

\[
= \frac{1}{2\pi} \sum_{l=0}^{\infty} I_l(z_0 - z_L) L_l(z_L)
\]

where the expansion coefficients \( L_l(z_L) \) are given by the M2L conversion formula:

\[
L_l(z_L) = (-1)^l \sum_{k=0}^{\infty} O_{k+l}(z_L - z_c) \mu_k(z_c).
\]
L2L translation. If the point of the local expansion is moved from $z_L$ to $z_{L'}$, we then have the following expression for the new local expansion coefficients:

$$
\int_{\Gamma \cap B} G(z_0, z)q(z) \, ds_z \approx \frac{1}{2\pi} \sum_{l=0}^{p} L_l(z_L)I_l(z_0 - z_L)
= \frac{1}{2\pi} \sum_{l=0}^{p} L_l(z_L)I_l(z_0 - z_{L'} + z_{L'} - z_L)
= \frac{1}{2\pi} \sum_{l=0}^{p} \sum_{m=0}^{l} L_l(z_L)I_m(z_0 - z_{L'})I_{l-m}(z_{L'} - z_L)
= \frac{1}{2\pi} \sum_{m=0}^{p} I_m(z_0 - z_{L'}) \sum_{l=m}^{p} L_l(z_L)I_{l-m}(z_{L'} - z_L).
$$

On the other hand, since

$$
\int_{\Gamma \cap B} G(z_0, z)q(z) \, ds_z \approx \frac{1}{2\pi} \sum_{m=0}^{p} L_m(z_{L'})I_m(z_0 - z_{L'}),
$$

we obtain

$$
L_m(z_{L'}) = \sum_{l=m}^{p} L_l(z_L)I_{l-m}(z_{L'} - z_L)
$$

which we refer to as the L2L translation formula.
Multipole expansions: Helmholtz equation in 2D

Graf’s addition theorem:

\[ C_n(w) e^{in\theta} = \sum_{m=-\infty}^{\infty} C_{n+m}(u) J_m(v) e^{im\alpha} \quad (|v e^{\pm i\alpha}| < |u|) \]

where \( C_n \) is \( J_n, Y_n \) or \( H_n^{(1)} \),

\[ w = \sqrt{u^2 + v^2 - 2uv \cos \alpha} \]

and

\[ u - v \cos \alpha = w \cos \theta, \quad v \sin \alpha = w \sin \theta. \]

The fundamental solution of the 2D Helmholtz equation can be expanded as:

\[ G_k(x, y) = \frac{i}{4} H_0^{(1)}(k|x-y|) = \frac{i}{4} \sum_{n=-\infty}^{\infty} O_n(x-y_c) I_{-n}(y-y_c), \quad |y-y_c| < |x-y_c| \]

where \( k \) is the wavenumber, \( y_c \) is an expansion point close to \( y \), and the two auxiliary function \( I_n \) and \( O_n \) are given by:

\[ I_n(x) = (-i)^n J_n(kr) e^{in\alpha}, \]

\[ O_n(x) = i^n H_n^{(1)}(kr) e^{in\alpha} \quad \text{with} \quad x = r(\cos \alpha, \sin \alpha). \]
Separability of the Helmholtz Green function

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

\[
G(x, y) = \frac{i}{4} H_0^{(1)}(k|x - y|).
\]

Assume that \( x \in A \) and \( y \in B \), where \( A \) and \( B \) are two well-separated boxes. 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 \( A \). For convenience, the box \( B \) is centered at the origin.

**Theorem.** Consider \( A \) and \( B \) as described above. For all \( p > 0 \), there exists a constant \( C_p(k) > 0 \) such that

\[
\left| G(x, y) - \frac{i}{4} \sum_{n=-p}^{p} O_n(x) I_{-n}(y) \right| \leq C_p(k) \left( \frac{r}{d} \right)^p.
\]
Separability of the Helmholtz Green function

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

\[ G(x, y) = \frac{i}{4} H_0^{(1)}(k|x - y|). \]

Assume that \( x \in A \) and \( y \in B \), where \( A \) and \( B \) are two well-separated boxes. 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 \( A \). For convenience, the box \( B \) is centered at the origin.

