18.337 Parallel Scientific Computing	March 2, 1995
Lecture 6	
Topic: Multipole Algorithm	*1995 Scribe: Cheng Wang*

Outline of The Lecture: Multipole Algorithm

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Introduction

For N-body simulations, sometimes, it is easier to work with the (gravitational) potential rather than with the force directly. The force can then be calculated as the gradient of the potential.

In two dimensions, the potential function at z_j due to the other bodies is given by

$$\begin{aligned}\phi(z_j) &= \sum_{i=1, i\neq j}^{n} q_i \log(z_j - z_i) \\ &= \sum_{i=1, i\neq j}^{n} \phi_{z_i}(z_j)\end{aligned}$$

with

$$\phi_{z_i}(z) = q_i \log|z - z_i|$$

where $z_1, \ldots, z_n$ the position of particles, and $q_1, \ldots, q_n$ the strength of particles. The potential due to the bodies in the rest of the space is

$$\phi(z) = \sum_{i=1}^{n} q_i \log(z - z_i)$$

which is *singular* at each potential body. (Note: actually the potential is $Re\ \phi(z)$ but we take the complex version for simplicity.)

With the Barnes and Hut scheme in term of potentials, each cluster may be regarded as an individual particle when the cluster is sufficiently far away from the evaluation point. The following sections will provide the details of the fast multipole algorithm developed by Greengard and Rokhlin.

Multipole Algorithm: An Overview

There are three important concepts in the multipole algorithm:

- function representations (multipole expansions and Taylor series)
- operators to change representations (SHIFTs and FLIPs)
- the general tree structure of the computation

Function Representation

Multipole expansions converge outside of a disk in the complex plane. By contrast, the more familiar Taylor series converge within a disk. A multipole expansion of $f(z)$ about a point z_c typically has the general form

$$f(z) = \sum_{k=1}^{\infty} a_k \frac{1}{(z - z_c)^k}$$

though other functions may be added to describe the behavior at ∞ such as

$$f(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} a_k \frac{1}{(z - z_c)^k}$$

A Taylor series about z_c has the form

$$f(z) = \sum_{k=0}^{\infty} a_k (z - z_c)^k$$

Operators to Change Representation

The same function $f(z)$ may be written as a multipole expansion or a Taylor series. The coefficients (and convergence properties) of the series depend on z_c. If

$$f(z) = \sum_{k=1}^{\infty} a_k \frac{1}{(z - z_c)^k} = \sum_{k=1}^{\infty} a'_k \frac{1}{(z - z'_c)^k}$$

then the operator that takes the a_k to the a'_k is known as a shift. Similarly if

$$f(z) = \sum_{k=0}^{\infty} a_k (z - z_c)^k = \sum_{k=0}^{\infty} a'_k (z - z'_c)^k$$

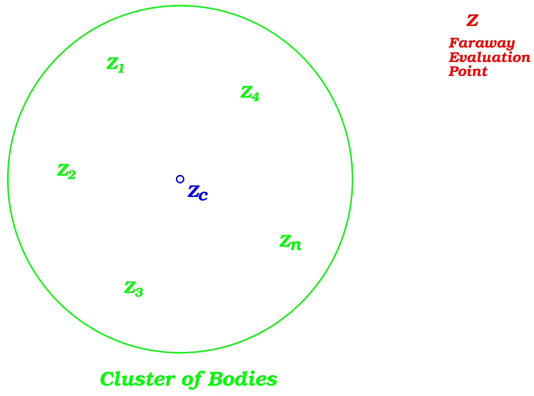

Figure 1: Potential of Faraway Particle due to Cluster

this operator is also known as a shift. Finally, if

$$\sum_{k=1}^{\infty} a_k \frac{1}{(z - z_c)^k} = \sum_{k=0}^{\infty} a'_k (z - z'_c)^k$$

then the operator converts the a_k to an a'_k is known as a flip. We will see that multipole expansions serve the purpose of broadcasting the news about a body to far away locations efficiently. On the other hand, Taylor expansions serve the purpose of locally computing all the needed information. The shifts allow the computations to occur on common ground.

