Harmonic Functions, Multipole Expansions, and the Fast Multipole Method

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1 Abstract

This paper explores the critical complex analysis tools for understanding the theory of harmonic potential functions, multipole expansions, and the Fast Multipole Method. Harmonic functions are vital in the study of numerous areas of physics, such as electromagnetism, gravitation, and fluid mechanics. We specifically delve into the theory of harmonic potentials in electrostatics, and by leveraging complex analysis, we can generate multipole expansions to discretize potential fields, allowing for efficient approximation of field values over spatial domains. We demonstrate the use of the multipole expansion by implementing the Fast Multipole Method and dive into the theoretical underpinnings of this method.

2 Attribution

Jaden worked on the introduction and mathematical formulation, Sudarshan worked on the mathematical formulation as well as conclusions and extensions, Kashyap worked on the the algorithm and conclusions and extensions.

3 Introduction

The study of potential fields generated by electrical charges or gravitational masses is central to many applications in physics and engineering. This paper focuses on the application of complex analysis to explore harmonic functions and multipole expansions, providing significant computational advancements through the Fast Multipole Method (FMM).

Harmonic functions offer an insight into potential theory as solutions to Laplace's equation. These functions represent the potential fields in various domains such as electrostatics and gravitational fields. Our exploration delves into the properties of these functions, utilizing complex analysis to explain their behavior and implications in physical systems.

Moreover, multipole expansions are integral for expressing potential fields with efficiency and accuracy. By decomposing a field into a series of simpler hierarchical terms, these expansions streamline the computation of interactions in large-scale simulations. Complex analysis plays a critical role in deriving and manipulating these expansions, which are pivotal in representing fields at various scales efficiently. This facilitates the handling of complex interactions in simulations involving large numbers of charges or masses, thereby reducing computational costs and improving accuracy.

The Fast Multipole Method dramatically improves the computation speed of interactions among large numbers of particles. We explain the mathematical foundation of FMM and its derivation from multipole expansions, showcasing its capability to reduce the computational complexity from $\mathcal{O}(n^2)$ to $\mathcal{O}(n \log n)$ or in special cases $\mathcal{O}(n)$. This method exemplifies the powerful application of complex analysis in transforming computational approaches to large-scale problems.

Through detailed mathematical formulations and practical implementations, this paper aims to illustrate the versatility and efficiency of complex analysis in tackling fundamental challenges in scientific computing. We provide examples, discuss potential enhancements, and demonstrate the broad applicability of these mathematical tools in solving complex physical problems.

The relevance of these techniques extends beyond theoretical applications to practical solutions in areas such as aerospace engineering, meteorological simulations, and the design of electronic devices. The ability to accurately predict and manipulate potential fields can lead to advancements in satellite technology, weather forecasting, and the miniaturization of electronic components. By applying complex analysis to these fields, we open up possibilities for new technologies and improvements in existing systems.

4 Mathematical Formulation

4.1 Legendre Polynomials

Before covering the relationship between the complex analysis of multipole expansion and Coulomb potential, it is vital to understand Legendre polynomials. A Legendre polynomial denoted as $P_n(x)$ is a specific set of orthogonal polynomials that are solutions to Legendre's differential equation

$$(1-x^2)\frac{d^2P_n(x)}{dx^2} - 2x\frac{dP_n(x)}{dx} + n(n+1)P_n(x) = 0$$

In the context of multipole expansion of Coulomb potential, Legendre polynomials arise when expressing the inverse distance between two points in terms of a power series.

4.2 Rodrigues Formula

Rodrigues' formula provides a systematic method for generating sequences of orthogonal polynomials that become useful in problems related to series expansions, as seen below. The formula ensures that each polynomial in the sequence satisfies orthogonality conditions for a given weight function over an interval.