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\]

In practice one needs to select \( p \) such that \( p > kr \).
We consider the approximation of the integral:

$$\int_{\Gamma \cap B} G(x, y)q(y) \, ds_y = \frac{i}{4} \sum_{n=-\infty}^{\infty} O_n(x - y_c) \int_{\Gamma \cap B} I_{-n}(y - y_c)q(y) \, ds_y,$$

where $y \in B$ and $x \in A$, $A$ and $B$ being well-separated boxes. We thus define the moments as:

$$\mu_n(y_c) = \frac{i}{4} \int_{\Gamma \cap B} I_{-n}(y - y_c)q(y) \, ds_y, \quad n \in \mathbb{Z}.$$

**M2M translation.** If the expansion point $y_c$ is moved to a new location $y_c'$ the moments can be “translated” by using the following intensity:

$$\mu_n(y_{c'}) = \int_{\Gamma \cap B} I_n(y - y_{c'})q(y) \, ds_y = \int_{\Gamma \cap B} I_n(y_2 + y_{c'} - y_{c'})q(y) \, ds_y$$

$$= \sum_{m=-\infty}^{\infty} I_{n-m}(y_c - y_{c'})\mu_m(y_c)$$
Multipole expansions: Helmholtz equation in 2D

**Local expansion and M2L conversion.** By the symmetry of the Green function we obtain the following local expansion:

\[
\int_{\Gamma \cap B} G(x, y)q(y) \, ds_y = \sum_{n=-\infty}^{\infty} I_{-n}(x - x_L) \frac{i}{4} \int_{\Gamma \cap B} O_n(y - x_L)q(y) \, ds_y
\]

where \( |x - x_L| < |y_c - x_L| \) (\( y_c \) denotes the center of the box \( B \)). Therefore, using the addition theorem we obtain the following M2L conversion formula:

\[
L_n(x_L) = \sum_{m=-\infty}^{\infty} (-1)^m O_{n-m}(x_L - y_c) \mu_m(y_c).
\]

**L2L translation.** If the point of the local expansion is moved from \( x_L \) to \( x_L' \), we then have the following expression for the new local expansion coefficients:

\[
L_n(x_{L'}) = \sum_{m=-\infty}^{\infty} I_m(x_{L'} - x_L)L_{n-m}(x_L).
\]

which we refer to as the L2L translation formula.
FMM algorithm

Initialization

Collect the points source locations $\mathbf{y}_j$ in boxes $B$ at all scales, and the observation locations $\mathbf{x}_i$ in boxes $A$ at all scales.

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

for all leaf boxes $B$:

Source-to-multipole (source-to-moment):

Compute $\mu^B_m = \mu_m(\mathbf{y}_c^B)$ where $\mathbf{y}_c^B$ is the center of the leaf box $B$.

end

Note that:

Laplace: $\mu_k(z_c) = \int_{\Gamma \cap B} I_k(z - z_c)q(z) \, ds_z, \quad k \geq 0.$

Helmholtz: $\mu_n(\mathbf{y}_c) = \frac{i}{4} \int_{\Gamma \cap B} I_{-n}(\mathbf{y} - \mathbf{y}_c)q(\mathbf{y}) \, ds_{\mathbf{y}}, \quad n \in \mathbb{Z}.$
FMM algorithm: leaf boxes

leaf boxes
FMM algorithm: interaction list IL(A)
FMM algorithm: $\text{far}(A)$
FMM algorithm: neighbor list NL(A)
FMM algorithm

Upward pass

for \( \ell = L - 1, \ldots, 1 \)
for \( B \) in tree at at level \( \ell \)
    M2M translation from \( B_c \) to \( B \):

\[
\mu^n_B = \mu_m(y^n_B) = \sum_{c} \sum_{m=-\infty}^{\infty} I_{n-m}(y^B_c - y^n_B) \mu^B_m.
\]

