MATH 393C: Fast Methods in Scientific Computing


Supplementary material on adaptive FMM – new material on page 25 onwards.

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The outgoing expansion

Let $\tau$ be a box (green).
Let $c_\tau$ be the center of $\tau$ (black).
Let $y_j$ be source locations in $\tau$ (red).
Let $q_j$ be the strength of source $j$.
Let $x_i$ be targets well separated from $\tau$ (blue).
Let $u$ denote the potential

$$ u(x_i) = \sum_j q_j \log(x_i - y_j). $$

The **outgoing expansion** of $\tau$ is a vector $\hat{q} = [\hat{q}_p]_{p=0}^P$ of complex numbers such that

(1) 

$$ u(x) \approx \hat{q}_0 \log |x - c_\tau| + \sum_{p=1}^P \hat{q}_p \frac{1}{(x - c_\tau)^p}, \quad x \in \Omega^{\text{far}}_{\tau}. $$

The outgoing expansion is a compact representation of the sources inside $\tau$
(it encodes both the source locations and the magnitudes).
The incoming expansion

Let $\tau$ be a box (green).
Let $c_\tau$ be the center of $\tau$ (black).
Let $y_j$ be sources well-separated from $\tau$ (red).
Let $q_j$ be strength of source $j$.
Let $x_i$ be targets inside $\tau$ (blue).
Let $u$ denote the potential
\[
u(x_i) = \sum_j q_j \log(x_i - y_j).
\]

The incoming expansion of $\tau$ is a vector $\hat{u} = [\hat{u}_p]_{p=0}^P$ of complex numbers such that
\[
\nu(x) \approx \sum_{p=0}^P \hat{u}_p(x - c_\tau)^p, \quad x \in \Omega_\tau.
\]

The incoming expansion is a compact representation of the sources well-separated from $\tau$ (it encodes both the source locations and the magnitudes).
The *outgoing-from-sources* translation operator $T_{\tau}^{(ofs)}$

Let $\tau$ be a box (green).

Let $c_\tau$ be the center of $\tau$ (black).

Let $\{y_j\}_{j}^{N_\tau}$ be source locations in $\tau$ (red).

Let $q_j$ be strength of source $j$.

The operator $T_{\tau}^{(ofs)}$ constructs the outgoing expansion directly from the vector of charges.

\[
\hat{q}_\tau = T_{\tau}^{(ofs)} q \quad (P + 1) \times 1 \quad (P + 1) \times N_\tau \quad N_\tau \times 1
\]

\[
T_{\tau,0,j}^{(ofs)} = 1 \quad 1 \leq j \leq N_\tau
\]

\[
T_{\tau,p,j}^{(ofs)} = -\frac{1}{p} (y_j - c_\tau)^p \quad 1 \leq p \leq P \quad 1 \leq j \leq N_\tau.
\]
The **outgoing-from-outgoing** translation operator $T_{\tau,\sigma}^{(ofo)}$

Let $\tau$ be a box (green).
Let $c_{\tau}$ be the center of $c_{\tau}$ (black).
Let $\sigma$ denote a box contained in $\tau$.
Let $c_{\sigma}$ denote the center of $\sigma$ (red).
Let $\hat{q}_{\sigma}$ be outgoing expansion of $\sigma$.

$T_{\tau,\sigma}^{(ofo)}$ constructs the outgoing expansion of $\tau$ from the outgoing expansion of $\sigma$

$$
\hat{q}_{\tau} = T_{\tau,\sigma}^{(ofo)} \hat{q}_{\sigma}
$$

$$(P + 1) \times 1 \quad (P + 1) \times (P + 1) \quad (P + 1) \times 1
$$

With $d = c_{\sigma} - c_{\tau}$, $T_{\tau,\sigma}^{(ofo)}$ is a lower tridiagonal matrix with entries

$$
T_{\tau,\sigma,0,0}^{(ofo)} = 1
$$

$$
T_{\tau,\sigma,p,0}^{(ofo)} = -\frac{1}{p} d \quad 1 \leq p \leq P
$$

$$
T_{\tau,\sigma,p,q}^{(ofo)} = \binom{p}{q} d^{p-q} \quad 1 \leq q \leq p \leq P.
$$
The \textit{incoming-from-outgoing} translation operator $T_{\tau,\sigma}^{(ifo)}$

Let $\sigma$ be a source box (red) with center $c_\sigma$.
Let $\tau$ be a target box (blue) with center $c_\tau$.
Let $\hat{q}_\sigma$ be the outgoing expansion of $\sigma$.
Let $\hat{u}_\tau$ represent the potential in $\tau$ caused by sources in $\sigma$.