The formula is derived as follows:

Let $(P_n(x))_{n=0}^{\infty}$ be a sequence of orthogonal polynomials on the interval $[a, b]$ satisfying the condition

$$\int_a^b P_m(x)P_n(x)w(x)\,dx = K_n\delta_{m,n},$$

with $w(x)$ being weight function, K_n is a constant, and $\delta_{m,n}$ represents the Kronecker delta. If the weight function $w(x)$ satisfies the Pearson's differential equation,

$$\frac{w'(x)}{w(x)} = \frac{A(x)}{B(x)},$$

where $A(x)$ is a linear expression or a constant and $B(x)$ is at most a quadratic. The limit of the weight function multiplied by $B(x)$ as x approaches the endpoints of the interval must go to 0,

$$\lim_{x\to a} w(x)B(x) = 0, \qquad \lim_{x\to b} w(x)B(x) = 0.$$

Then it can be shown that $P_n(x)$ can be represented as,

$$P_n(x) = \frac{c_n}{w(x)}\frac{d^n}{dx^n}\left[B(x)^n w(x)\right],$$

for some constants c_n. This relation is called Rodrigues' formula and will be useful in our application of multipole expansions to coulomb potentials[1].

4.3 Coulomb Potentials as Multipole Expansions

The crux of the multi-pole expansion in the application to the Coulomb potential relies on the expansion of

$$\frac{1}{|R-r|} = \frac{1}{\sqrt{R^2+r^2-2Rrcos\theta}} \tag{1}$$

into a power series in $\frac{r}{R}$ for $r << R$ taking $x = \cos(\theta)$. This expansion results in

$$\frac{1}{\sqrt{R^2 + r^2 - 2Rrcos\theta}} = \sum_{n=0}^{\infty} \frac{r^n}{R^{n+1}} \times P_n(cos\theta)$$

where $P_n(x)$ is a Legendre polynomial of degree n.

The proof of this expansion using the Rodrigues formula for the Legendre polynomials utilizes the residue method for contour integration in the complex plane. Starting with the Rodrigues formula for the Legendre polynomials

$$(c_n = \frac{1}{2^n n!}, B(x) = x^2 - 1, w(x) = 1)$$

,

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2 - 1)^n$$

. One can recognize that this formula represents the residue of an $n + 1$ order pole of a function $g(z) = \frac{f(z)}{(z-x)^{n+1}}$. Working backwards, the Legendre polynomials can be represented as

$$P_n(x) = \frac{1}{2^n} \oint_\Gamma \frac{dz}{2\pi i} \frac{(z^2 - 1)^n}{(z - x)^{n+1}}$$

for a contour Γ that encloses the pole at $z = x$.

Substituting the contour integral into equation (2) yields

$$\frac{1}{\sqrt{R^2 + r^2 - 2Rrcos\theta}} = \sum_{n=0}^{\infty} \frac{r^n}{R^{n+1}} \times P_n(\cos\theta) \tag{2}$$

$$= \sum_{n=0}^{\infty} \frac{r^n}{2^n R^{n+1}} \oint_\Gamma \frac{dz}{2\pi i} \frac{(z^2 - 1)^n}{(z - x)^{n+1}}. \tag{3}$$

Here, we can switch the integral and the sum because the sum converges uniformly. We can prove the sum is uniformly convergent by using the Weierstrass M-test. First, it is important to not that the Legendre polynomials $P_n(\cos\theta)$ are bounded for all n because they are continuous on the interval $[-1, 1]$ ($\cos\theta \in [-1, 1]$). This leads to the estimate of the terms of the series as follows:

$$|\frac{r^n}{R^{n+1}} P_n(cos\theta)| \leq \frac{r^n}{R^{n+1}}$$

This forms a geometric series in terms of $\frac{r}{R}$ for $r < R$ meaning

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{r^n}{R^{n+1}} &= \frac{1}{R} \sum_{n=0}^{\infty} (\frac{r}{R})^n \\ &= \frac{1}{R} * \frac{1}{1 - \frac{r}{R}} \\ &= \frac{1}{R - r}, \end{aligned}$$

thus proving uniform convergence allowing the integral and summation to be swapped. After swapping, the equation becomes

$$\sum_{n=0}^{\infty} \frac{r^n}{2^n R^{n+1}} \oint_\Gamma \frac{dz}{2\pi i} \frac{(z^2 - 1)^n}{(z - x)^{n+1}} = \oint_\Gamma \frac{dz}{2\pi i} \frac{1}{R(z - x)} \times \sum_{n=0}^{\infty} (\frac{r(z^2 - 1)}{2R(z - x)})^n.$$