\( y^B_c \) is the center of the box \( B \)
\( y^B_c \) is the center of the child box \( B_c \)

end

end

... in the case of the Laplace equation: (M2M translation)

\[
\mu^n_B = \mu_n(z^n_B) = \sum_{c} \sum_{l=0}^{n} I_{n-l}(z^B_c - z^n_B) \mu^B_l.
\]

moment associated to parent box

moments associated to child boxes
FMM algorithm

Upward pass: M2M translation
FMM algorithm

Downward pass
for $\ell = 0, \ldots, L$
  for $A$ in tree at level $\ell$
    Compute the local expansion coefficients:

\[
L_n(x_A^L) = \sum_{m=-\infty}^{\infty} I_m(x_A^L - x_{Lp}^A) L_{n-m}(x_{Lp}^A) + \sum_{B \in \text{IL}(A)} \sum_{m=-\infty}^{\infty} (-1)^m O_{n-m}(x_A^L - y_c^B) \mu_m(y_c^B) \tag{L2L}
\]

\[
\sum_{B \in \text{IL}(A)} \sum_{m=-\infty}^{\infty} (-1)^m O_{n-m}(x_A^L - y_c^B) \mu_m(y_c^B) \tag{M2L}
\]

$x_A^L$: is the center of the box $A$

$x_{Lp}^A$ is the center of the parent box $A_p$.

end

end

... in the case of the Laplace equation

\[
L_n(z_A^L) = \sum_{l=n}^p I_{l-n}(z_A^L - z_{Lp}^A) L_l(z_{Lp}^A) + \sum_{B \in \text{IL}(A)} \sum_{k=0}^{\infty} (-1)^n O_{k+n}(z_A^L - z_c^B) \mu_m(z_c^B). \]
FMM algorithm

Downward pass: L2L translation
FMM algorithm

Termination

for all leaf boxes $A$

Local-to-evaluation and diagonal interactions:

Helmholtz $\left\{ u(x_i) = u_i = \sum_{n=-\infty}^{\infty} I_n(x_i - x_L^A)L_n(x_L^A) + \sum_{B \in NL(A)} \int_{B \cap \Gamma} G(x_i, y) q(y) \, ds_y \right.$

$x_L^A$ is the center of the box $A$.

end

... in the case of the Laplace equation:

$u(x_i) = \frac{1}{2\pi} \sum_{\ell=0}^{\infty} \text{Re} \left\{ L_\ell(z_L^A) I_\ell(z_i - z_L^A) \right\} + \sum_{B \in NL(A)} \int_{B \cap \Gamma} G(x_i, y) q(y) \, ds_y$
FMM in 3D: Octree

Example: Neighbor list NL(A)
FMM in 3D: Octree

Example: Interaction list IL(A)
FMM in 3D: Octree

Example: Interaction list far(A)
Multipole expansions: Laplace equation in 3D

We proved that
\[ G(x, y) = \frac{1}{4\pi|x - y|} = \frac{1}{4\pi} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} S_{n,m}(x - y_c) R_{n,m}(y - y_c), \quad |y - y_c| < |x - y_c| \]

where

\[ R_{n,m}(x) = \frac{1}{(n + m)!} P_n^m(\cos \theta) e^{im\phi} r^n \]
\[ S_{n,m}(x) = (n - m)! P_n^m(\cos \theta) e^{im\phi} \frac{1}{r^{n+1}} \]

where \((\rho, \theta, \phi)\) are the coordinates of \(x\) in spherical coordinates.

Moments:
\[ \mu_{n,m}(y_c) = \int_{\Gamma \cap B} R_{n,m}(y - y_c) q(y) \, ds_y, \quad n \geq 0, |m| \leq n \]

\(y_c\): center of the 3D box \(B\).
Multipole expansions: Laplace equation in 3D

M2M translation:

\[ \mu_{n,m}(y_c') = \sum_{n'=0}^{n} \sum_{m'=-n'}^{n'} R_{n',m'}(y - y_c') \mu_{n-n',m-m'}(y_c). \]

M2L conversion:

\[ L_{n,m}(x_L) = (-1)^n \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \frac{S_{n+n',m+m'}(x_L - y_c) \mu_{n',m'}(y_c),}{|x-x_L| < |y_c-x_L|,} \]

\( x_L \) is the center of the 3D evaluation box \( A \). (\( A \) and \( B \) are well separated)

L2L translation:

\[ L_{n,m}(x_{L'}) = \sum_{n'=n}^{\infty} \sum_{m'=-n'}^{n'} R_{n'-n,m'-m}(x_{L'}) L_{n',m'}(x_L). \]