A short primer on the fast multipole method

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This is intended to be a short tutorial on fast multipole methods (FMM). These were mainly written to ease my understanding of the subject. We discuss the main technical concepts like singular potentials, factorization, and translation. Important topics like error analysis and the computational cost analysis are left out. The single level FMM is discussed in detail since the fast Gauss transform is based on the single level FMM. A brief discussion of multiple level FMM is given at the end. This primer is mainly based on the course offered by Dr. Ramani Duraiswami and Dr. Nail Gumerov at the University of Maryland, College Park.

[**FMM tutorial**]: April 8, 2006

Contents

1. INTRODUCTION

The fast multipole method has been called one of the ten most significant algorithms [Dongarra and Sullivan 2000][Board and Schulten 2000] in scientific computation discovered in the 20th century, and won its inventors, Vladimir Rokhlin and Leslie Greengard, the 2001 Steele prize, in addition to getting Greengard the ACM 1987 best dissertation award [Greengard 1988].

The algorithm allows the product of particular structured dense matrices with a vector to be evaluated approximately in $O(N)$ or $O(N \log N)$ operations, when direct multiplication requires $O(N^2)$ operations. Coupled with advances in iterative methods for the solution of linear systems, they provide $O(N)$ or $O(NlogN)$ time and memory complexity solutions of problems that hitherto required $O(N^3)$ or $O(N^2)$ time complexity and $O(N^2)$ memory complexity. For extremely large problems, the gain in efficiency and memory can be very significant, and enables the use of more sophisticated modeling approaches that, while known to be better, may have been discarded as computationally infeasible in the past.

Originally this method was developed for the fast summation of the potential fields generated by a large number of sources (charges), such as those arising in gravitational or electrostatic potential problems, that are described by the Laplace equation in two or three dimensions [Greengard and Rokhlin 1987]. This lead to the name for the algorithm. Since then FMM has also found application in many other problems, e.g. in non-parametric statistics, finance, chemistry, machine learning, computer vision etc.

We are interested in computing the following sum

$$v_j = \sum_{i=1}^{N} q_i \Phi(y_j, x_i), \quad j = 1, \ldots, M, \tag{1}$$

where

—$\{x_i \in \mathbf{R}^d\}_{i=1,\ldots,N}$ are called the *source points*,
—$\{y_j \in \mathbf{R}^d\}_{j=1,\ldots,M}$ are called the *target points*,
—$\{q_i \in \mathbf{R}\}_{i=1,\ldots,N}$ are the *source weights*,
—and Φ is the potential function.

$\Phi(y_j, x_i)$ is the contribution of source at x_i towards the target point y_j. The computational complexity to directly evaluate Eq. 1 is $O(MN)$.

The fast multipole methods look for computation of the same problem with complexity $O(M+N)$ and error $< \epsilon$. The FMM represents a fundamental change in the way of designing numerical algorithms, in that it solves the problem approximately, and trades complexity for exactness. However, practically this distinction is usually not important, as in general, we need the solution to any scientific problem only to a specified accuracy, and in any case the accuracy specified to the FMM can be arbitrary. In the case when the error of the FMM does not exceed the machine precision error there is no difference between the *exact* and *approximate* solution.

Compared to the FFT, the FMM does not require that the data be uniformly sampled, and in general it does not rely on discretization structure to achieve the speedup.

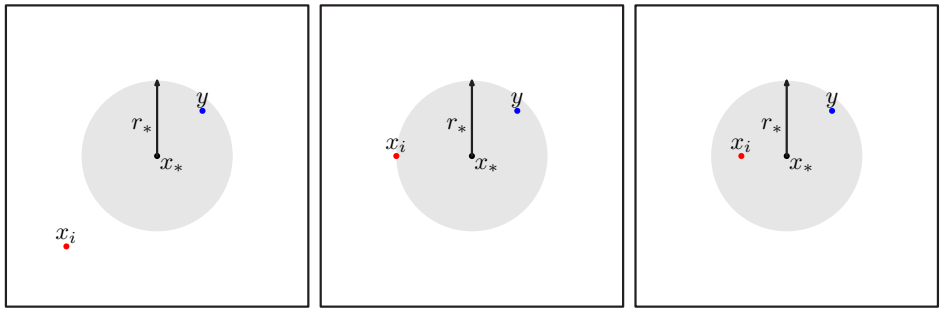


Fig. 1. Local R-expansion $B_{r_*}^<(x_*) = \{y \in \mathbf{R}^2 : \|y - x_*\| < r_*\}$ in case of (a) $r_* < \|x_i - x_*\|$, (b) $r_* = \|x_i - x_*\|$, and (c) $r_* > \|x_i - x_*\|$.

2. POTENTIALS AND FACTORIZATION

We refer to $\Phi(y, x_i)$ as the *field* or *potential* of the i^{th} unit source. We mainly focus on scalar fields. $\Phi(y, x_i)$ can either be *singular* or *regular*. For example the gravitational field is singular at the source point while the gaussian field is regular everywhere.

Gravity (singular at $x = x_i$).

$$\Phi(y, x_i) = \frac{1}{\|y - x_i\|} \tag{2}$$

Gaussian (regular everywhere).

$$\Phi(y, x_i) = e^{-\|y-x_i\|^2/h^2} \tag{3}$$

2.1 Regular (Local) Expansion: R-expansion

For any $x_* \in \mathbf{R}^d$ we call the expansion

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y - x_*) \tag{4}$$

regular (local) inside a sphere $B_{r_*}^<(x_*) = \{y \in \mathbf{R}^d : \|y - x_*\| < r_*\}$, if the series converges for all $y \in B_{r_*}^<(x_*)$. $a_m(x_i, x_*)$ are the *expansion coefficients* and $R_m(y - x_*)$ are the *regular basis functions*. x_* is also referred to as the *expansion center*.

Eq. 4 is referred as the *R-expansion* of the potential $\Phi(y, x_i)$. For a regular potential the region of convergence $B_{r_*}^<(x_*)$ can be quite arbitrary (the R-expansion is valid for all the three cases shown in Fig. 1). However for a singular potential $B_{r_*}^<(x_*)$ cannot include the singular point (only Fig. 1(a) and (b) are valid, where the singular point x_i is outside $B_{r_*}^<(x_*)$).

Example 1: R-expansion of a regular function
Consider the one-dimensional Gaussian function which is regular everywhere,

$$\Phi(y, x_i) = e^{-(y-x_i)^2/h^2}. \tag{5}$$

For any $x_* \in \mathbf{R}$ and $\|y - x_*\| < r_* < \infty$, making use of the Taylor's series, the R-expansion can be written as follows.

$$\begin{aligned}
\Phi(y, x_i) &= e^{-[(y-x_*)-(x_i-x_*)]^2/h^2} \\
&= e^{-(y-x_*)^2/h^2} e^{-(x_i-x_*)^2/h^2} e^{2(y-x_*)(x_i-x_*)/h^2} \\
&= e^{-(y-x_*)^2/h^2} e^{-(x_i-x_*)^2/h^2} \sum_{m=0}^{\infty} \frac{2^m}{m!} \left(\frac{y-x_*}{h}\right)^m \left(\frac{x_i-x_*}{h}\right)^m \\
&= \sum_{m=0}^{\infty} \left[\frac{2^m}{m!} e^{-(x_i-x_*)^2/h^2} \left(\frac{x_i-x_*}{h}\right)^m\right] e^{-(y-x_*)^2/h^2} \left(\frac{y-x_*}{h}\right)^m \\
&= \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y - x_*), \qquad (6)
\end{aligned}$$

where

$$a_m(x_i, x_*) = \frac{2^m}{m!} e^{-(x_i-x_*)^2/h^2} \left(\frac{x_i-x_*}{h}\right)^m. \qquad (7)$$

$$R_m(y - x_*) = e^{-(y-x_*)^2/h^2} \left(\frac{y-x_*}{h}\right)^m. \qquad (8)$$

Example 2: R-expansion of a singular function.
Consider the one-dimensional gravitational field which is singular at $y = x_i$,

$$\Phi(y, x_i) = \frac{1}{y - x_i}. \qquad (9)$$

For any $x_* \in \mathbf{R}$ and $\|y - x_*\| < r_* \leq \|x_i - x_*\|$ (to make sure we do not include the singular point x_i), [We make use of the Geometric progression.]

$$\begin{aligned}
\Phi(y, x_i) &= \frac{1}{(y-x_*)-(x_i-x_*)} = -\frac{1}{(x_i-x_*)[1-\frac{y-x_*}{x_i-x_*}]} \\
&= -\frac{1}{(x_i-x_*)} \left[1 - \frac{y-x_*}{x_i-x_*}\right]^{-1} \\
&= -\frac{1}{(x_i-x_*)} \sum_{m=0}^{\infty} \frac{(y-x_*)^m}{(x_i-x_*)^m}, \text{since} \|y-x_*\| < \|x_i-x_*\| \\
&= \sum_{m=0}^{\infty} \left[\frac{-1}{(x_i-x_*)^{m+1}}\right] (y-x_*)^m \\
&= \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y - x_*), \qquad (10)
\end{aligned}$$

where

$$a_m(x_i, x_*) = \frac{-1}{(x_i-x_*)^{m+1}}. \qquad (11)$$

$$R_m(y - x_*) = (y - x_*)^m. \qquad (12)$$

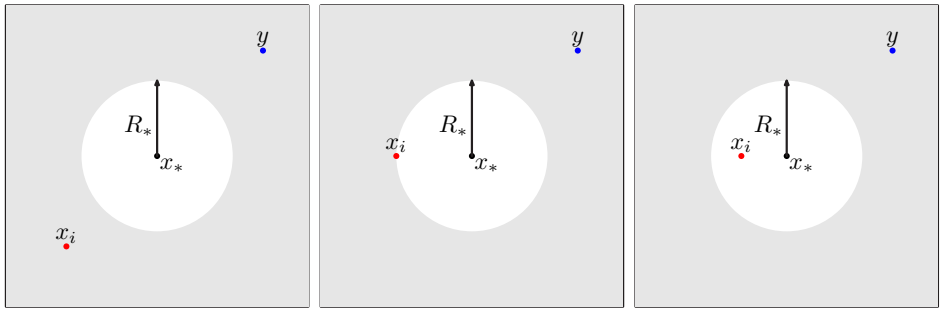


Fig. 2. Far field S-expansion $B^{>}_{R_*}(x_*) = \{y \in \mathbf{R}^2 : \|y - x_*\| > R_*\}$ in case of (a) $R_* < \|x_i - x_*\|$, (b) $R_* = \|x_i - x_*\|$, and (c) $R_* > \|x_i - x_*\|$.

2.2 Far Field Expansion: S-expansion

For any $x_* \in \mathbf{R}^d$ we call the expansion

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*) \tag{13}$$

far field expansion outside a sphere $B^{>}_{R_*}(x_*) = \{y \in \mathbf{R}^d : \|y - x_*\| > R_*\}$, if the series converges for all $y \in B^{>}_{R_*}(x_*)$. $b_m(x_i, x_*)$ are the expansion coefficients and $S_m(y - x_*)$ are the basis function (which can be singular at $y = x_*$). Eq. 13 is referred as the *S-expansion* of the potential $\Phi(y, x_i)$. For a regular potential $B^{>}_{R_*}(x_*)$ can be quite arbitrary (the S-expansion is valid for all the three cases shown in Fig. 2) but for a singular potential $B^{>}_{R_*}(x_*)$ cannot include the singular point (only Fig. 2(b) and (c) are valid, where the singular point x_i is not in $B^{>}_{R_*}(x_*)$).

Example 1: S-expansion of a regular function
For a regular potential the R-expansion can serve as the S-expansion since the potential does not have any singular points. However it is desirable to use rapidly converging series. Consider the one-dimensional Gaussian function which is regular everywhere.

$$\Phi(y, x_i) = e^{-(y - x_i)^2/h^2}. \tag{14}$$

For any $x_* \in \mathbf{R}$ and $\|y - x_*\| > R_* < \infty$,

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*), \tag{15}$$

where

$$b_m(x_i, x_*) = \frac{2^m}{m!} e^{-(x_i - x_*)^2/h^2} (x_i - x_*)^m. \tag{16}$$

$$S_m(y - x_*) = e^{-(y - x_*)^2/h^2} (y - x_*)^m. \tag{17}$$

Example 2: S-expansion of a singular function.
Consider the one-dimensional gravitational field which is singular at $y = x_i$,

$$\Phi(y, x_i) = \frac{1}{y - x_i} = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*), . \tag{18}$$

For any $x_* \in \mathbf{R}$ and $\|y - x_*\| > R_* \geq \|x_i - x_*\|$ (to make sure we do not include the singular point x_i),

$$\begin{aligned}
\Phi(y, x_i) &= \frac{1}{(y - x_*) - (x_i - x_*)} = \frac{1}{(y - x_*)[1 - \frac{x_i - x_*}{y - x_*}]} \\
&= \frac{1}{(y - x_*)} \left[1 - \frac{x_i - x_*}{y - x_*}\right]^{-1} = \frac{1}{(y - x_*)} \sum_{m=0}^{\infty} \frac{(x_i - x_*)^m}{(y - x_*)^m} \\
&= \sum_{m=0}^{\infty} \left[\frac{1}{(y - x_*)^{m+1}}\right] (x_i - x_*)^m \\
&= \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*),
\end{aligned} \tag{19}$$

where,

$$b_m(x_i, x_*) = (x_i - x_*)^m, \;\; S_m(y - x_*) = \frac{1}{(y - x_*)^{m+1}}. \tag{20}$$

2.3 Why R- and S-expansions?

If the potential has a singular point x_i, then we use R-expansion for all $\|y - x_*\| < \|x_i - x_*\|$, and S-expansion for all $\|y - x_*\| > \|x_i - x_*\|$. Note that the singular point x_i is at the boundary of the regions for R- and S-expansions. Also in case of regular potentials depending upon how far y is from x_* either the S-expansion or the R-expansion will converge much more rapidly than the other.

3. MIDDLEMAN METHOD

3.1 For regular potentials

Consider a potential which is regular everywhere. Then we can use the R-expansion about a point x_* for factorizing the potential. The field at y_j can be evaluated as follows.

$$\begin{aligned}
v_j &= \sum_{i=1}^{N} q_i \Phi(y_j, x_i) \\
&= \sum_{i=1}^{N} q_i \left[\sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y_j - x_*)\right] \;\; \text{[R-expansion]} \\
&= \sum_{i=1}^{N} q_i \left[\sum_{m=0}^{p-1} a_m(x_i, x_*) R_m(y_j - x_*) + error(p, x_i, y_j, x_*)\right]
\end{aligned} \tag{21}$$

The truncation number p is chosen based on the desired error. One of the trickiest part in designing a good FMM algorithm lies in getting a pretty tight bound for

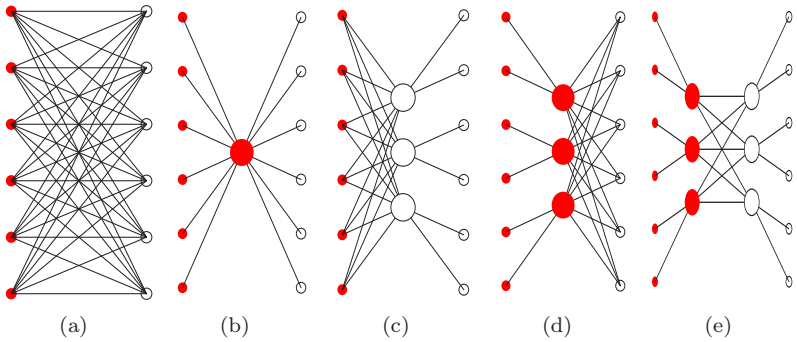


Fig. 3. (a) Direct computation (b) Middleman method (c) middleman with target clusters (d) middleman with source clusters (e) Single level FMM.

$error(p, x_i, y_j, x_*)$. Ignoring the error term we have,

$$\begin{aligned}\hat{v}_j &= \sum_{i=1}^{N} q_i \left[\sum_{m=0}^{p-1} a_m(x_i, x_*) R_m(y_j - x_*)\right] \\ &= \sum_{m=0}^{p-1} \left[\sum_{i=1}^{N} q_i a_m(x_i, x_*)\right] R_m(y_j - x_*) \\ &= \sum_{m=0}^{p-1} A_m R_m(y_j - x_*) \end{aligned} \tag{22}$$

where $A_m = \sum_{i=1}^{N} q_i a_m(x_i, x_*)$, which depends only on the source and can be computed in one pass for different m. The computational complexity for computing $\{A_m\}_{m=0}^{p-1}$ if $O(pN)$ and for computing $\{\hat{v}_j\}_{j=1}^{M}$ is $O(pM)$. Hence the total computational cost is $O(pN + pM)$. As long as $p \ll \min(M, N)$ we have a reduction in the computational complexity.

This approach is called the *middleman method* since we are computing the set of coefficients $\{A_m\}_{m=0}^{p-1}$ at a single expansion center x_* (see Fig. 3(b)). The reader should realize that this approach will work only for regular potentials. Also it can be seen that the middleman method need not use only one expansion center. We can use multiple expansion centers and them consolidate the contribution of all the expansion centers (see Fig. 3(c)).

3.2 For singular potentials

For singular potentials we can use the middleman approach if the source and the target points are well separated. [See Fig. 4(a) and (b)]. In (a) and (b) we will use the R-expansion at the center of each target clusters and in (d) and (e) we will use the S-expansion at the center of each source clusters.

If the sources and targets are not well separated we do a space partitioning. For example let us say we partition with respect to the target points. For each target cluster we use the R-expansion for all sources outside a neighborhood of the cluster. There will be some sources which happen to lie within the neighborhood of these

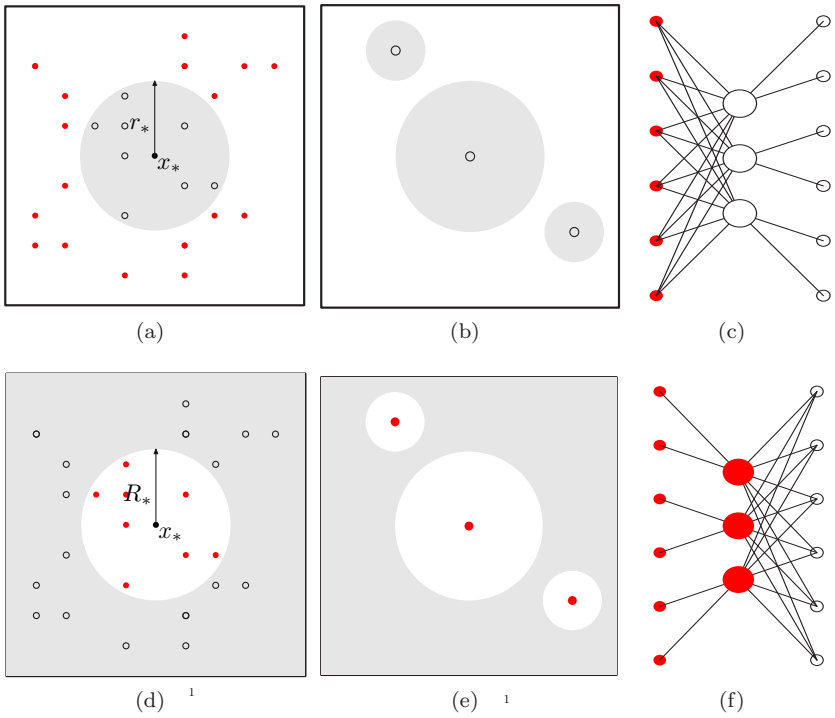


Fig. 4. For singular potentials we can use the middleman approach if the source and the target points are well separated. In (a) and (b) we will use the R-expansion at the center of each target clusters and in (d) and (e) we will use the S-expansion at the center of each source clusters. The red filled circles are the source points and the back circles are the target points.

clusters, where the potential happens to be singular at each of these source points. If the number of such sources is few we can directly sum the contribution of these sources. However if they are large in number, this leads to the idea of a single level FMM to be discussed in the next section.

4. TRANSLATIONS (RE-EXPANSIONS)

Let $\{F_n(y-x_{*1})\}_{n=0}^{\infty}$ and $\{G_m(y-x_{*2})\}_{m=0}^{\infty}$ be two sets of basis functions centered at x_{*1} and x_{*1} such that $\Phi(y,x_i)$ can be represented by two uniformly and absolutely convergent series as,

$$\Phi(y,x_i) = \sum_{n=0}^{\infty} a_n(x_i,x_{*1})F_n(y-x_{*1}), \quad \forall y \in \Omega_1 \subset \mathbf{R}^d. \tag{23}$$

$$\Phi(y,x_i) = \sum_{m=0}^{\infty} b_m(x_i,x_{*2})G_m(y-x_{*2}), \quad \forall y \in \Omega_2 \subset \Omega_1. \tag{24}$$

$(F|G)(t)$ is called a *translation operator* which relates the two sets of coefficients as,

$$\{b_m(x_i,x_{*2})\} = (F|G)(t)\{a_n(x_i,x_{*1})\}, \quad t = x_{*2} - x_{*1}. \tag{25}$$

4.1 R|R re-expansion (Local to Local)

Refer to Fig. 5(a). Consider the R expansion of a potential $\Phi(y, x_i)$ about the expansion center $x_* \in \mathbf{R}^d$

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y - x_*), \quad \forall y \in B_r^<(x_*) = \{y \in \mathbf{R}^d : \|y - x_*\| < r\}$$

We are interested in writing the same function over a shifted basis $R_n(y-(x_*+t))$ about the expansion center $x_* + t \in B_r^<(x_*)$

$$\Phi(y, x_i) = \sum_{n=0}^{\infty} \widetilde{a_n}(x_i, x_* + t) R_n(y - (x_* + t)), \quad \forall y \in B_{r1}^<(x_* + t) \subset B_r^<(x_*),$$

where $B_{r1}^<(x_* + t) = \{y \in B_r^<(x_*) : \|y - (x_* + t)\| < r1 = r - \|t\|\}$. The matrix operator $(R|R)(t)$ relates the coefficients $a_m(x_i, x_*)$ and $\widetilde{a_n}(x_i, x_* + t)$ as,

$$\widetilde{a_n}(x_i, x_* + t) = \sum_{m=0}^{\infty} (R|R)_{nm}(t) a_m(x_i, x_*). \tag{26}$$

4.2 S|S re-expansion (Multipole to Multipole)

Refer to Fig. 5(b). Consider the S expansion of a potential $\Phi(y, x_i)$ about the expansion center $x_* \in \mathbf{R}^d$ ($\|x_i - x_*\| \leq r$)

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*), \quad \forall y \in B_r^>(x_*) = \{y \in \mathbf{R}^d : \|y - x_*\| > r\}$$

We are interested in writing the same function over a shifted basis $S_n(y-(x_*+t))$ about the expansion center $x_* + t \in B_r^<(x_*)$

$$\Phi(y, x_i) = \sum_{n=0}^{\infty} \widetilde{b_n}(x_i, x_* + t) S_n(y - (x_* + t)), \quad \forall y \in B_{r1}^>(x_* + t) \subset B_r^>(x_*),$$

where $B_{r1}^>(x_* + t) = \{y \in B_r^>(x_*) : \|y - (x_* + t)\| > r1 = r + \|t\|\}$. The matrix operator $(S|S)(t)$ relates the coefficients $b_m(x_i, x_*)$ and $\widetilde{b_n}(x_i, x_* + t)$ as,

$$\widetilde{b_n}(x_i, x_* + t) = \sum_{m=0}^{\infty} (S|S)_{nm}(t) b_m(x_i, x_*). \tag{27}$$

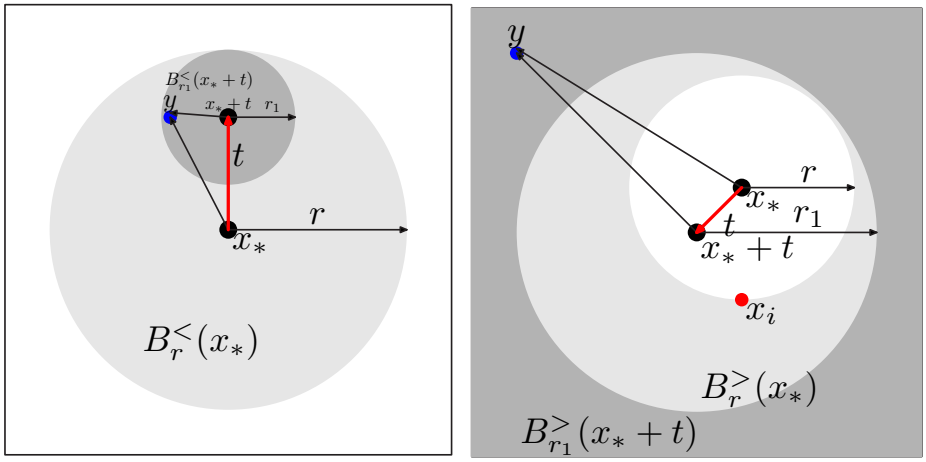
4.3 S|R re-expansion (Multipole to Local)

Refer to Fig. 5(c). Consider the S expansion of a potential $\Phi(y, x_i)$ about the expansion center $x_* \in \mathbf{R}^d$ ($\|x_i - x_*\| \leq r$)

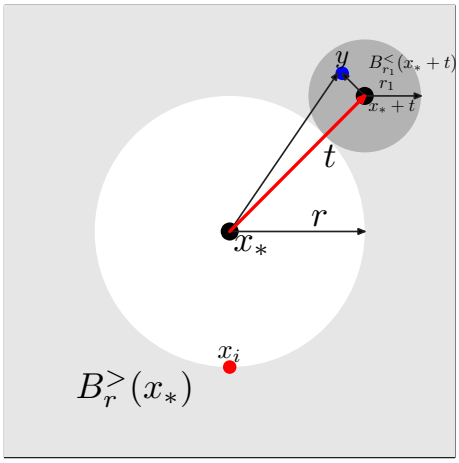
$$\Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*), \quad \forall y \in B_r^>(x_*) = \{y \in \mathbf{R}^d : \|y - x_*\| > r\}$$

We are interested in writing the same function over a shifted regular basis $R_n(y - (x_* + t))$ about the expansion center $x_* + t \in B_r^>(x_*)$

$$\Phi(y, x_i) = \sum_{n=0}^{\infty} \widetilde{a_n}(x_i, x_* + t) R_n(y - (x_* + t)), \quad \forall y \in B_{r1}^<(x_* + t) \subset B_r^>(x_*),$$



(a) R|R (b) S|S



(c) S|R

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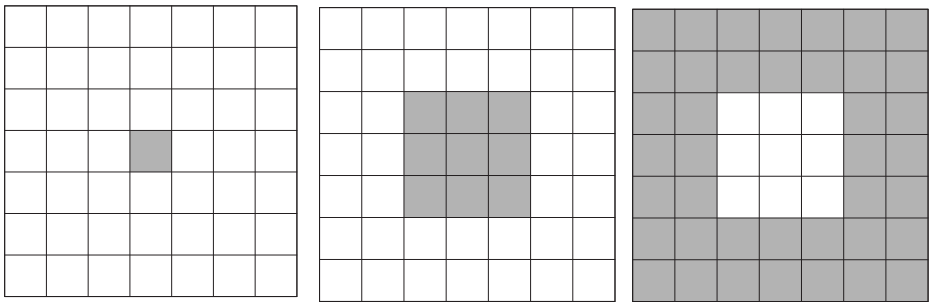
Fig. 5. Schematic illustrating (a) R|R re-expansion, (b) S|S re-expansion, and (c) S|R re-expansion

where $B^{<}_{r1}(x_* + t) = \{y \in B^{>}_{r}(x_*) : \|y - (x_* + t)\| < r1 = \|t\| - r\}$. The matrix operator $(S|R)(t)$ relates the coefficients $b_m(x_i, x_*)$ and $\widetilde{a_n}(x_i, x_* + t)$ as,

$$\widetilde{a_n}(x_i, x_* + t) = \sum_{m=0}^{\infty} (S|R)_{nm}(t) b_m(x_i, x_*). \tag{28}$$

4.4 R|S re-expansion (Local to Multipole)

Theoretically it is possible to have R|S re-expansion also. But in practice since the domain of S expansion is larger than the domain of R expansion, this is either not useful (due to large error bounds) or can be avoided in algorithms. Most FMM algorithms do not use R|S re-expansion.



(a) $I_1(n)$ (b) $I_2(n)$ (c) $I_3(n)$

Fig. 6. The three spatial domains.

5. SINGLE LEVEL FMM

5.1 What is the problem with middleman ?

For a regular potential even though the expansion is valid everywhere, the truncation number can be huge for large domains to provide the desired accuracy. For singular potentials the middleman approach can be used only when either the source or targets are naturally grouped.

5.2 Space subdivison

Given these series representations and translation operators, the single level FMM proceeds as follows. First the space is partitioned into boxes. Each box will contain a certain number of sources and targets. For any box n we define the following three spatial domains [See Fig. 6].

$$\begin{aligned} I_1(n) &= \{n\} \\ I_2(n) &= \{\text{Neighbors}(n)\} \bigcup \{n\} \\ I_3(n) &= \{\text{All boxes}\} - \{I_2(n)\} \end{aligned} \tag{29}$$

Let the target point $y \in n$. We define the following three potentials,

$$\begin{aligned} \Phi_1^n(y) &= \sum_{x_i \in I_1(n)} q_i \Phi(y, x_i) \\ \Phi_2^n(y) &= \sum_{x_i \in I_2(n)} q_i \Phi(y, x_i) \\ \Phi_3^n(y) &= \sum_{x_i \in I_3(n)} q_i \Phi(y, x_i) \end{aligned} \tag{30}$$

Since $E_3(n)^c = E_2(n)$ the total potential can be written as,

$$\Phi(y) = \sum_{i=1}^{N} q_i \Phi(y, x_i) = \sum_{x_i \in \{I_2(n) \bigcup I_3(n)\}} q_i \Phi(y, x_i) = \Phi_2^n(y) + \Phi_3^n(y). \tag{31}$$

5.3 R expansion

The potential $\Phi_3^n(y)$ has to be computed using the local R expansion of $\Phi(y, x_i)$ about the box center x_c^n. Exchanging the order of summation and consolidating the source terms we have,

$$\begin{aligned}
\Phi_3^n(y) &= \sum_{x_i \in I_3(n)} q_i \Phi(y, x_i) \\
&= \sum_{x_i \in I_3(n)} q_i \left[\sum_{m=0}^{\infty} a_m(x_i, x_c^n) R_m(y - x_c^n) \right] \\
&= \sum_{m=0}^{\infty} \left[\sum_{x_i \in I_3(n)} q_i a_m(x_i, x_c^n) \right] R_m(y - x_c^n) \\
&= \sum_{m=0}^{\infty} A_m^n R_m(y - x_c^n) \qquad (32)
\end{aligned}$$

where $A_m^n = \sum_{x_i \in I_3(n)} q_i a_m(x_i, x_c^n)$.

5.4 S expansion

If y is close to x_c^n then the local R-expansion series will converge quickly. However if y is faraway then the series may converge very slowly or may nor converge at all. We need a larger radius of convergence so that the number of boxes are small. Also since we will be truncating the above series, if the series converges slowly larger radius will imply a very large truncation number. For this reason we use the S-expansions, and translate it to an R-expansion via the S|R translation operator. The S expansions are computed about the box centers for all the boxes. Exchanging the order of summation and consolidating the source terms we have $\Phi_1^l(y)$ the potential at $y \in I_3(l)$ due to all sources $x_i \in I_1(l)$

$$\begin{aligned}
\Phi_1^l(y) &= \sum_{x_i \in I_1(l)} q_i \Phi(y, x_i) \\
&= \sum_{x_i \in I_1(l)} q_i \left[\sum_{m=0}^{\infty} b_m(x_i, x_c^l) S_m(y - x_c^l) \right] \\
&= \sum_{m=0}^{\infty} \left[\sum_{x_i \in I_1(l)} q_i b_m(x_i, x_c^l) \right] S_m(y - x_c^l) \\
&= \sum_{m=0}^{\infty} B_m^l S_m(y - x_c^l) \qquad (33)
\end{aligned}$$

where $B_m^l = \sum_{x_i \in I_1(l)} q_i b_m(x_i, x_c^l)$.

5.5 S|R Translation

Now we want to write the potential $\Phi_1^l(y)$ (expanded using an S expansion around x_c^l) as an R expansion around x_c^n.

$$\begin{aligned}
\Phi_1^l(y) &= \sum_{x_i \in I_1(l)} q_i \left[\sum_{m=0}^{\infty} b_m(x_i, x_c^l) S_m(y - x_c^l) \right] \\
&= \sum_{x_i \in I_1(n)} q_i \left[\sum_{k=0}^{\infty} \widetilde{a_k}\left(x_i, x_c^l + (x_c^n - x_c^l)\right) R_k\left(y - \left(x_c^l + (x_c^n - x_c^l)\right)\right) \right] \\
&= \sum_{k=0}^{\infty} \left[\sum_{x_i \in I_1(l)} q_i \widetilde{a_k}\left(x_i, x_c^l + (x_c^n - x_c^l)\right) \right] R_k(y - x_c^n) \\
&= \sum_{k=0}^{\infty} \left[\sum_{x_i \in I_1(l)} q_i \left\{ \sum_{m=0}^{\infty} (S|R)_{km}(x_c^n - x_c^l) b_m(x_i, x_c^l) \right\} \right] R_k(y - x_c^n) \\
&= \sum_{k=0}^{\infty} \left[\sum_{m=0}^{\infty} (S|R)_{km}(x_c^n - x_c^l) \left\{ \sum_{x_i \in I_1(l)} q_i b_m(x_i, x_c^l) \right\} \right] R_k(y - x_c^n) \\
&= \sum_{k=0}^{\infty} \left[\sum_{m=0}^{\infty} (S|R)_{km}(x_c^n - x_c^l) B_m^l \right] R_k(y - x_c^n) \\
&= \sum_{k=0}^{\infty} \widetilde{A_k^{nl}} R_k(y - x_c^n) \qquad (34)
\end{aligned}$$

where $\widetilde{A_k^{nl}} = \sum_{m=0}^{\infty} (S|R)_{km}(x_c^n - x_c^l) B_m^l$. The R expansions about the box center x_c^n,

$$\Phi_3^n(y) = \sum_{m=0}^{\infty} A_m^n R_m(y - x_c^n) \qquad (35)$$

where $A_m^n = \sum_{x_i \in I_3(n)} q_i a_m(x_i, x_c^n) = \sum_{l \in I_3(n)} \widetilde{A_m^{nl}}$. So we have R expansions about the box centers, and very few points for which valid expansions could not be constructed. These are evaluated directly and added to the R expansions evaluated at the evaluation points. The speedup is achieved by appropriately truncating each series.

6. MULTI LEVEL FMM

We give a brief description of the multi level FMM without going into the details. Given these series representations and translation operators, the multilevel FMM proceeds as follows. First the space is partitioned into boxes at various levels, and outer S expansions computed about box centers at the finest level, for points within the box. These expansions are consolidated, and they are translated S|S using translations in an upward pass up the hierarchy. The coefficients of these box-centered expansions at each level are stored. In the downward pass, the consolidated S expansions are expanded as local R expansions about boxes in the evaluation

Algorithm 1: Single Level Fast Multipole Method

Input :

$x_i \in \mathbf{R}^d \ i = 1, \ldots, N$ /* N sources in d dimensions. */
$q_i \in \mathbf{R}^+ \ i = 1, \ldots, N$ /* source weights. */
$y_j \in \mathbf{R}^d \ j = 1, \ldots, M$ /* M targets in d dimensions. */
$\Phi(y, x_i)$ /* potential at y due to source x_i. */
$\epsilon > 0$ /* Desired error. */

Output: Computes an approximation $\hat{\Phi}(y_j)$ to $\Phi(y_j) = \sum_{i=1}^{N} q_i \Phi(y_j, x_i)$ such that the $|\hat{\Phi}(y_j) - \Phi(y_j)| \leq \epsilon$.

Step 0 *Partition the space into boxes.*;

Step 1 *Decide the truncation numbers* p_1 *and* p_2 *such that the error is* $\leq \epsilon$;

Step 2 *S- and R-expansion of the potential function about each box center.*
$\forall x_i \in I_1(l) \ \forall y \in I_3(l) \ \Phi(y, x_i) = \sum_{r=0}^{p_1-1} b_r(x_i, x_c^l) S_r(y - x_c^l)$
$\forall x_i \in I_3(l) \ \forall y \in I_1(l) \ \Phi(y, x_i) = \sum_{q=0}^{p_2-1} a_q(x_i, x_c^l) R_q(y - x_c^l)$;

Step 3 *Consolidate the S-expansion coefficients for each box.*
$B_r^l = \sum_{x_i \in I_1(l)} q_i b_r(x_i, x_c^l)$ *for* $r = 0, \ldots, p_1 - 1$;

Step 4 *S|R translate the expansion coefficients.*
$\widetilde{A_q^{nl}} = \sum_{r=0}^{p_1-1} (S|R)_{qr}(x_c^n - x_c^l) B_r^l$ *for* $q = 0, \ldots, p_2 - 1$
$A_q^n = \sum_{l \in I_3(n)} \widetilde{A_q^{nl}}$ *for* $q = 0, \ldots, p_2 - 1$;

Step 5 *Final summation.*
$\Phi(y \in I_1(n)) = \sum_{x_i \in I_2(n)} q_i \Phi(y, x_i) + \sum_{q=0}^{p_2-1} A_q^n R_q(y - x_c^n)$;

hierarchy, using the S|R translation, for boxes for which the expansion is valid (it is in the domain of validity of the particular S expansion). At finer levels, the R expansions at the higher levels are R|R translated to the new box centers and to these are added the coefficients of the S|R translations from boxes at finer levels of the source hierarchy, which were excluded at the previous level(s). At the finest level of the evaluation hierarchy we have R expansions about the box centers, and very few points for which valid expansions could not be constructed. These are evaluated directly and added to the R expansions evaluated at the evaluation points.

REFERENCES

Board, J. and Schulten, K. 2000. The fast multipole algorithm. *Computing in Science and Engineering 2,* 1, 76–79. 2

Dongarra, J. and Sullivan, F. 2000. The top ten algorithms of the century. *Computing in Science and Engineering 2,* 1, 22–23. 2

Greengard, L. and Rokhlin, V. 1987. A fast algorithm for particle simulations. *J. of Comp. Physics 73,* 2, 325–348. 2

Greengard, L. F. 1988. *The Rapid Evaluation of Potential Fields in Particle Systems.* The MIT Press. 2