$T_{\tau,\sigma}^{(ifo)}$ constructs the incoming expansion of $\tau$ from the outgoing expansions of $\sigma$:

$$\hat{u}_\tau = T_{\tau,\sigma}^{(ifo)} \hat{q}_\sigma$$

$(P + 1) \times 1$ $(P + 1) \times (P + 1)$ $(P + 1) \times 1$

With $d = c_\sigma - c_\tau$, $T_{\tau,\sigma}^{(ifo)}$ is a matrix with entries

$$T_{\tau,\sigma,p,q}^{(ifo)} = ?$$
The incoming-from-incoming translation operator $T^{(ifi)}_{\tau,\sigma}$

Let $\tau$ be a box (green) with center $c_\tau$ (black).
Let $\sigma$ be a box (blue) containing $\tau$ with center $c_\sigma$.
Let $\hat{u}_\sigma$ be an incoming expansion for $\sigma$.

$T^{(ifi)}_{\tau,\sigma}$ constructs the incoming expansion of $\tau$ from the incoming expansion of $\sigma$

$$
\hat{u}_\tau = T^{(ifi)}_{\tau,\sigma} \hat{u}_\sigma \\
(P + 1) \times 1 \quad (P + 1) \times (P + 1) \quad (P + 1) \times 1
$$

With $d = c_\sigma - c_\tau$, $T^{(ifi)}_{\tau,\sigma}$ is a matrix with entries

$$
T^{(ifi)}_{\tau,\sigma,p,q} = ?
$$
The *targets-from-incoming* translation operator $T^{(t,fi)}_{\tau}$

Let $\tau$ be a box (green).

Let $c_\tau$ be the center of $\tau$ (black).

Let $\{x_i\}_{i}^{N_\tau}$ be target locations in $\tau$ (blue).

Let $\hat{u}_\tau$ be the incoming expansion of $\tau$.

$T^{(t,fi)}_{\tau}$ constructs the potentials in $\tau$ from the incoming expansion

$$
\begin{align*}
    u_\tau &= T^{(t,fi)}_{\tau} \hat{u}_\tau \\
    &\quad \text{in} \ N_\tau \times 1 \quad N_\tau \times (P + 1) \quad (P + 1) \times 1
\end{align*}
$$

$$
T^{(t,fi)}_{\tau, i, p} = (x_i - c_\tau)^p \\
1 \leq i \leq N_\tau \quad 0 \leq p \leq P.
$$
How do you compute the expansions of a box?
Computing the outgoing expansion of a leaf

Let $\tau$ be a box (green).

Let $c_\tau$ be the center of $\tau$ (black).

Let $\{y_j\}_{j=1}^{N_\tau}$ be source locations in $\tau$ (red).

Let $q_j$ be strength of source $j$.

There is an analytic formula:

$$\hat{q}_0 = \sum_{j=1}^{N_\tau} q_j$$
$$\hat{q}_p = -\frac{1}{p} \sum_{j=1}^{N_\tau} q_j (y_j - c_\tau)^p, \quad p = 1, 2, \ldots, P.$$

We write the formula compactly as

$$\hat{q}_\tau = T_\tau^{(ofs)} q_\tau.$$
Computing the outgoing expansion of a parent

Let $\tau$ be a box (green).
Let $c_\tau$ be the center of $\tau$ (black).
Let $\mathcal{L}_\tau^{(\text{child})}$ denote the children of $\tau$.
Let $c_\sigma$ be the center of child $\sigma$.
Let $\hat{q}_\sigma$ be the outgoing expansion of child $\sigma$.