Multipole Expansion

The multipole algorithm flips between two point of views, or to be more precise, two representations for the potential function. One of them, which considers the cluster of bodies corresponding to many far away evaluation points, is treated in detail here. This part of the algorithm is often called the *Multipole Expansion*.

In elementary calculus, one learns about Taylor expansions for functions. This power series represents the function perfectly within the radius of convergence. A multipole expansion is also a perfectly valid representation of a function which typically converges *outside* a circle rather than inside. For example, it is easy to show that

$$\begin{aligned} \phi_{z_i}(z) &= q_i \log(z - z_i) \\ &= q_i \log(z - z_c) + \sum_{k=1}^{\infty} -\frac{q_i}{k} \left(\frac{z_i - z_c}{z - z_c} \right)^k \end{aligned}$$

where z_c is any complex number. This series converges in the region $|z - z_c| > |z - z_i|$, i.e., outside of the circle containing the singularity. The formula is particularly useful if $|z - z_c| \gg |z - z_i|$, i.e., if we are far away from the singularity.

Note that

$$\phi_{z_i}(z) = q_i \log(z - z_i)$$

$$
\begin{aligned}
&= q_i \log[(z - z_c) - (z_i - z_c)] \\
&= q_i \left[\log(z - z_c) + \log(1 - \frac{z_i - z_c}{z - z_c})\right]
\end{aligned}
$$

The result follows from the Taylor series expansion for $\log(1 - x)$. The more terms in the Taylor series that are considered, the higher is the order of the approximation.

By substituting the single potential expansion back into the main equation, we obtain the multipole expansion as following

$$
\begin{aligned}
\phi(z) &= \sum_{i=1}^{n} \phi_{z_i}(z) \\
&= \sum_{i=1}^{n} q_i \log(z - z_c) + \sum_{i=1}^{n} \sum_{k=1}^{\infty} q_i \left(-\frac{1}{k}\left(\frac{z_i - z_c}{z - z_c}\right)^k\right) \\
&= Q \log(z - z_c) + \sum_{k=1}^{\infty} a_k \left(\frac{1}{z - z_c}\right)^k
\end{aligned}
$$

where

$$
a_k = -\sum_{i=1}^{n} \frac{q_i (z_i - z_c)^k}{k}
$$

When we truncate the expansion due to the consideration of computation cost, an error is introduced into the resulting potential. Consider a $p - term$ expansion

$$
\phi_p(z) = Q \log(z - z_c) + \sum_{k=1}^{p} a_k \frac{1}{(z - z_c)^k}
$$

An error bound for this approximation is given by

$$
||\phi(z) - \phi_p(z)|| \leq \frac{A}{\left(\left|\frac{z - z_c}{r}\right| - 1\right)} \left|\frac{r}{z - z_c}\right|^p
$$

where r is the radius of the cluster and

$$
A = \sum_{i=1}^{n} |q_i|
$$

This result can be shown as the following

$$
\begin{aligned}
\text{Error} &= \left|\sum_{k=p+1}^{\infty} a_k \frac{1}{(z - z_c)^k}\right| \\
&= \left|-\sum_{k=p+1}^{\infty} \sum_{i=1}^{n} \frac{q_i}{k} \left(\frac{z_i - z_c}{z - z_c}\right)^k\right| \\
&\leq \sum_{k=p+1}^{\infty} \sum_{i=1}^{n} |q_i| \left|\frac{r}{z - z_c}\right|^k
\end{aligned}
$$

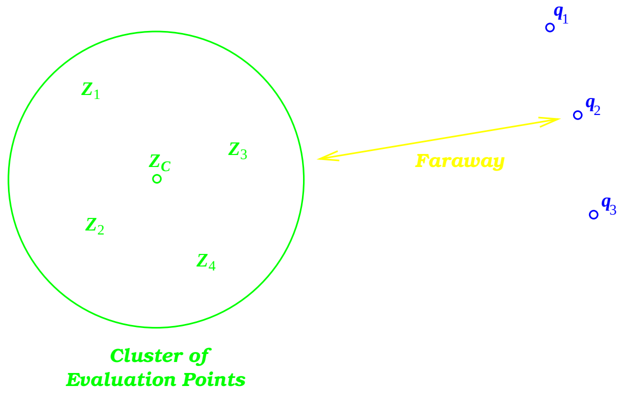

Figure 2: Potential of Particle Cluster

$$
\begin{aligned}
&\le A \sum_{k=p+1}^{\infty} \left| \frac{r}{z - z_c} \right|^k \\
&\le A \frac{\left| \frac{r}{z-z_c} \right|^{p+1}}{1 - \left| \frac{r}{z-z_c} \right|} \\
&\le \frac{A}{\left(\left| \frac{z-z_c}{r} \right| - 1 \right)} \left| \frac{r}{z - z_c} \right|^p
\end{aligned}
$$

At this moment, we are able to calculate the potential of each particle due to cluster of far away bodies, through multipole expansion.

Taylor Expansion

In this section, we will briefly discuss the other point of view for the multipole algorithm, which considers the cluster of evaluation points with respect to many far away bodies. It is called *Taylor Expansion*. For this expansion, each processor "ownes" the region of the space defined by the cluster of evaluation points, and compute the potential of the cluster through a Taylor series about the center of the cluster z_c.

Generally, the local Taylor expansion for cluster denoted by C (with center z_c) corresponding to some body z has the form

$$\phi_{C,z_c}(z) = \sum_{k=0}^{\infty} b_k (z - z_c)^k$$

Denote $z - z_i = (z - z_c) - (z_i - z_c) = -(z_i - z_c)(1 - \xi)$. Then for z such that $|z - z_c| < \min(z_c, C)$, we have $|\xi| < 1$ and the series $\phi_{C,z_c}(z)$ converge:

$$\phi_{C,z_c}(z) \;=\; \sum_C q_i \log(-(z_i - z_c)) + \sum_C q_i \log(1 - \xi)$$

$$
\begin{aligned}
&= \sum_C q_i \log(-(z_i - z_c)) + \sum_{k=1}^{\infty} \left(\sum_C q_i \right) k^{-1} (z_i - z_c)^{-k} (z - z_c)^k \\
&= b_0 + \sum_{k=1}^{\infty} b_k (z - z_c)^k
\end{aligned}
$$

where formulæ for coefficients are

$$
b_0 = \sum_C q_i \log(-(z_i - z_c)) \quad \text{and} \quad b_k = k^{-1} \sum_C q_i (z_i - z_c)^{-k} \quad k > 0.
$$

Define the $p - order$ truncation of local expansion ϕ^p_{C,z_c} as follows

$$
\phi^p_{C,z_c}(z) = \sum_{k=0}^{p} b_k (z - z_c)^k.
$$

We have error bound

$$
\begin{aligned}
\left| \phi_{C,z_c}(z) - \phi^p_{C,z_c}(z) \right| &= \left| \sum_{k=p+1}^{\infty} k^{-1} \sum_C q_i \left(\frac{z - z_c}{z_i - z_c} \right)^k \right| \\
&\leq \frac{1}{p+1} \sum_C |q_i| \sum_{k=p+1}^{\infty} \left| \frac{z - z_c}{\min(z_c, C)} \right|^k = \frac{A}{(1+p)(1-c)} c^{p+1},
\end{aligned}
$$

where $A = \sum_C |q_i|$ and $c = |z - z_c| / \min(z_c, C) < 1$.

By now, we can also compute the local potential of the cluster through the Taylor expansion. During the process of deriving the above expansions, it is easy to see that

- Both expansions are singular at the position of any body;
- Multipole expansion is valid outside the cluster under consideration;
- Taylor expansion converges within the space defined the cluster.

At this point, we have finished the basic concepts involved in the multipole algorithm. Next, we will begin to consider some of the operations that could be performed on and between the expansions.

Operation No.1 — SHIFT

Sometimes, we need to change the location of the center of the reference for the expansion series, either the multipole expansion or the local Taylor expansion. To accomplish this goal, we will perform the SHIFT operation on the expansion series.

For the multipole expansion, consider some far away particle with position z such that both series ϕ_{z_0} and ϕ_{z_1} , corresponding to different center of reference z_0 and z_1, converge: $|z - z_0| > \max(z_0, C)$ and $|z - z_1| > \max(z_1, C)$. Note that

$$
z - z_0 = (z - z_1) - (z_0 - z_1) = (z - z_1) \left(1 - \frac{z_0 - z_1}{z - z_1} \right) = (z - z_1)(1 - \xi)
$$

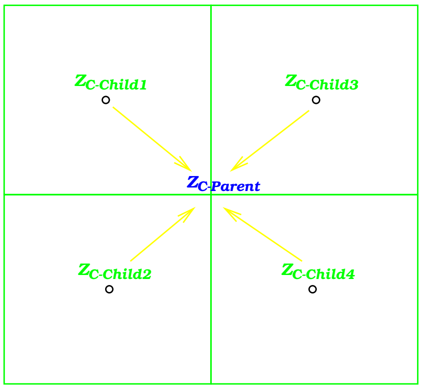

Figure 3: SHIFT the Center of Reference

for appropriate ξ and if we also assume z sufficiently large to have $|\xi| < 1$, we get identity

$$(1-\xi)^{-k} = \left(\sum_{l=0}^{\infty} \xi^l\right)^k = \sum_{l=0}^{\infty} \binom{k+l-1}{l} \xi^l.$$

Now, we can express the SHIFT operation for multipole expansion as

$$\begin{aligned}
\phi_{z_1}(z) &= SHIFT\left(\phi_{z_0}(z), z_0 \Rightarrow z_1\right) \\
&= SHIFT\left(a_0 \log(z-z_0) + \sum_{k=1}^{\infty} a_k (z-z_0)^{-k}, z_0 \Rightarrow z_1\right) \\
&= a_0 \log(z-z_1) + a_0 \log(1-\xi) + \sum_{k=1}^{\infty} a_k (1-\xi)^{-k} (z-z_1)^{-k} \\
&= a_0 \log(z-z_1) - a_0 \sum_{k=1}^{\infty} k^{-1} \xi^k + \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} a_k \binom{k+l-1}{l} \xi^l (z-z_1)^{-k} \\
&= a_0 \log(z-z_1) + \sum_{l=1}^{\infty} \left(\sum_{k=1}^{l} a_k (z_0-z_1)^{l-k} \binom{l-1}{k-1} - a_0 l^{-1} (z_0-z_1)^l \right) (z-z_1)^{-l}
\end{aligned}$$

We can represent $\phi_{z_1}(z)$ as a sequence of its coefficients a'_k:

$$a'_0 = a_0 \quad \text{and} \quad a'_l = \sum_{k=1}^{l} a_k (z_0-z_1)^{l-k} \binom{l-1}{k-1} - a_0 l^{-1} (z_0-z_1)^l \quad l > 0.$$

Note that a'_l depends only on $a_0, a_1, \ldots, a_l$ and not on the higher coefficients. It shows that given $\phi^p_{z_0}$ we can compute $\phi^p_{z_1}$ *exactly*, that is without any further error! In other words, operators SHIFT and truncation commute on multipolar expansions:

$$SHIFT(\phi^p_{z_0}, z_0 \Rightarrow z_1) = \phi^p_{z_1}.$$

Similarly, we can obtain the SHIFT operation for the local Taylor expansion, by extending the operator on the domain of local expansion, so that $SHIFT(\phi_{C,z_0}, z_0 \Rightarrow z_1)$ produces

ϕ_{C,z_1}. Both series converges for z such that $|z - z_0| < \min(z_0, C)$, $|z - z_1| < \min(z_1, C)$. Then

$$\begin{aligned}
\phi_{C,z_1}(z) &= SHIFT\left(\phi_{C,z_0}(z), z_0 \Rightarrow z_1\right) \\
&= \sum_{k=0}^{\infty} b_k((z - z_1) - (z_0 - z_1))^k \\
&= \sum_{k=0}^{\infty} b_k \sum_{l=0}^{\infty} (-1)^{k-l} \binom{k}{l} (z_0 - z_1)^{k-l} (z - z_1)^l \\
&= \sum_{l=0}^{\infty} \left(\sum_{k=l}^{\infty} b_k (-1)^{k-l} \binom{k}{l} (z_0 - z_1)^{k-l} \right) (z - z_1)^l
\end{aligned}$$

Therefore, formula for transformation of coefficients b_k of ϕ_{C,z_0} to b'_l of ϕ_{C,z_1} are

$$b'_l = \sum_{k=l}^{\infty} a_k (-1)^{k-l} \binom{k}{l} (z_0 - z_1)^{k-l}.$$

Notice that in this case, b'_l depends only on the higher coefficients, which means knowledge of the coefficients $b_0, b_1, \ldots, b_p$ from the truncated local expansion in z_0 does *not* suffice to recover the coefficients $b'_0, b'_1, \ldots b'_p$ at another point z_1. We do incur an error by the SHIFT operation applied to truncated local expansion:

$$\begin{aligned}
\left| SHIFT(\phi^p_{C,z_0}, z_0 \Rightarrow z_1) - \phi^p_{C,z_1} \right| &= \left| \sum_{l=0}^{\infty} \left(\sum_{k=p+1}^{\infty} b_k (-1)^{k-l} (z_0 - z_1)^{k-l} \right) (z - z_1)^l \right| \\
&\leq \left| \sum_{k=p+1}^{\infty} b_k (z_1 - z_0)^k \right| \left| \sum_{l=0}^{\infty} \left(\frac{z - z_1}{z_1 - z_0} \right)^l \right| \\
&= \left| \sum_{k=p+1}^{\infty} k^{-1} \sum_C q_i \left(\frac{z_1 - z_0}{z_i - z_0} \right)^k \right| \left| \sum_{l=0}^{\infty} \left(\frac{z - z_1}{z_0 - z_1} \right)^l \right| \\
&\leq \frac{A}{(p+1)(1-c)(1-D)} c^{p+1},
\end{aligned}$$

where $A = \sum_C |q_i|$. $c = |z_1 - z_0| / \min(z_0, C)$ and $D = |z - z_1| / |z_0 - z_1|$.

At this moment, we have obtained all the information needed to perform the SHIFT operation for both multipole expansion and local Taylor expansion. Next, we will consider the operation which can transform multipole expansion to local Taylor expansion.

Operation No.2 — FLIP

At this section, we will introduce the more powerful operation in multipole algorithm, namely the FLIP operation. For now, we will consider only the transformation in the direction from the multipole expansion $\phi_{z_0}(z)$ to the local Taylor expansion $\phi_{C,z_1}(z)$, denoted by

$$FLIP(\phi_{z_0}, z_0 \Rightarrow z_1) = \phi_{C,z_1}$$

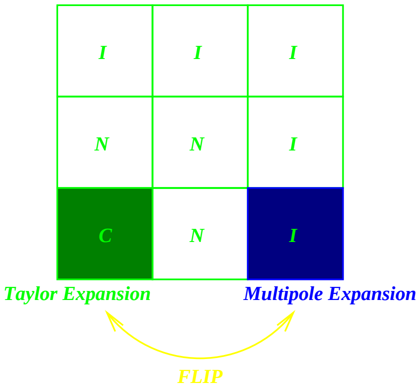

Figure 4: FLIP from Multipole to Taylor Expansion

For $|z-z_0| > \max(z_0, C)$ and $|z-z_1| < \min(z_1, C)$ both series converge. Note that

$$z - z_0 = -(z_0 - z_1)(1 - \frac{z - z_1}{z_0 - z_1}) = -(z_0 - z_1)(1 - \xi)$$

and assume also $|\xi| < 1$. Then,

$$\begin{aligned}
\phi_{z_0}(z) &= a_0 \log(z - z_0) + \sum_{k=1}^{\infty} a_k (z - z_0)^{-k} \\
&= a_0 \log(-(z_0 - z_1)) + a_0 \log(1 - \xi) + \sum_{k=1}^{\infty} a_k (-1)^k (z_0 - z_1)^{-k} (1 - \xi)^{-k} \\
&= a_0 \log(-(z_0 - z_1)) + \sum_{l=1}^{\infty} -a_0 l^{-1} \xi^l + \sum_{k=1}^{\infty} (-1)^k a_k (z_0 - z_1)^{-k} \sum_{l=0}^{\infty} \binom{k+l-1}{l} \xi^l \\
&= \left(a_0 \log(-(z_0 - z_1)) + \sum_{k=1}^{\infty} (-1)^k a_k (z_0 - z_1)^{-k} \right) + \\
&\qquad \sum_{l=1}^{\infty} \left(a_0 l^{-1} (z_0 - z_1)^{-l} + \sum_{k=1}^{\infty} (-1)^k a_k \binom{k+l-1}{l} (z_0 - z_1)^{-(k+l)} \right) (z - z_1)^l.
\end{aligned}$$

Therefore coefficients a_k of ϕ_{z_0} transform to coefficients b_l of ϕ_{C,z_1} by the formula

$$\begin{aligned}
b_0 &= a_0 \log(-(z_0 - z_1)) + \sum_{k=1}^{\infty} (-1)^k a_k (z_0 - z_1)^{-k} \\
b_l &= a_0 l^{-1} (z_0 - z_1)^{-l} + \sum_{k=1}^{\infty} (-1)^k a_k \binom{k+l-1}{l} (z_0 - z_1)^{-(k+l)} \quad l > 0
\end{aligned}$$

Note that FLIP does *not* commute with truncation since one has to know all coefficients $a_0, a_1, \ldots$ to compute $b_0, b_1, \ldots, b_p$ exactly. For more information on the error in case of truncation, see Greengard and Rokhlin (1987).

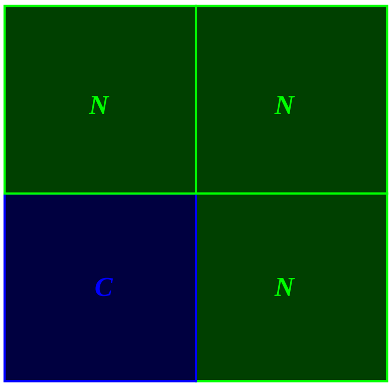

Figure 5: First Level of Quad Tree

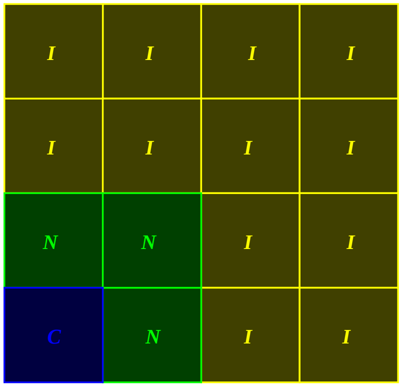

Figure 6: Second Level of Quad Tree

Application on Quad Tree

In this section, we will go through the application of multipole algorithm on quad tree in detail. During the process, we will also look into the two different operations $SHIFT$ and $FLIP$, and gain some experience on how to use them in real situations.

We will start at the lowest level h of the tree. For every node of the tree, it computes the multipole expansion coefficients for the bodies inside, with origin located at the center of the cell. Next, it will shift all of the four centers for the children cells into the center of the parent node, which is at the $h-1$ level, through the SHIFT operation for the multipole expansion. Adding up the coefficients from the four shifted expansion series, the multipole expansion of the whole parent node is obtained. And this SHIFT and ADD process will continue upward for every level of the tree, until the multipole expansion coefficients for each node of the entire tree are stored within that node. The computational complexity for this part is $O(N)$.

Before we go to the next step, some terms have to be defined first.

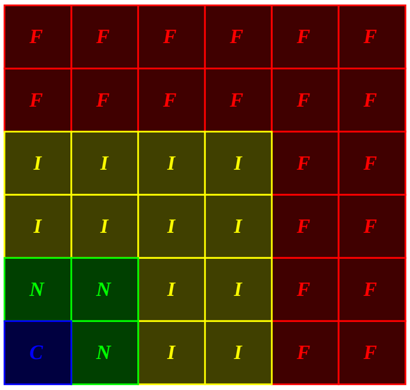

Figure 7: Third Level of Quad Tree

- NEIGHBOR — a neighbor N to a cell C is defined as any cell which shares either an edge or a corner with C
- INTERACTIVE — an interactive cell I to a cell C is defined as any cell whose parent is a neighbor to parent of C, excluding those which are neighbors to C
- FARAWAY — a faraway cell F to a cell C is defined as any cell which is neither a neighbor nor an interactive to C

Now, we start at the top level of the tree. For each cell C, FLIP the multipole expansion for the interactive cells and combine the resulting local Taylor expansions into one expansion series. After all of the FLIP and COMBINE operations are done, SHIFT the local Taylor expansion from the node in this level to its four children in the next lower level, so that the information is conserved from parent to child. Then go down to the next lower level where the children are. To all of the cells at this level, the faraway field is done (which is the interactive zone at the parent level). So we will concentrate on the interactive zone at this level. Repeat the FLIP operation to all of the interactive cells and add the flipped multipole expansion to the Taylor expansion shifted from parent node. Then repeat the COMBINE and SHIFT operations as before. This entire process will continue from the top level downward until the lowest level of the tree. In the end, add them together when the cells are *close* enough.

Expansion from 2-D to 3-D

For 2-D N-body simulation, the potential function is given as

$$\phi(z_j) = \sum_{i=1}^{n} q_i \log(z_j - z_i)$$

where $z_1, \ldots, z_n$ the position of particles, and $q_1, \ldots, q_n$ the strength of particles. The corresponding multipole expansion for the cluster centered at z_c is

$$\phi_{z_c}(z) = a_0 \log(z - z_c) + \sum_{k=1}^{\infty} a_k \frac{1}{(z - z_c)^k}$$

The corresponding local Taylor expansion looks like

$$\phi_{C,z_c}(z) = \sum_{k=0}^{\infty} b_k \frac{1}{(z - z_c)^k}$$

In three dimensions, the potential as well as the expansion series become much more complicated. The 3-D potential is given as

$$\Phi(x) = \sum_{i=1}^{n} q_i \frac{1}{||x - x_i||}$$

where $x = f(r, \theta, \phi)$. The corresponding multipole expansion and local Taylor expansion as following

$$\begin{aligned} \Phi_{multipole}(x) &= \sum_{n=0}^{\infty} \frac{1}{r^{n+1}} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta, \phi) \\ \Phi_{Taylor}(x) &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} r^n b_n^m Y_n^m(\theta, \phi) \end{aligned}$$

where $Y_n^m(\theta, \phi)$ is the *Spherical Harmonic* function. For a more detailed treatment of 3-D expansions, see Nabors and White (1991).

References

[1] J. Barnes and P. Hut. A hierarchical $O(n \log n)$ force calculation algorithm *Nature*, 324 (1986) pp446-449.

[2] L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *J. Comp. Phys.* 73 (1987) pp325-348.

[3] K. Nabors and J. White. A multipole accelerated 3-D capacitance extraction program. *IEEE Trans. Comp. Des.* 10 (1991) v11.