The sum inside the integral is a geometric series as $\frac{r(z^2-1)}{2R(z-x)} < 1$ because $\frac{r}{2R} << 1$. The sum can be simplified to

$$\sum_{n=0}^{\infty}(\frac{r(z^2-1)}{2R(z-x)})^n = \frac{1}{1-\frac{r(z^2-1)}{2R(z-x)}}.$$

Plugging back into the previous equation gives

$$\oint_{\Gamma} \frac{dz}{2\pi i}\frac{1}{R(z-x)}\sum_{n=0}^{\infty}(\frac{r(z^2-1)}{2R(z-x)})^n = \oint_{\Gamma} \frac{dz}{2\pi i}\frac{-2}{rz^2-2Rz+2Rx-r}.$$

This derivation moved the poles at $z = x$ and $z = \infty$ to $z_1 \approx \frac{2R}{r} \to \infty$ and $z_2 \approx x$. To complete the proof, we must solve equation (3) by creating a integration contour Γ that only encloses $z_2 \approx x$, and using the residue method to solve the integral.

$$\begin{aligned}\oint_{\Gamma} \frac{dz}{2\pi i}\frac{-2}{rz^2-2Rz+2Rx-r} &= \text{Residue}[\frac{-2}{rz^2-2Rz+2Rx-r}]_{z=z_2} \\ &= \frac{-2}{r}\frac{1}{z_2-z_1} \\ &= \frac{1}{\sqrt{R^2-2rRx+r^2}} \\ &= \frac{1}{\sqrt{R^2+r^2-2Rrcos\theta}}.\end{aligned}$$

Thus proving that

$$\frac{1}{|R-r|} = \frac{1}{\sqrt{R^2+r^2-2Rrcos\theta}} = \sum_{n=0}^{\infty}\frac{r^n}{R^{n+1}} \times P_n(cos\theta).[4]$$

4.4 Harmonics, Complex Potentials, and Multipoles

The work in the following sections is based off Leslie Greengard's dissertation on Potential Theory [3].

Many physical processes are described by two-dimensional models due to their computational simplicity a fact often exploited in computer simulations. The dimensonality reduction has two major advantages: fewer particles are required to simulate a meaningful physical model and numerical methods are better developed and easier to implement. In this paper we focus specifically on potentials and force fields that are independent of one of the Cartesian coordinates, the z dimension. In other words we consider potentials and force fields for coordinates of the form $(x, y, 0)$. The governing equation for potential problems is the two-dimensional Laplace Equation:

$$\nabla^2\Phi = \frac{\partial^2\Phi}{\partial^2 x} + \frac{\partial^2\Phi}{\partial^2 y} = 0 \tag{4}$$

Functions that satisfy Laplace's equation are referred to as harmonic.

The physical model we consider consists of a set of N charged particles lying in the (x, y) plane. In these 2-D systems, the force of attraction between two particles is inversely proportional to the distance between them. Specifically, if a 2-D point charge is located at the point $(x_0, y_0) = \vec{x_0} \in \mathbb{R}^2$ then for any $\vec{x} \in \mathbb{R}^2$ such that $\vec{x_0} = \vec{x}$, the potentials and electrostatic fields due to the charge are described by the following expressions:

$$\phi_{x_0}(x, y) = -\log(||x - x_0||) \tag{5}$$

$$E_{x_0}(x,y) = \frac{(x-x_0)}{||x-x_0||^2} \tag{6}$$

For every harmonic function u there exits an analytic function w such that $w : \mathbb{C} \to \mathbb{C}$ and $u(x,y) = Re(w(x,y))$ and w is unique except for an additive constant. For the rest of this paper we work solely with analytic functions and make no distinction between a point $(x,y) \in \mathbb{R}^2$ and a point $x+iy = z \in \mathbb{C}$. Furthermore we note that:

$$\phi_{z_0} = Re(-\log(z-z_0)) \tag{7}$$

We will refer to the analytic function $log(z)$ as the potential due to a charge and take the standard branch.

The following lemma is an immediate consequence of the Cauchy-Riemann Equations:

Lemma 1 If $u(x,y) = Re(w(x,y))$ describes the potential field at (x,y), then the corresponding force field is given by

$$\nabla u = (u_x, u_y) = (Re(w'), -Im(w')),$$

where w' is the derivative of w.

The following lemma is used in obtaining the multipole expansion for the field due to m charges.

Lemma 2 Let a point charge of intensity q be located at z_0. Then for any z such that $|z| \geq |z_0|$,

$$\phi_{z_0}(z) = q\log(|z-z_0|) = q\left(\log(|z|) - \sum_{k=1}^{\infty} \frac{1}{k}\left(\frac{z_0}{z}\right)^k\right) \tag{8}$$

Proof: Note first that $\log(|z-z_0|) - \log(|z|) = \log\left(1-\frac{z_0}{z}\right)$ and that $\left|\frac{z_0}{z}\right| < 1$. The lemma now follows from the expansion

$$\log(1-w) = (-1)\sum_{k=1}^{\infty} \frac{w^k}{k},$$

which is valid for any w such that $|w| < 1$.

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

$$\phi(z) = Q\log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k}, \tag{9}$$

where

$$Q = \sum_{i=1}^{m} q_i \quad \text{and} \quad a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k}.$$

For any $p \geq 1$ we can bound Equation 9 as follows:

$$\left|\phi(z) - Q\log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k}\right| \leq \frac{|r|^{p+1}}{|z|^{p+1}}\left(\frac{A}{c-1}\right)^p, \tag{10}$$

where

$$c = \frac{|z|}{r}, \quad A = \sum_{i=1}^{m} |q_i|, \quad \text{and} \quad \alpha = \frac{A}{1-\frac{r}{|z|}}.$$

Proof: The form of the multipole expansion is an immediate consequence of the preceding lemma and the fact that $\phi(z) = \sum_{i=1}^{m} \phi_i(z)$. To obtain the error bound, observe that

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

$$\left| \sum_{k=p+1}^{\infty} \frac{a_k}{z^k} \right| \leq A \sum_{k=p+1}^{\infty} \frac{r^k}{|z|^k} \leq A \sum_{k=p+1}^{\infty} \left|\frac{r}{z}\right|^k = \alpha \left|\frac{r}{z}\right|^{p+1} = \left(\frac{A}{c-1}\right)\left(\frac{1}{c}\right)^p.$$

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

$$\left| \phi(z) - Q\log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq A \left(\frac{1}{2}\right)^p. \tag{11}$$

4.5 Error Bounds

We now describe tools for shifting the center of a multipole expansion, converting expansions into local Taylor expansions in a circular region of analyticity, and derive error bounds associated with these translation operators to perform numerical computations with specified accuracies

Lemma 3 Suppose that

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k}, \tag{12}$$

is a multipole expansion of the potential due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$, 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,

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

where

$$b_l = \frac{-a_0 z_0^l}{l} + \sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1},$$

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

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

Proof: The coefficients of the shifted expansion are obtained by expanding into a Taylor Series the expression with respect to z_0. For the error bound we observe the terms $\{b_l\}$ are the coefficients of the unique multipole expansion about the origin of those charges contained in a circle D. This means the Multipole Expansion Theorem immediately applies with r replaced by $|z_0| + R$.

Once the values of $a_0, \ldots, a_p$ in the expansion about z_0 are computed we can obtain $\{b_1, \ldots, b_p\}$ exactly. In other words we can shift the center of a truncated multipole expansion without any loss of precision.

Lemma 4 Conversion of a Multipole Expansion into a Local Expansion Suppose that m charges of strengths $q_1, q_2, \ldots, q_m$ 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 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:

$$\phi(z) = \sum_{l=0}^{\infty} b_l \cdot z^l, \tag{13}$$

where

$$b_0 = a_0 \log(-z_0) + \sum_{k=1}^{\infty} \frac{a_k}{z_0^k}(-1)^k \qquad \text{and} \quad b_l = \frac{-a_0}{l \cdot z_0^l} + \sum_{k=1}^{l} \frac{a_k}{z_0^k} \left(\frac{l+k-1}{k-1} \right) (-1)^k, \quad \text{for } l \geq 1.$$

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

$$\left| \phi(z) - \sum_{i=0}^{p} b_i \cdot z^i \right| < \frac{A(4e(p+c)(c+1)+c^2)}{c(c-1)} \left(\frac{1}{c} \right)^{p+1}, \tag{14}$$

where A is defined above

Proof: We obtain the coefficients of the local expansion from MacLaurin's theorem applied to the multipole expansion. To derive the error bound , we let $\gamma_0 = a_0 \log(-z_0)$, $\gamma_l = -\frac{a_0}{l \cdot z_0^l}$ for $l \geq 1$, and $\beta_l = b_l - \gamma_l$ for $l \geq 0$.

$$\phi(z) - \sum_{l=0}^{p} b_l \cdot z^l = \sum_{l=p+1}^{\infty} b_l \cdot z^l = S_1 + S_2, \tag{15}$$

Such that S_1 and S_2 are defined as

$$S_1 = \sum_{l=p+1}^{\infty} \gamma_l \cdot z^l \qquad S_2 = \sum_{l=p+1}^{\infty} \beta_l \cdot z^l.$$

We bound S_1 by observing that

$$|S_1| = \left| \sum_{l=p+1}^{\infty} \gamma_l \cdot z^l \right| \leq |a_0| \sum_{l=p+1}^{\infty} \frac{1}{l \cdot |z_0|^l} \cdot |z|^l \leq A \sum_{l=p+1}^{\infty} \left(\frac{1}{c+1} \right)^l < A \left(\frac{1}{c} \right)^p, \tag{16}$$

Since $\frac{1}{c+1} < \frac{1}{c}$. To obtain a bound for S_2, let C be a circle of radius s where $s = cR\left(\frac{p}{p-1}\right)$ (Figure 2.2). Note first that for any $p \geq \frac{2c}{c-1}$,

$$R < \frac{cR+R}{2} < s < cR.$$

Defining the function $\phi_1 : \mathbb{C} \setminus D_1 \to \mathbb{C}$ by the expression

$$\phi_1(z) = \phi(z) - a_0 \cdot \log(z - z_0),$$

Using Taylor's Theorem leads to:

$$S_2 = \left| \phi_1(z) - \sum_{l=0}^{p} \beta_l z^l \right| = \left| \sum_{l=p+1}^{\infty} \beta_l z^l \right| \leq \frac{M}{1 - \frac{|z|}{s}} \left(\frac{|z|}{s} \right)^{p+1},$$

where

$$M = \max_{\mathbb{C}} |\phi_1(t)|.$$

For any t lying on C,

$$|\phi_1(t)| \leq \sum_{k=1}^{\infty} \left| \frac{a_k}{(t-z_0)^k} \right|,$$

From there we get

$$|a_k| \leq AR^k \quad \text{and} \quad |t - z_0| \geq R + cR - s = R + \frac{cR}{p}.$$

Which implies

$$M \leq A\left(\frac{pR+cR}{cR}\right) \quad \text{and} \quad 1-\frac{|z|}{s} \geq \frac{cR-R}{cR+R}.$$

Observe that for any positive integer n and any integer $p \geq 2$,

$$\left(1+\frac{1}{n}\right)^n \leq e \quad \text{and} \quad \left(1+\frac{1}{p-1}\right)^2 \leq 4,$$

Finally

$$S_2 \leq \ A\left(\frac{pR+cR}{cR(cR-R)}\right)\left(\frac{|z|}{cR}\right)^{p+1} \ \leq A\left(\frac{p+c}{c(c-1)}\right)\left(\frac{1}{c}\right)^{p+1}\left(1+\frac{1}{p-1}\right)^{p-1} \ \leq 4Ae\left(\frac{p+c}{c(c-1)}\right)\left(\frac{1}{c}\right)^{p+1}.$$

Adding the error bound of S_2 to the error bound for S_1 completes the proof.

Lemma 5 Translation of a Local Expansion For any complex z_0, z and $\{a_k\}, k = 0, 1, 2, \ldots, n$,

$$\sum_{k=0}^{n} a_k(z-z_0)^k = \sum_{l=0}^{n}\left(\sum_{k=l}^{n} a_k\binom{k}{l}(-z_0)^{k-l}\right)z^l. \tag{17}$$

The lemma above is an immediate consequence of a MacLaurin Series and describes the exact translation operation with a finite number of terms and when no error bound is needed.

5 Fast Multipole Method

We will now go through the algorithm for the Fast Multipole Method (FMM), with the caveat that this specific algorithm is for free-space problems, where the only interactions to be accounted for involve the particles within the computational box themselves, and the boundary conditions are ignored. This method is from [3] and [2].

Consider a unit cube centered at the origin containing N particles. We introduce a hierarchical mesh termed "refinements," where each level splits the box into four sub-boxes. At level 0, the entire box is present, and at level l, there are 4^l boxes. This setup forms a tree structure (quadtree), with each box at level l having four children at level $l+1$. Two boxes, each with side $2s$, are considered well-separated if their distance is at least $2s$, with their encompassing disks' radii at $\sqrt{2}s$ and separated by at least $4(1-\sqrt{2})s$. Using c $= \frac{4-\sqrt{2}}{\sqrt{2}} \approx 1.828$, interactions are computed only for well-separated boxes to achieve precision e by choosing $p = \lceil -\log(e) \rceil$. Each box at level l has: $\Phi_{i,l}$: the p-term multipole expansion for distant potentials, $\Psi_{i,l}$: the p-term local expansion capturing external potentials, excluding immediate neighbors, $\tilde{\Psi}_{i,l}$: similar to $\Psi_{i,l}$ but includes potentials from beyond immediate and adjacent neighbors. Lastly, we define the term interaction list which for a box i at level l consists of the children of the nearest neighbors of box i's parent that are well-separated from box i. Additionally, every local expansion is described by the coefficients of a p-term, and the direct evaluation of this p-term polynomial gives a potential.

Initialization
Choose a level of refinement $n \approx \log_4 N$, a precision ε, and set $p = \lceil -\log_c(\varepsilon) \rceil$, applying the error bounds from 4.4, 4.5, and 14.

Upward Pass

Step 1 Form multipole expansions of potential field due to particles in each box about the box center at the finest refinement. We iterate through every single particle from 1 to 4^n and form a p-term multipole expansion for each $\Phi_{n,i}$, by using the Multipole Expansion Theorem 4.4. The complexity here is Np since every particle contributes to one expansion at this refinement.

Step 2 From level l=n-1...0, and for each box from i=1...4^l within each level, form a p-term Multipole Expansion $\Phi_{l,i}$ using the Translation of a Multipole Expansion 4.5 to shift the center of each child box's expansion to the current box center and adding them together. The complexity here is Np^2 since at the lth level, 4^l shifts involving order p^2

Downward Pass

Step 3 For all levels from l=1...n-1, and for each box from i=1...4^l in level l, we'd go through each box on each level and form our $\Psi_{l,i}$ by using the Conversion of a Multipole Expansion into a Local Expansion Lemma 4.5 in order to convert the multipole expansion $\Phi_{l,j}$ of each box j in the interaction list of each box i to a local expansion about the center of box i, and we add those together and add the result to our $\tilde{\Psi}_{l,i}$. Additionally, we also form the expansion for i's children $\tilde{\Psi}_{l+1,i}$ by using the Translation of a Local Expansion 17 Lemma to expand $\Psi_{l,i}$ about the children box's centers. The complexity here is $\leq 28Np^2$ there are at most 27 elements on the interaction list for each box at each level, and an extra Np^2 is required for the second loop.

Step 4 Once we reach the n level (the finest refinement), we repeat the last step with all of the expansions except only at level n. At this point, we have the local expansions at the finest refinement now available, and these can be used in order to generate the potential due to all particles outside the nearest neighbor boxes at this refinement. The complexity here is $\leq 27Np^2$, since there are at most 27 elements on the interaction list and around N boxes.

Step 5 At this step, once we're still in the nth refinement, for every box i from 1 to 4^n, we evaluate local expansions at each particle p_j's positions at z_j and evaluate $\Psi_{n,i}(z_j)$, where j each element on the interaction list of each box i. The complexity here is Np, since one p term expansion is evaluated for each particle.

Step 6 Once we reach this step, we have calculated all of the potentials for every particle except the nearest neighbors, and thus for every box i from 1 to 4^n, at each particle p_j in box i, we directly compute its interactions with all other particles within the box and its nearest neighbors. The complexity reduces to $\frac{9}{4}Nk_n$ by bounding particles per box at k_n and halving the interaction computations with 8 neighbors via Newton's 3rd law.

Step 7 For every particle in box i, we add direct and far-field terms together. The complexity here is n since that's just adding 2 terms for each particle.

Overall we can see our time complexity as we add everything up results in $\mathcal{O}(N)$, as the coefficients for N are all constants, since calculating, we get $N\left(-2 \cdot a \cdot p + 56 \cdot b \cdot p^2 + 4.5 \cdot d \cdot k_n + e\right)$ which results in $\mathcal{O}(N)$

6 Conclusion and Extension

We have explored the utilization of complex analysis tools in the examination of multipole expansions, emphasizing their crucial role in solutions for harmonic potential theory and the Fast Multipole Method. By employing the sophisticated mathematical architecture of complex analysis, we have successfully delineated the process and advantages of multipole expansions in decomposing potential fields into simpler computational elements.

The implementation of the Fast Multipole Method notably marks a substantial progression beyond traditional $\mathcal{O}(n^2)$ methods for the N-Body problem. By diminishing the computational complexity to $\mathcal{O}(n\log(n))$ or even $\mathcal{O}(n)$ under specific circumstances, this method significantly augments the practicality of conducting large-scale simulations. It becomes an essential instrument within both academic research and industry applications. Our discussion about the error bounds pertinent to various implementations further solidifies the robustness and flexibility of the Fast Multipole Method.

Looking ahead, the extension of the Fast Multipole Method to three-dimensional configurations holds the potential to aid additional fields, such as quantum mechanics and acoustic wave propagation. The theoretical foundations laid out in this paper provide a solid basis for such expansions, suggesting a wide spectrum of potential research

directions. Moreover, ongoing enhancements in algorithmic efficiency and the exploration of different boundary conditions may unlock new possibilities for advanced computational methods in complex systems.

The extension to three dimensions is particularly promising as it aligns with the natural complexity of many physical systems. In three-dimensional space, interactions are not merely planar and involve additional degrees of freedom, which can be efficiently managed using the 3D Fast Multipole Method through the use of spherical harmonics and Legendre Polynomials. This extension can better model real-world phenomena, thereby improving the accuracy and efficiency of simulations in aerospace, meteorology, and beyond [2].

Another extension we would have liked to discuss is the kernel free approach for the Fast Multipole Method. Traditionally, FMM relies on mathematical expressions of the kernel functions, which describe the interaction between particles, to efficiently compute potential fields and forces. These kernels are usually specific to the type of interaction (e.g., gravitational, electrostatic) and are often algebraically complex. Kernel-free approaches, however, do not require explicit forms of these kernel functions. Instead, they use numerical approximations to evaluate the interactions directly from the fundamental equations governing the system. This approach offers greater flexibility and can be applied to a wider range of problems where the kernel might not be easily expressible in a closed form. Unlike classical FMM, which optimizes performance based on the analytical properties of the kernels, kernel-free methods leverage high-performance computing techniques to manage the increased computational load of numerical evaluations, thus maintaining efficiency without being constrained by the need for explicit kernel functions [5].

By recognizing the depth of the mathematical structures and their practical implications discussed herein, this study not only underscores the significance of complex analysis in theoretical physics but also emphasizes its pivotal role in propelling forward computational techniques.

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Appendix

Algorithm 1: Fast Multipole Method

Input:
N particles, unit cube at origin, precision ε, levels n ($n \approx \log_4 N$)
Output:
Potentials at each particle location
Initialization:
Compute the number of terms p for the expansions: $p = \lceil -\log_c(\varepsilon) \rceil$, where $c = \frac{4-\sqrt{2}}{\sqrt{2}}$

Upward Pass:

Step 1:
for $i = 1$ *to* 4^n **do**
    Compute multipole expansion $\Phi_{n,i}$ for each particle in box i

Step 2:
for *each level* l *from* $n-1$ *down to* 0 **do**
    :
    for *each box* $i = 1$ *to* 4^l **do**
    :
    Form $\Phi_{l,i}$ by translating and adding multipole expansions of child boxes

Downward Pass:

Step 3:
for *each level* l *from* 1 *to* $n-1$ **do**
    :
    for *each box* $i = 1$ *to* 4^l **do**
    :
    Form local expansions $\Psi_{l,i}$ from interaction lists using multipole-to-local conversions
    Translate local expansions to children to form $\Psi_{l+1,i}$

Step 4: At level n, compute local expansions $\Psi_{n,i}$ from interaction lists

Step 5: Evaluate local expansions at particle positions within each box at level n

Step 6: Directly compute interactions within each box and with immediate neighbors

Step 7: Sum direct and far-field potentials for each particle

return the computed potentials for all particles