The outgoing expansion of $\tau$ can be computed from the outgoing expansions of its children:

$$\hat{q}_\tau = \sum_{\sigma \in \mathcal{L}_\tau^{(\text{child})}} T_{\tau,\sigma}^{(\text{ofo})} \hat{q}_\sigma.$$
Computing the incoming expansions on level 2

Let $\tau$ be a box on level 2 (green).
Let $c_{\tau}$ be the center of $\tau$ (black).
The well-separated boxes on level 2 are red.

The incoming expansion of $\tau$ is computed from the outgoing expansions of boxes in its interaction list

$$\hat{u}_\tau = \sum_{\sigma \in \mathcal{L}^{(\text{int})}_\tau} T^{(ifo)}_{\tau,\sigma} \hat{q}_\sigma.$$
Computing the incoming expansions on level \( \ell \) when \( \ell > 2 \)

Let \( \tau \) be a box on level \( \ell = 3 \) (green).

Let \( \nu \) be the parent of \( \tau \) (blue).

Let \( u_{\text{in}}^\tau \) denote the potential caused by charges that are well-separated from \( \tau \) — these are charges in the boxes marked with red dots and crosses. We have

\[
u_{\text{in}}^\tau = u_{\text{in}}^\nu + v,
\]

where \( u_{\text{in}}^\nu \) is the incoming field for \( \tau \)'s parent (caused by the boxes with red crosses), and \( v \) is the field caused by boxes in the interaction list of \( \tau \) (boxes with a red dot).

The field \( u_{\text{in}}^\nu \) was computed on the previous level and is represented by \( \hat{u}_\nu \).

The field \( v \) is computed by transferring the outgoing expansions \( \hat{q}_\sigma \) for \( \sigma \in L_\tau^{(\text{int})} \).

\[
\hat{u}_\tau = T_{\tau,\nu}^{(\text{ifi})} \hat{u}_\nu + \sum_{\sigma \in L_\tau^{(\text{int})}} T_{\tau,\sigma}^{(\text{ifo})} \hat{q}_\sigma
\]

\[
\sim u_{\text{in}}^\tau \quad \sim u_{\text{in}}^\nu \quad \sim v
\]
The classical Fast Multipole Method in \( \mathbb{R}^2 \)

1. Construct the tree and all “interaction lists.”

2. For each leaf node, compute its outgoing expansion directly from the charges in the box via the \textit{outgoing-from-sources operator}.

3. For each parent node, compute its outgoing expansion by merging the expansions of its children via the \textit{outgoing-from-outgoing operator}.

4. For each node, compute its incoming expansion by transferring the incoming expansion of its parent (via the \textit{incoming-from-incoming operator}), and then add the contributions from all charges in its interaction list (via the \textit{incoming-from-outgoing operator}).

5. For each leaf node, evaluate the incoming expansion at the targets (via the \textit{targets-from-incoming operator}), and compute near-field interactions directly.
Construct the tree and all interaction lists.

Let $L$ denote the number of levels in the tree.
Set all potentials to zero:

For all boxes $\tau$

$\hat{u}_\tau = 0$

$\hat{q}_\tau = 0$.

Set the potential to zero:

$u = 0$. 
Compute the outgoing expansion on each leaf via application of the **outgoing-from-source operators**:

**loop** over all leaf nodes \( \tau \)

\[
\hat{q}_\tau = T^{(ofs)}_\tau q(J_\tau)
\]

**end loop**
Compute the outgoing expansion of each parent by merging the expansions of its children via application of the *outgoing-from-outgoing operators*:

**loop** over levels \( \ell = L - 1, L - 2, \ldots, 2 \)

**loop** over all nodes \( \tau \) on level \( \ell \)

\[
\hat{q}_\tau = \sum_{\sigma \in \mathcal{L}_\tau}^{(child)} T_{\tau,\sigma}^{(ofo)} \hat{q}_\sigma
\]

**end loop**

**end loop**

![Diagram of a grid with a selected node](image-url)
Add contributions from boxes in the interaction list of each box via the *incoming-from-outgoing operators*:

**loop** over all nodes $\tau$

$$\hat{u}_\tau = \hat{u}_\tau + \sum_{\sigma \in \mathcal{L}^{(\text{int})}_\tau} T^{(\text{ifo})}_{\tau,\sigma} \hat{q}_\sigma.$$ 

