

# Fast Multipole Method

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# Contents

<b>1</b>	<b>Physics Background</b>	<b>2</b>
1.1	Electric potential . . . . .	2
<b>2</b>	<b>Mathematical Preliminaries</b>	<b>3</b>
2.1	multipole expansion . . . . .	3
2.2	Convert multipole expansion into a local expansion . . . . .	6
2.3	Transfer the Center of Multipole and Local Expression . . . . .	7
<b>3</b>	<b>The Fast Multipole Algorithm</b>	<b>10</b>
3.1	2D domain and quadtree . . . . .	10
3.2	The $O(N \log N)$ Algorithm . . . . .	11
3.3	The $O(N)$ Algorithm . . . . .	12
3.4	A Fast Algorithm for Particle Simulations . . . . .	15

# Chapter 1

## Physics Background

### 1.1 Electric potential

In electrodynamics, we can express electric potential in this Poisson's equation

$$\nabla^2\Phi = -\rho/\varepsilon_0 \quad (1.1)$$

If in a region where there are no charges or currents,  $\rho$  will vanish, and the Poisson's equation will become Laplace's equation

$$\nabla^2\Phi = 0 \quad (1.2)$$

Let us consider the electric potential in two dimensional which caused by a point charge. In this situation, the  $\rho$  will be a delta function, and can be expressed in this form

$$\nabla^2\Phi(x, x_0) = \delta(x - x_0) \quad (1.3)$$

And for two dimensional Poisson equation, we have

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \quad (1.4)$$

In order to get the fundamental solutions, we will use polar coordinates and apply the divergence theorem, we can get

$$1 = \int \int \delta(x)dV = \int \int \nabla \cdot (\nabla G)dV = \oint \nabla G \cdot ndl = \oint g'(r)dl = 2\pi Rg'(R) \quad (1.5)$$

So we obtain expression of the electric potential in two dimensional

$$\Phi(x, y) = -\log(\|x - x_0\|) \quad (1.6)$$

Where the target point  $x$  and source point  $x_0$  are defined by

$$x_0 = (x_0, y_0) \quad (1.7)$$

$$x = (x, y) \quad (1.8)$$

Above all, we have finished all the background. And we also want to mention the electric potential in three dimensional. It can be express in this form

$$1 = \int \int \int \delta(x)dV = \int \int \int \nabla \cdot (\nabla G)dV \quad (1.9)$$

$$= \int \int \nabla G \cdot ndS = \int \int g'(r)dS \quad (1.10)$$

$$= 4\pi R^2g'(R) \quad (1.11)$$

So the form of fundamental solution is

$$\Phi = -\frac{1}{\|x - x_0\|} \quad (1.12)$$

## Chapter 2

# Mathematical Preliminaries

In this chapter, we will show all mathematical preliminaries in order to develop a fast algorithm to calculate the expansion

$$\phi(x, y) = -\log(\|x - x_0\|) \quad (2.1)$$

### 2.1 multipole expansion

To begin with the multipole expansion, we first point that the equation

$$\phi(x, y) = -\log(\|x - x_0\|) \quad (2.2)$$

is not a harmonic function because it has singular at the source point, which by the equation

$$\nabla^2 \phi(x, x_0) = \delta(x - x_0) \quad (2.3)$$

But if we consider the region which not included the source point, then this function will be a harmonic function in any region not containing the point  $x_0$ . For every harmonic function  $u$ , there exists an analytic function  $w$ , such that  $u(x, y) = \text{Re}(w(x, y))$  and  $w$  is unique except for an additive constant. In the remainder of the note, we will work with analytic functions, making no distinction between a point  $(x, y) \in \mathbb{R}^2$  and a point  $x + iy = z \in \mathbb{C}$ . So we can rewrite the expression

$$\phi(x) = \text{Re}(-\log(z - z_0)) \quad (2.4)$$

Where  $z$  is the target point and  $z_0$  is the source point.

For a point charge of intensity  $q$  be located at  $z_0$ . Then for any  $z$  such that  $|z| > |z_0|$

$$\phi(x) = q \log(z - z_0) \quad (2.5)$$

And for the electric potential which caused by many charges, we have

$$\phi(z) = \sum_{i=1}^m q_i \log(z - z_i) \quad (2.6)$$

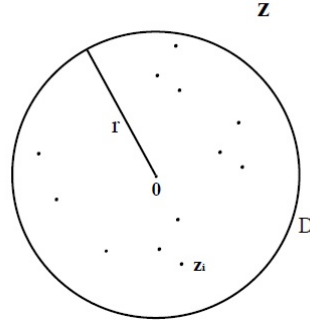
From this equation, we can find that in order to obtain the result, we need to calculate the logarithm which related both source point and target point. This calculate will cost  $N^2$  times float arithmetic. If we want to make calculation fast, we need to find an expression to calculate source point and target point separately.

$$\phi(z) = \sum_i^m q_i \log(z - z_i) \quad (2.7)$$

$$= \sum_i^m q_i \log\left(z \cdot \left(z - \frac{z_i}{z}\right)\right) \quad (2.8)$$

$$= \sum_i^m q_i \log z + \sum_i^m q_i \log\left(1 - \frac{z_i}{z}\right) \quad (2.9)$$

$$= \sum_i^m q_i \log z + \sum_i^m q_i (-1) \sum_{k=1}^{\infty} \frac{1}{k} \left(\frac{z_i}{z}\right)^k \quad (2.10)$$



So we get this multiple expansion.

**Theorem 2.1.** Suppose that  $m$  charges of strengths  $\{q_i, i = 1, \dots, m\}$  are located at points  $\{z_i, i = 1, \dots, m\}$ , with  $|z_i| < r$ . Then for any  $z \in C$  with  $|z| > r$ , the potential  $\phi(z)$  is given by

$$\phi(z) = Q \log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k} \quad (2.11)$$

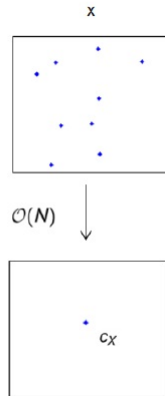
where

$$Q = \sum_{i=1}^m q_i \quad (2.12)$$

and

$$a_k = \sum_{i=1}^m \frac{-q_i z_i^k}{k} \quad (2.13)$$

If we first calculate the coefficient of the expression, which  $Q$  and  $a_k$ , we will find that the expression is only related to the target point. This means that we collect all the source points into one point equivalently. Namely, we finish the step in this picture.



In order to get  $\phi$ , we have to calculate infinite coefficient in the second term. This is impossible, so we need to reconsider this problem. We truncate the polynomial and use an expression to evaluate this truncate as below.

**Theorem 2.2.** If we truncate the second term in the equation 2.11, and only keep first  $p$  term, then the error will be

$$\left| \phi(z) - Q \log(z) - \sum_{k=1}^p \frac{a_k}{z^k} \right| \leq \alpha \left( \frac{r}{p} \right)^{p+1} \leq \left( \frac{A}{c-1} \right) \left( \frac{1}{c} \right)^p \quad (2.14)$$

where

$$c = \left| \frac{z}{r} \right| \quad (2.15)$$

$$A = \sum_{i=1}^m |q_i| \quad (2.16)$$

$$\alpha = \frac{A}{1 - |r/z|} \quad (2.17)$$

Now we give the prove for this theorem.

$$\left| \phi(z) - Q \log(z) - \sum_{k=1}^p \frac{a_k}{z^k} \right| = \left| \sum_{k=p+1}^{\infty} \frac{a_k}{z^k} \right| \quad (2.18)$$

$$= \left| \sum_{k=p+1}^{\infty} \frac{1}{z^k} \cdot \sum_{i=1}^m \frac{(-q_i) z_i^k}{k} \right| \quad (2.19)$$

$$\leq \left| \sum_{k=p+1}^{\infty} \frac{1}{z^k} \cdot \sum_{i=1}^m \frac{(-q_i) r^k}{k} \right| \quad (2.20)$$

$$= \left| \sum_{k=p+1}^{\infty} \frac{r^k}{z^k \cdot k} \sum_{i=1}^m (-q_i) \right| \quad (2.21)$$

$$= A \sum_{k=p+1}^{\infty} \frac{1}{k} \left| \frac{r}{z} \right|^k \quad (2.22)$$

$$\leq A \sum_{k=p+1}^{\infty} \left| \frac{r}{z} \right|^k \quad (2.23)$$

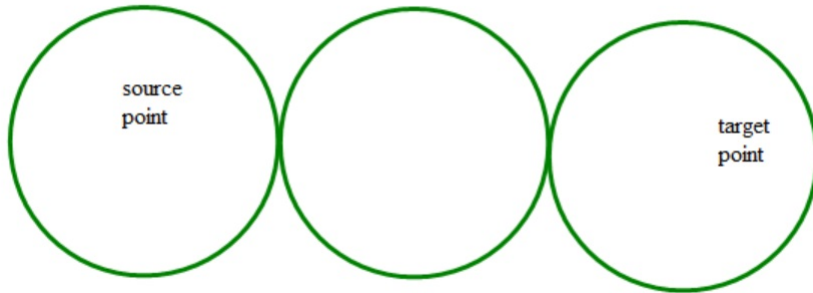
$$= \alpha \left| \frac{r}{z} \right|^{p+1} \quad (2.24)$$

$$= \left( \frac{A}{c-1} \right) \left( \frac{1}{c} \right)^p \quad (2.25)$$

In particular, if  $c \geq 2$ , then

$$\left| \phi(z) - Q \log(z) - \sum_{k=1}^p \frac{a_k}{z^k} \right| \leq A \left( \frac{1}{2} \right)^p \quad (2.26)$$

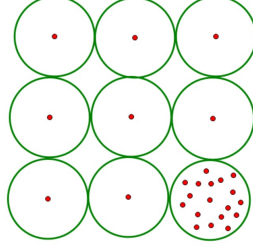
Now I want to talk about what is the meaning of this equation. As I mentioned before, this fast multipole method will have a certain error band. In order to accelerate calculation, we need truncate the polynomial, and it will bring a error band into our calculation. So the calculation step is as follow, first, according the problem, we decide what precision we need in the calculation; then, bring this precision into the equation 2.26, we can get from which term we need to truncate the polynomial; after this, we can calculate the equation 2.11.



Next, I want to talk about what  $c = 2$  means. From the theorem, we find  $c = z/r$ , and we get  $z = 2r$ . It means that we can only use truncate to the points which source points and target points have a distance larger than  $2r$ ; and for those points which distance smaller than  $2r$ , we cannot use this truncate, and we need calculate them directly. In the other words, we can use truncate for the interaction between left region and right region, but we cannot use truncate for the interaction between central region and right region. If we want to calculate the interaction between central region and right region, we have to directly or use other ways to calculate them.

## 2.2 Convert multipole expansion into a local expansion

Suppose the source region have been divided into several subregion, and for each subregion we have collect all source points into one source point equivalently. At this time, for every subregion, there is one equivalent point in it, we denote the number of the total equivalent points (= the number of the total subregion)  $N'$ . We can find that if we direct calculate the electric potential between equivalent points and the target points, we need  $N' \times N$  float arithmetic. This is also an  $N^2$  float arithmetic. If the number of subregion is extreme huge, this calculation is also very time consuming. So we need to find some steps to further reduce the flout arithmetic.



In order to further reduce the float arithmetic, we find an expression which convert multipole expansion into a local expansion. This local expansion describes the interaction for any target points in a circular region, which caused by all the source points outside the circular region.

This theorem described as below.

**Theorem 2.3.** *Suppose that  $m$  charges of strengths  $q_1, q_2, \dots, q_m$  are located inside the circle  $D_1$  with radius  $R$  and center at  $z_0$ , and that  $|z_0| > (c+1)R$  with  $c > 1$ . Then the corresponding multipole expansion, which is*

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k} \quad (2.27)$$

converges inside the circle  $D_2$  of radius  $R$  centered about the origin. Inside  $D_2$ , the potential due to the charges is described by a power series:

$$\phi(z) = \sum_{l=0}^{\infty} b_l \cdot z^l \quad (2.28)$$

where

$$b_0 = \sum_{k=1}^{\infty} \frac{a_k}{z_0^k} (-1)^k + a_0 \log(-z_0) \quad (2.29)$$

and

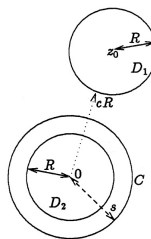
$$b_l = \left( \frac{1}{z_0^l} \sum_{k=1}^{\infty} \frac{a_k}{z_0^k} \binom{l+k-1}{k-1} (-1)^k \right) - \frac{a_0}{l \cdot z_0^l} \quad \text{for } l \geq 1 \quad (2.30)$$

Furthermore, for any  $p \geq \max(2, 2c/(c-1))$ , an error bound for the truncated series is given by

$$\left| \phi(z) - \sum_{l=0}^p b_l \cdot z^l \right| < \frac{A(4e(p+c)(c+1) + c^2)}{c(c-1)} \left( \frac{1}{c} \right)^{p+1} \quad (2.31)$$

where  $e$  is the base of natural logarithms.

The theorem can be shown as following picture.



In here, we only give simple prove for the equation 2.28 , and for the prove of the error bound, people can refer ” A Fast Algorithm for Particle Simulations ”. We can get equation 2.28 by using these two expressions

$$\log(z - z_0) = \log\left(-z_0 \left(1 - \frac{z}{z_0}\right)\right) \quad (2.32)$$

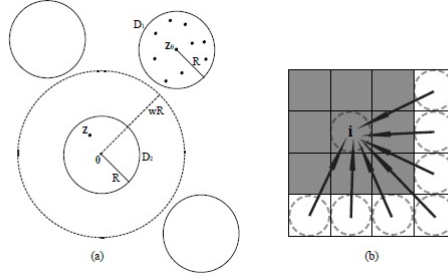
$$= \log(-z_0) - \sum_{l=1}^{\infty} \frac{1}{l} \left(\frac{z}{z_0}\right)^l \quad (2.33)$$

and

$$(z - z_0)^{-k} = \left(\frac{1}{-z_0}\right)^k \left(\frac{1}{1 - \frac{z}{z_0}}\right)^k \quad (2.34)$$

$$= \left(\frac{1}{-z_0}\right)^k \sum_{l=0}^{\infty} \binom{l+k-1}{k-1} \left(\frac{z}{z_0}\right)^l \quad (2.35)$$

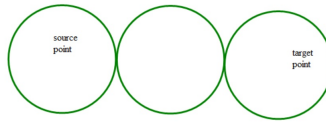
After doing this, we have convert the multipole expression into a local expression, which is, we convert the expression which describe the interaction of any target points outside the source points circle to the expression which describe the interaction of any target point inside the target points circle. After we get this expression, we can calculate all the interaction of the target point by substituting the target point coordinate  $z$  into the expression. However, in order to make further development, after we get the expression, we do not directly substitute coordinate  $z$  to get the interaction.



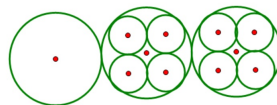
In the above pictures, Fig.(a) shows that the multipole expansion about region  $D_1$  can be converted to a local expansion about the regio  $D_2$ . Fig.(b) shows the similar behavior of the quad tree structure.

### 2.3 Transfer the Center of Multipole and Local Expression

As we mentioned before, in the below picture, we can only calculate the potential between left region and right region, and we cannot calculate the potential between central region and right region due to the limit  $c = 2$ . If central region has many source points, it will cost huge float arithmetic. So we need to find a way to calculate the interaction between central region and right region.



The way is that we divided the central region and right region, and use the subregion (which keep  $c = 2$  conditions) to calculate interaction.



As above picture shows, we divided central region and right region into subregions, for every subregion, the radius become small and the condition ( $c = 2$ ) may be fitted for several subregion. Then, we can calculate the interaction between these subregions and leave those subregion which not fit the conditions ( $c = 2$ ) uncalculated. We can repeat these step until the left subregion is very small and only few points in it, then we will calculate



these left subregion directly.

So the next step is to find the expression divided region. We will show that, the desired expression is very simple and we only need to transfer the center of the multipole expansion and local expression.



The next theorem provides a formula for shifting the center of a multipole expansion.

**Theorem 2.4.** *Suppose that*

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k} \quad (2.36)$$

is a multipole expansion of the potential due to a set of  $m$  charges of strengths  $q_1, q_2, \dots, q_m$ , all of which are located inside the circle  $D$  of radius  $R$  with center at  $z_0$ . Then for  $z$  outside the circle  $D_1$  of radius  $(R + |z_0|)$  and center at the origin,

$$\phi(z) = a_0 \log(z) + \sum_{l=1}^{\infty} \frac{b_l}{z^l} \quad (2.37)$$

where

$$b_l = \left( \sum_{k=1}^l a_k z_0^{l-k} \binom{l-1}{k-1} \right) - \frac{a_0 z_0^l}{l} \quad (2.38)$$

with  $\binom{l}{k}$  the binomial coefficients. Furthermore, for any  $p \geq 1$ ,

$$\left| \phi(z) - a_0 \log(z) - \sum_{l=1}^p \frac{b_l}{z^l} \right| \leq \left( \frac{A}{\left(1 - \frac{|z_0|+R}{|z|}\right)} \right) \cdot \left| \frac{|z_0|+R}{z} \right|^{p+1} \quad (2.39)$$

This theorem can be proved by using these two equations.

$$\log(z - z_0) = \log \left( z \left( 1 - \frac{z_0}{z} \right) \right) = \log(z) - \sum_{l=1}^{\infty} \frac{1}{l} \left( \frac{z_0}{z} \right)^l \quad (2.40)$$

and

$$(z - z_0)^{-k} = \sum_{l=k}^{\infty} \binom{l-1}{k-1} \frac{z_0^{l-k}}{z^l} \quad (2.41)$$

Once the values  $\{a_0, a_1, \dots, a_p\}$  in the expansion 2.36 about  $z_0$  are computed, we can obtain  $\{b_1, b_2, \dots, b_p\}$  exactly by 2.38. In the other words, we may shift the center of a truncate multipole expansion without any loss of precision.

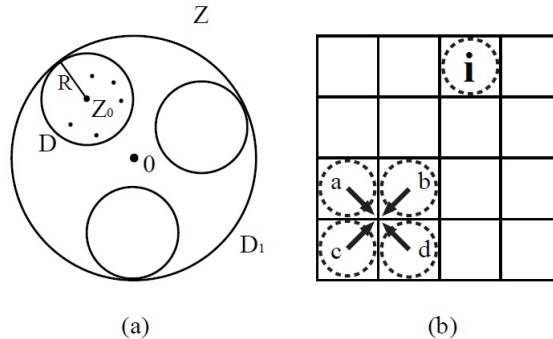


Fig.(a) shows that the multipole expansion about child subregion  $D$  can be translated to the multipole expansion about the parent region  $D_1$ . Fig.(b) shows the similar behavior of the quadtree structure.

**Observation 2.1.** *Suppose that we have created the multipole expansion for each of the four children of some box in the mesh hierarchy. We would like to form a single expansion for the parent box without re-examining each particle. This theorem provides just such a mechanism at the cost of  $4p^2$  operations, since each shift requires  $p^2$  work.*

After this theorem, we will introduce a mechanism for shifting the center of a Taylor expansion within a region of analyticity. This following theorem is an immediate consequence of Maclaurin's theorem. It describes an exact translation operation with an finite number of terms, and no error bound is needed.

**Theorem 2.5.** For any complex  $z_0, z$  and  $\{a_k\}$ ,  $k = 0, 1, 2, \dots, n$ ,

$$\sum_{k=0}^n a_k (z - z_0)^k = \sum_{l=0}^n \left( \sum_{k=l}^n a_k \binom{k}{l} (-z_0)^{k-l} \right) \cdot z^l \quad (2.42)$$

This theorem means that translation of a complex polynomial centered about  $z_0$

$$\sum_{k=0}^p a_k (z - z_0)^k \quad (2.43)$$

into a complex polynomial centered about origin

$$\sum_{k=0}^n b_k z^k \quad (2.44)$$

can be achieved by the complete Horner scheme in the following:

```

1  for j from 0 to p-1 do
2      for k from p-j-1 to p-1 do
3           $a_k := a_k - z_0 * a_{k+1}$ 
4      end
5  end

```

which given the vector of coefficients  $a$  overwrites it with  $b$ . This is Horner calculation algorithm, and for people who not familiar with it, we refer reader to read related papers.

**Observation 2.2.** Suppose that we have a local expansion for a box  $b$  which describes the field induced by all particles outside  $b$ 's nearest neighbors. We would like to transmit this information to  $b$ 's children. This theorem provides just such a mechanism at the cost of  $4p^2$  operations, since each shift requires  $p^2$  work.

Now we have finished this chapter and we will introduce the fast multipole algorithm in the next chapter.

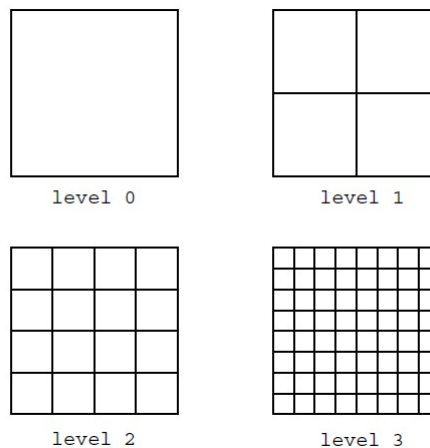
# Chapter 3

## The Fast Multipole Algorithm

### 3.1 2D domain and quadtree

As we mentioned before, if we want to calculate the potential between central region and right region, we need divide central region and right region, then use the subregion to calculate. In order to do this, it is natural rise to talk about the space division.

First, we introduce the level of the quadtree. The level shows as below.

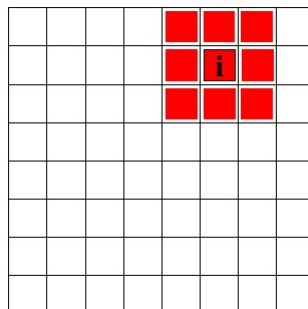


For each parent box, we divided it into four children subboxes in the next level. The number of level will be determined by how many points we want to directly calculate.

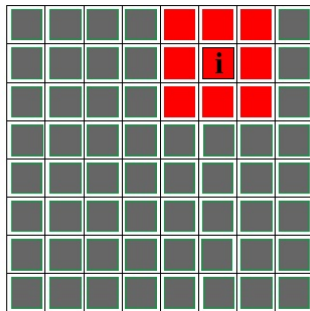
Next we want to introduce the definition of near neighbour box, well-separated box and interaction list box.

**Definition 3.1** (Near Neighbour). *Two boxes are said to be near neighbors if they are at the same refinement level and share a boundary point. A box is a near neighbor of itself.*

The near neighbor boxes is shown below in red color as an example.



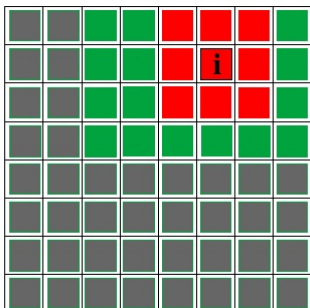
**Definition 3.2** (well separated). *Two boxes are said to be well separated if they are at the same refinement level and are not near neighbors.*



The well separated boxes is shown below in grey color as an example.

**Definition 3.3** (interaction list). *Each box  $i$  has its own interaction list, consisting of the children of the near neighbors of  $i$ 's parent which are well separated from box  $i$ .*

The interaction list boxes is shown below in green color as an example.



After this, we have divided a region into near neighbor region, well separated region and interaction list region.

## 3.2 The $O(N \log N)$ Algorithm

This algorithm is a typical  $N \log N$  quadtree algorithm, and it do not use our theorem which introduced in chapter two, in the next section, I will improve this algorithm into  $N$  with the help of the theorem introduced in chapter two.

The quadtree is a typical fast calculation algorithm. We introduce a hierarchy of boxes which refine the computational domain into smaller and smaller regions. At refinement level 0, we have the entire computational domain. Refinement level  $l+1$  is obtained recursively from level  $l$  by subdivision of a box at level  $l$  are considered its children.

In order to make description clear, we also define near neighbor region, well separated region and interaction list region.

The basic idea is to consider cluster of particles at successive levels of spatial refinement, and to compute interactions between distant clusters by means of multipole expansions when possible. It is clear that at levels 0 and 1, there are no pairs of boxes which are well separated. At level 2, on the other hand, 16 boxes have been created and there are a number of well separated pairs. Multipole expansions can then be used to compute interactions between these well separated pairs with rigorous bounds on the error. In fact, the bound equation 2.26 is valid so that given a precision  $\epsilon$ , we need to use  $p = \log_2(1/\epsilon)$  terms.

It remains to compute the interactions between particles contained in each box with those contained in the box's near neighbors, and this is where recursion enters the picture. After each level 2 box is refined to create level 3, we seek to determine which other boxes can be interacted with by means of multipole expansions. But notice that those boxes outside the region of the parent's nearest neighbors are already accounted for (at level 2) and that interactions with current near neighbors cannot accurately be computed by means of an expansion. The remaining boxes correspond exactly to the interaction list defined above.

The nature of the recursion is now clear. At every level, the multipole expansion is formed for each box due to the particles it contains. The resulting expansion is then evaluated for each particle in the region covered by its interaction list.

We halt the recursive process after roughly  $\log N$  levels of refinement. The amount of work done at each level is of the order  $O(N)$ . To see this, note first that approximately  $Np$  operations are needed to create all expansions, since each particle contributes to  $p$  expansion coefficients. Secondly, from the point of view of a single particle, there are at most 27 boxes (the maximum size of the interaction list) whose expansions are computed, so that  $27Np$  operations are needed for all evaluations.

At the finest level, we have created roughly  $4^{\log_4 N} = N$  boxes and it remains only to compute interactions between nearest neighbors. By the assumption of homogeneity, there are  $O(1)$  particles per box, so that this last step requires about  $8N$  operations. The total cost is approximately

$$28Np \log(N) + 8N \tag{3.1}$$

### 3.3 The $O(N)$ Algorithm

Above we have shows the  $O(N \log N)$  algorithm to calculate multipole expansion, and How to improve it into a  $O(N)$  algorithm?

The difference in performance can be seen as arising from the fact that each point must be visited at each level of the tree structure, both to create a box's series expansion and evaluate the expansion from each well separated box. If we could instead visit only every box at each level, caching sufficient information about the expansion, we would require only  $O(N)$  operations.

So the improvement can be achieved in two aspects. The first is in computing the source expansion — naively, we compute moments for each box  $b$  by evaluating a sum  $N_b$  ( $N_b$  is the particle number in box  $b$ ) terms. We may avoid this by designing a means of converting the finer scale's moment expansions to an expansion at the next coarser scale. The second is in evaluating at the target locations. We would like to accumulate terms from several source boxes and combine them so that they may be evaluated at the target only once. This requires two things — a translation of several expansions' origins to a common point (enabling them to be summed), typically the target box center, and a translation of an expansion about the target box center to expansions about each of its subregions ( enabling expansions from different levels to be combined easily). These required expansions are there theorems which we have told in chapter two.

Now we will show the outline of the  $O(N)$  algorithm.

```

1 Initialization
2 Choose a number of levels so that there are, on average,  $s$  particles per box at the
   finest level. (The number of boxes is then approximately  $N/s$ .)
3 Upward Pass
4 In the NlogN scheme, we proceeded from the coarsest to the finest level, forming
   multipole expansions for every box. In the FMM, we begin at the finest level, and
   create multipole expansions from the source positions and strengths. The expansions
   for all boxes at all higher levels are then formed by the merging procedure
   delineated in Observation 1.
5 Downward Pass
6 In the NlogN scheme, whenever a box  $b$  was under consideration, we used its multipole
   expansion to compute interactions with all particles contained in the boxes of  $b$ 's
   interaction list. In the FMM, we convert the multipole expansion into a local
   expansion about the center of all boxes in  $b$ 's interaction list.
7
8
9 After these calculations are completed, we are left with a local expansion in each box
   at each level. Beginning at the coarsest level, these local expansion are shifted
   to the children's level and added to the children's local expansions, as described
   in Observation 2. After this recursive process reaches the finest refinement level,
   a local expansion will have been created for each box which describes the field
   due to all particles outside the box's near neighbors. It is only this expansion
   which is evaluated. The near neighbor interactions, as before, are computed
   directly.

```

And we can approximately estimate the total operation is

$$Np + 29 \left( \frac{N}{s} \right) p^2 + Np + 9Ns \tag{3.2}$$

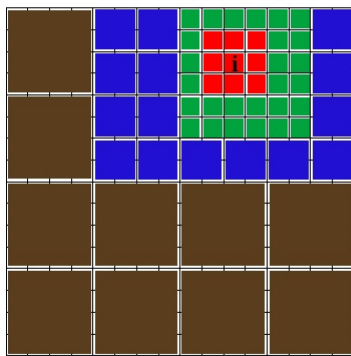
This equation correspond to formation of the multipole expansion, shifting the expansions, evaluation of the local expansions and computation of the near neighbor interaction.

Now we will show this scheme more details and use 5 levels for example to illustrate. First, I will show some notation used in the description of the algorithm include

- \*  $P_{i,nnb}^l$ : the potential due to the particles inside of  $i$ 's near neighbor
- \*  $P_{i,list}^l$ : the potential due to the particles inside of  $i$ 's interaction list
- \*  $P_{i,out}^l$ : the potential due to the particles outside of  $i$ 's parent's near neighbors, which can be computed recursively
- \*  $P_{j,list}^{l-1}$ :  $j$  is the parent box of box  $i$
- \*  $P_{k,list}^{l-2}$ :  $k$  is the grandparent box of box  $i$

The definition we can see in below picture.

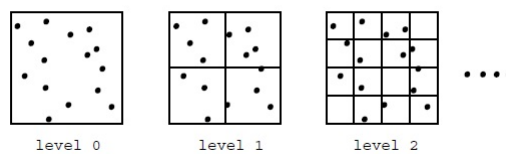
Notice:  $P_{x,S}^\ell$  is the potential (Local Expansion) centered around  $x$ , due to the particles set  $S$ .



- $P_{i,nnb}^\ell$ : the potential due to the particles inside of  $i$ 's **near neighbors**.
- $P_{i,list}^\ell$ : the potential due to the particles inside of  $i$ 's **interaction list**.
- $P_{i,out}^\ell$ : the potential due to the particles outside of  $i$ 's parent's near neighbors, which can be computed recursively.
- $P_{j,list}^{\ell-1}$ :  $j$  is the **parent box** of box  $i$ .
- $P_{k,list}^{\ell-2}$ :  $k$  is the **grandparent box** of box  $i$ .

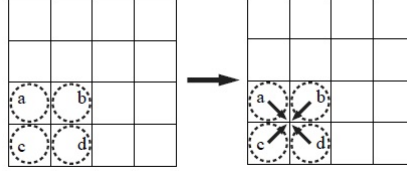
And the initialization we will do these steps.

- \* Given  $N$  particles distributed in a square domain.
- \* Construct a quadtree with  $L + 1$  levels.
- \* The indices of levels will be  $0, 1, 2, \dots, L - 1, L$ .
- \* Assume that, on average,  $s$  particles per box in the finest level.
- \*  $4^l \cdot s = N$ , or equivalently,  $L = \log_4(N/s)$ .



Next we will do upward pass process:

- \* Start with the finest level, construct multipole expansions for each box
- \* Translate the multipole expansion to coarser levels.
- \* The multipole expansion about every box in the coarser levels will be constructed by the merging procedure.



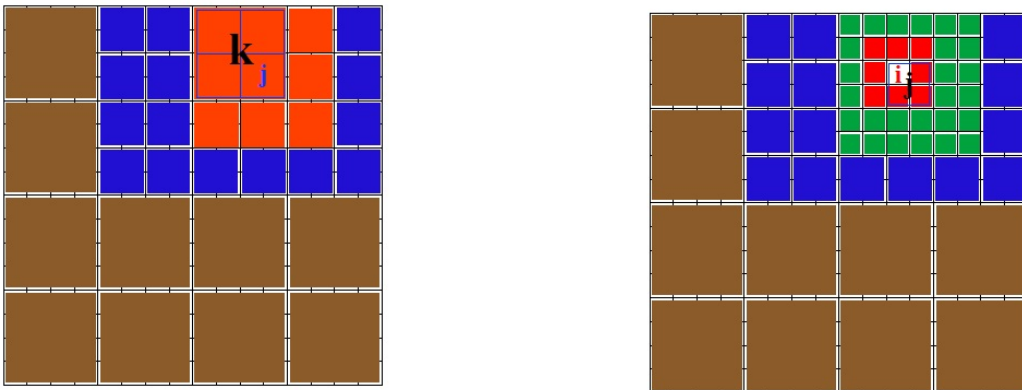
And then, for the downward pass process.

- \* Start with the coarsest level, in fact, level 2, where each box  $k$  has its interaction list. Construct the local expansions  $P_{k,list}^2$ .
- \* Repeat this for every finer level. For simplicity, assume finest level  $L = 4$ .
- \* Let box  $i$  at level 4 be the target. We already have  $P_{i,list}^4$ ,  $P_{j,list}^3$ ,  $P_{k,list}^2$ , where  $j$  is the parent of  $i$ , and  $k$  is the parent of  $j$ .
- \* Start with the coarsest level again, translate the local expansion from the parent to its children.
- \*

$$P_{k,list}^2 \Rightarrow P_{j,out}^3 \quad (3.3)$$

$$P_{j,out}^3 + P_{j,list}^3 \Rightarrow P_{i,out}^4 \quad (3.4)$$

- \* Finally,  $P_{i,out}^4 + P_{i,list}^4 + P_{i,nnb}^4$  will be the total potential centered at  $i$  due to all the other particles.



This picture show the region for level 3 and level 4, and the finally potential can be expressed as follow:

$$P_{i,out}^4 + P_{i,list}^4 + P_{i,nnb}^4 \quad (3.5)$$

Now we show the cost of FMM.

For Upward Pass.

- \* In the finest level, to form the multipole expansion centered at each box, we need about  $Np$  operations, where  $p$  is the number of terms in the multipole expansion.
- \* Then for the translations for the higher levels, we need about  $(\frac{N}{s})p^2$  operations, where  $s$  is the average number of particles in each box of the finest level.

and

For Downward Pass.

- \* To convert the multipole expansions about all boxes in the interaction list of each box in an arbitrary level, we need about  $27(\frac{N}{s})p^2$  operations.
- \* Then for the translations from the parent to its children, we need about  $(\frac{N}{s})p^2$  operations.
- \* For the evaluation of a local expansion in the finest level and computing potential directly from the near neighbor, we need about  $Np$  and  $9Ns$  respectively.

Totally, the cost of FMM is

$$Np + (\frac{N}{s})p^2 + 27(\frac{N}{s})p^2 + (\frac{N}{s})p^2 + Np + 9Ns \quad (3.6)$$

### 3.4 A Fast Algorithm for Particle Simulations

Now we will show the program in details and analysis time complexity in details. The algorithm is offered by L.Greengard and V.Rokhlin "A Fast Algorithm for Particle Simulations" P.334 — P.339.

First, in order to show problem more clear, we redefine the region and notation of the algorithm.

We introduce a hierarchy of meshes which refine the computational box into smaller and smaller regions. Mesh level 0 is equivalent to the entire box, while mesh level  $l + 1$  is obtained from level  $l$  by subdivision of each region into four equal parts. The number of the distinct boxes at mesh level is equal to  $4^l$ . A tree structure is imposed on this mesh hierarchy, so that if  $ibox$  is a fixed box at level  $l$ , the four boxes at level  $l + 1$  obtained by subdivision of  $ibox$  are considered its children.

And the notation defined by

**Definition 3.4.**  $\Phi_{l,i}$  denote the  $p$ -term multipole expansion (about the box center) of the potential field created by the particles contained inside box  $i$  at level  $l$

**Definition 3.5.**  $\Psi_{l,i}$  denote the  $p$ -term local expansion about the center of box  $i$  at level  $l$ , describing the potential field due to all particles outside the box and its nearest neighbors.

**Definition 3.6.**  $\tilde{\Psi}_{l,i}$  denote the  $p$ -term local expansion about the center of box  $i$  at level  $l$ , describing the potential field due to all particles outside  $i$ 's parent box and the parent box's nearest neighbors.

Suppose now that at level  $l - 1$ , the local expansion  $\Psi_{l-1,i}$  has been obtained for all boxes. Then, by using Theorem 2.5 to shift (for all  $i$ ) the expansion  $\Psi_{l-1,i}$  to each of box  $i$ 's children, we have, for each box  $j$  at level  $l$ , a local representation of the potential due to all particles outside of  $j$ 's parent's neighbors, namely  $\tilde{\Psi}_{l,j}$ . The interaction list is, therefore, precisely that set of boxes whose contribution to the potential must be added to  $\tilde{\Psi}_{l,j}$  in order to creat  $\Psi_{l,j}$ . This is done by using Theorem 2.3 to convert the multipole expansions of these interaction boxes to local expansions about the current box center and adding them to the expansion obtained from the parent. Note also that with free-space boundary conditions,  $\Psi_{0,i}$  and  $\Psi_{1,i}$  are equal to zero since there are no well-separated boxes to consider, and we can begin forming local expansion at level 2.

The following is the formal description of the algorithm.

#### Initialization

Choose a level of refinement  $n \approx \log_4 N$ , a precision  $\varepsilon$ , and set  $p \approx \log_2(\varepsilon)$ .

#### Upward Pass



## Step One

```
1
2   Comment 3.1. Form multipole expansions of potential field due to particles in each box about the box center at
3   the finest mesh level
4   do ibox=1,...,4n
5     Form a p-term multipole expansion  $\Phi_{n,ibox}$ , by using Theorem 2.1 .
6   enddo
```

**Remark 3.1.** Each particle contributes to one expansion at the finest level. In order to calculate first  $p$ -term  $a_k$  in theorem 2.3, we need  $p$  complexity for each particle. Therefore, the total complexity of this step is  $Np$ .

## Step Two

```
1
2   Comment 3.2. Form multipole expansions about the centers of all boxes at all coarser mesh levels, each
3   expansion representing the potential field due to all particles contained in one box
4   do l = n - 1, ..., 0
5     do ibox=1,...,4l
6       Form a p-term multipole expansion  $\Phi_{l,ibox}$ , by using Theorem 2.4 to shift the center
7       of each child box's expansion to the current box center and adding them
8       together .
9     enddo
10  enddo
```

**Remark 3.2.** In this step, the total complexity is  $Np^2$ . At the  $l$ th level,  $4^l$  shifts involving order  $p^2$  work per shift must be performed.

### Downward Pass

## Step Three

```
1
2   Comment 3.3. Form a local expansion about the center of each box at each mesh level  $l \leq n - 1$ . This local
3   expansion describes the field due to all particles in the system that are not contained in the current box or its nearest
4   neighbors. Once the local expansion is obtained for a given box, it is shifted, in the second inner loop to the centers of
5   the box's children, forming the initial expansion for the boxes at the next level.
6   Set  $\tilde{\Psi}_{1,1} = \tilde{\Psi}_{1,2} = \tilde{\Psi}_{1,3} = \tilde{\Psi}_{1,4} = (0, \dots, 0)$ 
7   do l = 1, ..., n-1
8     do ibox = 1, ..., 4l
9       Form  $\Psi_{l,ibox}$  by using Theorem 2.3 to convert the multipole expansion  $\Phi_{l,j}$  of each
10      box j in interaction list of box ibox to a local expansion about the center
11      of box ibox, adding these local expansions together, and adding the result
12      to  $\tilde{\Psi}_{l,ibox}$  .
13    enddo
14    do ibox = 1, ..., 4l
15      Form the expansion  $\tilde{\Psi}_{l+1,j}$  for ibox's children by using 2.5 to expand  $\Psi_{l,ibox}$  about
16      the children's box centers .
17    enddo
18  enddo
```

**Remark 3.3.** There are at most 27 entries in the interaction list for each box at each level. An extra order  $Np^2$  work is required for the second loop. The total complexity is  $28Np^2$ .

## Step Four

```
1
2   Comment 3.4. Compute interactions at finest mesh level
```

```

2 do  $ibox = 1, \dots, 4^n$ 
3   Form  $\Psi_{l,ibox}$  by using Theorem 2.3 to convert the multipole expansion  $\Phi_{l,j}$  of each box
   j in interaction list of box  $ibox$  to a local expansion about the center of box
    $ibox$ , adding these local expansions together, and adding the result to  $\tilde{\Psi}_{l,ibox}$ .
4 enddo

```

**Remark 3.4.** *There are at most 27 entries in the interaction list for each box and  $\approx N$  boxes. The total complexity is  $27Np^2$ .*

## Step Five

```

1
   Comment 3.5. Evaluate local expansions at particle positions.
2 do  $ibox = 1, \dots, 4^n$ 
3   For every particle  $p_j$  located at the point  $z_j$  in box  $ibox$ , evaluate  $\Phi_{n,ibox}(z_j)$ .
4 enddo

```

**Remark 3.5.** *One  $p$ -term expansion is evaluated for each particle.*

## Step Six

```

1
   Comment 3.6. Compute potential due to nearest neighbors
2 do  $ibox = 1, \dots, 4^n$ 
3   For every particle  $p_j$  located at the point  $z_j$  in box  $ibox$ , evaluate  $\Phi_{n,ibox}(z_j)$ .
4 enddo

```

**Remark 3.6.** *Let  $k_n$  be a bound on the number of particles per box at the finest mesh level. Interactions must be computed within the box and its eight nearest neighbors, but using Newton's third law, we need only compute half of the pairwise interactions. The total complexity is  $\frac{9}{2}Nk_n$ .*

## Step Seven

```

1 do  $ibox = 1, \dots, 4^n$ 
2   For every particle in box  $ibox$ , add direct and far-field terms together.
3 enddo

```

**Remark 3.7.** *Adding two terms for each particle. The total complexity is  $N$ .*

$$s = 1 \tag{3.7}$$

$$= 2 \tag{3.8}$$