**end loop**
Add contributions from boxes in the interaction list of each box via the *incoming-from-outgoing operators*:

**loop** over all nodes $\tau$

$$\hat{u}_\tau = \hat{u}_\tau + \sum_{\sigma \in \mathcal{L}^{(int)}_{\tau}} T^{(ifo)}_{\tau,\sigma} \hat{q}_\sigma.$$ 

**end loop**
Add contributions from the parent of each box via via the *incoming-from-incoming operators*:

**loop** over levels $\ell = 2, 3, 4, \ldots, L - 1$

  **loop** over all nodes $\tau$ on level $\ell$

    **loop** over all children $\sigma$ of $\tau$

    $\hat{u}_\sigma = \hat{u}_\sigma + T^{(ifi)}_{\sigma, \tau} \hat{u}_\tau$.

  **end loop**

**end loop**

**end loop**
Compute the potential on every leaf by expanding its incoming potential via the \textit{targets-from-incoming} operators:

\textbf{loop} over all leaf nodes \( \tau \)

\[ u(J_\tau) = u(J_\tau) + T_{\tau}^{(t\!f\!i)} \hat{u}_\tau \]

\textbf{end loop}
Add to the leaf potentials the interactions from direct neighbors:

\[ \text{loop over all leaf nodes } \tau \]

\[ u(J_\tau) = u(J_\tau) + A(J_\tau, J_\tau) q(J_\tau) + \sum_{\sigma \in L_\tau^{(\text{nei})}} A(J_\tau, J_\sigma) q(J_\sigma) \]

end loop
Set $\hat{u}_\tau = 0$ and $\hat{q}_\tau = 0$ for all $\tau$.

**loop** over all leaf nodes $\tau$

$\hat{q}_\tau = T^{(ofs)}_\tau q(J_{\tau})$

**end loop**

**loop** over levels $\ell = L, L - 1, \ldots, 2$

**loop** over all nodes $\tau$ on level $\ell$

$\hat{q}_\tau = \sum_{\sigma \in \mathcal{L}_\tau^{(child)}} T^{(ofo)}_{\tau,\sigma} \hat{q}_\sigma$

**end loop**

**end loop**

**loop** over all nodes $\tau$

$\hat{u}_\tau = \hat{u}_\tau + \sum_{\sigma \in \mathcal{L}_\tau^{(int)}} T^{(ifo)}_{\tau,\sigma} \hat{q}_\sigma$

**end loop**

**loop** over levels $\ell = 2, 3, 4, \ldots, L - 1$

**loop** over all nodes $\tau$ on level $\ell$

**loop** over all children $\sigma$ of $\tau$

$\hat{u}_\sigma = \hat{u}_\sigma + T^{(ifi)}_{\sigma,\tau} \hat{u}_\tau$

**end loop**

**end loop**

**end loop**

**loop** over all leaf nodes $\tau$

$u(J_{\tau}) = T^{(tfi)}_\tau \hat{u}_\tau$

**end loop**

**loop** over all leaf nodes $\tau$

$u(J_{\tau}) = u(J_{\tau}) + A(J_{\tau}, J_{\tau}) q(J_{\tau})$

$+ \sum_{\sigma \in \mathcal{L}_\tau^{(nei)}} A(J_{\tau}, J_{\sigma}) q(J_{\sigma})$

**end loop**
Now let us consider a non-uniform tree.
Construct the tree and all interaction lists.

Let $L$ denote the number of levels in the tree.
Set all potentials to zero:

For all boxes $\tau$

\[
\hat{u}_\tau = 0
\]

\[
\hat{q}_\tau = 0.
\]

Set the potential to zero:

\[
u = 0.
\]
Compute the outgoing expansion on each leaf via application of the *outgoing-from-source operators*:

**loop** over all leaf nodes $\tau$

\[ \hat{q}_\tau = T_{\tau}^{(ofs)} q(J_{\tau}) \]

**end loop**
Compute the outgoing expansion on each leaf via application of the *outgoing-from-source operators*:

**loop** over all leaf nodes \( \tau \)

\[
\hat{q}_\tau = T^{(ofs)}_\tau q(J_\tau)
\]

**end loop**
Compute the outgoing expansion of each parent by merging the expansions of its children via application of the *outgoing-from-outgoing operators*:

**loop** over levels $\ell = L - 1, L - 2, \ldots, 2$

**loop** over all nodes $\tau$ on level $\ell$

$$\hat{q}_\tau = \sum_{\sigma \in \mathcal{L}_\tau^{(\text{child})}} T_{\tau,\sigma}^{(\text{ofo})} \hat{q}_\sigma$$

**end loop**

**end loop**

![Diagram of a tree structure with nodes and edges indicating the flow of information.]
Add contributions from the parent of each box via via the *incoming-from-incoming operators*:

**loop** over levels $\ell = 2, 3, 4, \ldots, L - 1$

**loop** over all nodes $\tau$ on level $\ell$

**loop** over all children $\sigma$ of $\tau$

$\hat{u}_\sigma = \hat{u}_\sigma + T_{\sigma,\tau}^{(ifi)} \hat{u}_\tau$.

end loop

end loop

end loop
New: Some leaves $\tau$ (e.g. the green one below) must collect contributions to their potentials from outgoing expansions on boxes $\sigma$ (red) on finer levels via the \textit{targets-from-outgoing operator}:

\begin{align*}
\text{loop} \text{ over all nodes leaf } \tau \\
\quad u(J_\tau) &= u(J_\tau) + \sum_{\sigma \in \mathcal{L}_\tau^{(3)}} T^{(t\text{f}o)}_{\tau,\sigma} \hat{q}_\sigma \\
\text{end loop}
\end{align*}
**New:** Some leaves $\tau$ (e.g. the green one below) must collect contributions to their potentials from outgoing expansions on boxes $\sigma$ (red) on finer levels via the \textit{targets-from-outgoing operator}:

\begin{equation*}
\textbf{loop} \text{ over all nodes leaf } \tau \\
u(J_\tau) = u(J_\tau) + \sum_{\sigma \in \mathcal{L}_\tau^{(3)}} T_{\tau,\sigma}^{(tfo)} \hat{q}_\sigma.
\end{equation*}

\textbf{end loop}
New: Some boxes $\tau$ (e.g. the green one) must collect contributions to their incoming expansions directly from the sources in some leaves $\sigma$ (red) via the \textit{incoming-from-sources operator}:

\textbf{loop} over all nodes $\tau$

$$\hat{u}_\tau = \hat{u}_\tau + \sum_{\sigma \in \mathcal{L}_\tau^{(4)}} \mathcal{T}_{\tau,\sigma}^{\text{ifs}} q(J_\sigma).$$

\textbf{end loop}
**New:** Some boxes $\tau$ (e.g. the green one) must collect contributions to their incoming expansions directly from the sources in some leaves $\sigma$ (red) via the *incoming-from-sources operator*:

**Loop** over all nodes $\tau$

$$\hat{u}_\tau = \hat{u}_\tau + \sum_{\sigma \in \mathcal{L}_\tau^{(4)}} T^{(ifs)}_{\tau,\sigma} q(J_\sigma).$$

**End loop**
Add contributions from the parent of each box via the *incoming-from-incoming operators*:

\[
\textbf{loop} \text{ over levels } \ell = 2, 3, 4, \ldots, L - 1 \\
\quad \textbf{loop} \text{ over all nodes } \tau \text{ on level } \ell \\
\quad \quad \textbf{loop} \text{ over all children } \sigma \text{ of } \tau \\
\quad \quad \quad \hat{u}_\sigma = \hat{u}_\sigma + T_{\sigma,\tau}^{(ifi)} \hat{u}_\tau. \\
\quad \textbf{end loop} \\
\quad \textbf{end loop} \\
\textbf{end loop}
\]
Compute the potential on every leaf by expanding its incoming potential via the *targets-from-incoming operators*:

**loop** over all leaf nodes \( \tau \)

\[
u(J_\tau) = u(J_\tau) + (T^{(t_{fi})}_{\tau}) \hat{u}_{\tau}
\]

**end loop**
Add to the leaf potentials the interactions from direct neighbors:

\[ \text{loop over all leaf nodes } \tau \]
\[ u(J_\tau) = u(J_\tau) + A(J_\tau, J_\tau) q(J_\tau) + \sum_{\sigma \in L_\tau^{\text{nei}}} A(J_\tau, J_\sigma) q(J_\sigma) \]

end loop
Add to the leaf potentials the interactions from direct neighbors:

**Loop** over all leaf nodes $\tau$

$$u(J_\tau) = u(J_\tau) + A(J_\tau, J_\tau) q(J_\tau) + \sum_{\sigma \in L^{\text{(nei)}}_\tau} A(J_\tau, J_\sigma) q(J_\sigma)$$

**end loop**
Set $\hat{u}_\tau = 0$ and $\hat{q}_\tau = 0$ for all $\tau$.

**loop** over all leaf nodes $\tau$

$\hat{q}_\tau = T_{\tau}^{(ofs)} q(J_\tau)$

**end loop**

**loop** over levels $\ell = L, L - 1, \ldots, 2$

**loop** over all nodes $\tau$ on level $\ell$

$\hat{q}_\tau = \sum_{\sigma \in \mathcal{L}_\tau^{(child)}} T_{\tau,\sigma}^{(ofs)} \hat{q}_\sigma$

**end loop**

**end loop**

**loop** over all nodes $\tau$

$\hat{u}_\tau = \hat{u}_\tau + \sum_{\sigma \in \mathcal{L}_\tau^{(int)}} T_{\tau,\sigma}^{(ifo)} \hat{q}_\sigma$

**end loop**

**loop** over all nodes $\tau$

$u(J_\tau) = T_{\tau}^{(tifi)} \hat{u}_\tau$

**end loop**

**loop** over all nodes $\tau$

$u(J_\tau) = u(J_\tau) + \sum_{\sigma \in \mathcal{L}_\tau^{(3)}} T_{\tau,\sigma}^{(ifo)} \hat{q}_\sigma$

**end loop**

**loop** over all leaf nodes $\tau$

$u(J_\tau) = u(J_\tau) + \sum_{\sigma \in \mathcal{L}_\tau^{(4)}} T_{\tau,\sigma}^{(ifs)} q(J_\sigma)$

**end loop**

**loop** over levels $\ell = 2, 3, 4, \ldots, L - 1$

**loop** over all nodes $\tau$ on level $\ell$

**loop** over all children $\sigma$ of $\tau$

$\hat{u}_\sigma = \hat{u}_\sigma + T_{\sigma,\tau}^{(ifi)} \hat{u}_\tau$

**end loop**

**end loop**

**end loop**

**loop** over all leaf nodes $\tau$

$u(J_\tau) = A(J_\tau, J_\tau) q(J_\tau)$

$+ \sum_{\sigma \in \mathcal{L}_\tau^{(nee)}} A(J_\tau, J_\sigma) q(J_\sigma)$

**end loop**
A summary of the lists needed:

$\mathcal{L}_\tau^{(\text{child})}$ The children of $\tau$.

$\mathcal{L}_\tau^{(\text{parent})}$ The parent of $\tau$.

$\mathcal{L}_\tau^{(\text{nei})}$ For a leaf box $\tau$, this is a list of the leaf boxes that directly border $\tau$.
For a non-leaf box, $\mathcal{L}_\tau^{(\text{nei})}$ is empty.

$\mathcal{L}_\tau^{(\text{int})}$ A box $\sigma \in \mathcal{L}_\tau^{(\text{int})}$ iff $\sigma$ and $\tau$ are on the same level,
$\sigma$ and $\tau$ are well-separated,
but the parents of $\sigma$ and $\tau$ are not well-separated.

$\mathcal{L}_\tau^{(3)}$ For a leaf box $\tau$, a box $\sigma \in \mathcal{L}_\tau^{(3)}$ iff $\sigma$ lives on a finer level than $\tau$,
$\tau$ is well-separated from $\sigma$, but $\tau$ is not well-separated from the parent of $\sigma$.
For a non-leaf box $\tau$, $\mathcal{L}_\tau^{(3)}$ is empty.

$\mathcal{L}_\tau^{(4)}$ The dual of $\mathcal{L}_\tau^{(3)}$. In other words, $\sigma \in \mathcal{L}_\tau^{(4)}$ if and only if $\tau \in \mathcal{L}_\sigma^{(3)}$. 
A summary of the translation operators: