

Implementing Fast-Multipole Methods with High-Level Interpreted Languages

Srinath Kailasa

A thesis submitted in partial fulfillment of the requirements
for the degree Master of Science



Department of Physics
University College London
August 17, 2020

Declaration

I, Srinath Kailasa, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Abstract

The Fast Multipole Method (FMM) is a numerical method to accelerate the solution of the N -Body problem, which appears in numerous contexts in science and engineering, for example in solving for gravitational or electrostatic potentials in multi-particle systems. It does so by approximating the Green's function of the system with analytic infinite series expansions (the origin of the 'multipole' in its name), and coalescing the effect of distinct distant sources together so as to greatly reduce the number of computations. The analytic expansions of the original Fast Multipole Method depend on the Green's function of the system in question (Helmholtz, Laplace etc.), and in practice a new implementation must be written for a given system.

The Kernel-Independent Fast Multipole Method (KIFMM), first presented by Ying et al. [5], is a similar approach that replaces the analytic series expansions with a continuous distribution of so called 'equivalent density' supported at discrete points on a box enclosing a set of particles. These equivalent densities are found by matching the potential they generate to those generated by the original sources at another surface in the far field. Usefully, this approach doesn't require multipole expansions of the Green's functions of a system, and therefore can be programmed in an agnostic way, hence the origin of it's name.

This thesis presents a Python implementation of the KIFMM, with investigations made into both mathematical and computational techniques for the acceleration of the algorithm. Python is chosen as it has emerged as a standard for scientific and data intensive computing in recent years, with a huge increase in adoption, and a well supported ecosystem of libraries and tools available for accelerating numerical codes. The wider context of this thesis is an ongoing collaboration with the ExaFMM Project [6] to produce a Pythonic implementation of the KIFMM that sacrifices as little performance as possible. This thesis introduces the relevant theoretical background, before proceeding to discuss the strategies used in the practical implementation of the software. Key bottlenecks in the implementation are examined and addressed, with the speed and accuracy of the software benchmarked for the Laplace kernel for electrostatic problems. Finally, future avenues of investigation and software development are discussed, in the context of the wider literature.

Contents

Glossary	3
1 Introduction	4
1.1 Overview of the Analytic FMM	4
1.1.1 Motivation	4
1.1.2 Algorithm structure	8
1.1.3 Analysis	8
1.2 Overview of the Kernel-Independent FMM	9
1.2.1 Motivation	9
1.2.2 Algorithm Structure	9
1.2.3 Analysis	9
2 Strategy for Practical Implementation	10
2.1 Bottleneck Analysis	10
2.2 Space-Filling Curves	11
2.3 Operator Caching	11
2.4 SVD Compression	11
2.5 Software Design	11
3 Experiments & Results	12
3.1 Section 1	12
4 Conclusion	14
4.1 Section 1	14
A Appendix	15
A.1 FMM Algorithm Specification	15
A.2 Analytic FMM Operators for 3D Laplace Kernel	16
Bibliography	19

Glossary

FMM The Fast Multipole Method. . 1, 4

KIFMM The ‘Kernel Independent’ Fast Multipole Method. . 1

near neighbours Two boxes in computational tree are near neighbours if they are at the same level of refinement, and share a boundary point. . 15

well separated Two boxes in computational tree are near neighbours if they are at the same level of refinement, and are not near neighbours. . 15

Introduction

1.1 Overview of the Analytic FMM

1.1.1 Motivation

The paradigmatic problem of Fast Multipole Methods (**FMM**)¹ is the so called N -Body problem. This classic problem refers to the calculation of the pairwise interactions between N particles over a potentially long-range, for example in gravitational or electrostatic systems. The straightforward calculation can be written in the form of the following sum,

$$\Phi(x_j) = \sum_{i=1}^N w_i K(x_i, x_j) \quad (1.1)$$

Where $i, j \in [1, N]$ and $K(x, y)$ is called a kernel function where we are generally concerned with coordinates of particles in an $n = 2$ or 3 dimensional Hilbert space taking $\{(x, y) | x, y \in \mathbb{R}^n\}$. Additionally, each summand is weighted by w_i . For calculating electrostatic problems in three dimensions, which is used as a model problem throughout this thesis, this goes to,

$$\Phi(x_j) = \sum_{i=1}^N q_i K(x_i, x_j) \quad (1.2)$$

where q_i refers to a charge density and,

$$K(x, y) = \frac{1}{4\pi\epsilon_0} \frac{1}{|x - y|} \quad (1.3)$$

the constant ϵ_0 is the permittivity of free space. It's easy to see how a naive direct application of this equation over N particles results in an algorithm of $O(N^2)$ complexity, therefore it's only practicable for systems of moderate size. In realistic systems, we may be interested in interactions involving 10^6 to 10^8 particles, making it impossible to directly compute all interactions.

The analytic FMM represented a sea change for N -Body simulation as it manages to trade off computations for error to achieve an asymptotic complexity of just $O(N)$. First presented by Greengard [3], the analytic FMM comes equipped with rigorous error bounds, making accurate massive N -Body simulations feasible on available computing hardware.

Notes from [2]

¹The first usage of a technical term or abbreviation listed in the glossary is highlighted throughout the text for ease of reference.

Accurate N-Body simulations (stars in a galaxy, atoms in a protein) require $\mathcal{O}(n^2)$ calculations. Using multipole expansions in the far field, and hierarchical partitioning of the space. Comes equipped with rigorous error bounds.

Notes from [3]

- particle simulation important in many fields: e.g. celestial mechanics
- 2 approaches, (1) solving N2L with given initial conditions and find trajectories as function of time
- or, (2) find equilibrium configuration by solving for potential.

Potential of the form

$$\Phi = \Phi_{\text{near}} + \Phi_{\text{external}} + \Phi_{\text{far}} \quad (1.4)$$

1. Φ_{external} , underlying potential (background).
2. Φ_{near} , rapid decaying (e.g. Van Der Waals)
3. Φ_{far} , far field, e.g Coulombic, Gravitational.

1 and 2 are $\mathcal{O}(n)$ to evaluate at N points. 3 decays slower, so all particles must be accounted for, naively evaluating results in $\mathcal{O}(n^2)$

Shows up in celestial mechanics, plasma physics, molecular dynamics etc

Notes from [1]

Again, reference efficacy in particle simulations for computing pairwise interactions. As this is where they are most easily understood. Equally useful in the solution of certain partial differential equations by first recasting as integral equations.

‘Atomic’ problem of many probs in comp. phys. boils down to,

Examples of physical problems,

Gravitational potential 3D

$$\phi(x_j) = \sum_{i=1, i \neq j}^N \frac{m_i}{r_{i,j}} \quad (1.5)$$

Gravitational field 3D.

$$\mathbf{E}(\mathbf{x}_j) = \sum_{i=1, i \neq j}^N m_i \frac{\mathbf{x}_j - \mathbf{x}_i}{r_{i,j}^3} \quad (1.6)$$

Same as electrostatics, where coulomb’s law used instead, mass \rightarrow charge.

Can turn into integral, for continuous distributions of mass/charge. (Biot-Savart law etc)

Acoustic Scattering and diffusion, examples given too. Probably wont write in report.

Each physical problem results in integral equation,

$$u(\mathbf{x}) = \int K(\mathbf{x}, \mathbf{y}) w(\mathbf{y}) d\mathbf{y} \quad (1.7)$$

Discrete case,

$$u(\mathbf{x}) = \sum_{i=1}^N w_i K(\mathbf{x}, \mathbf{y}_i) \quad (1.8)$$

Direct evaluations obviously quadratic computational cost. Most famous fast summation method FFT $\sum_{k=1}^N e^{\frac{2\pi i j k}{N}} w_k$ in $\mathcal{O}(n \log(n))$. FFT different, it's exact method, based on symmetry (algebra) - requires uniform spatial grid (geometry dep). FMM are approximate - i.e. based on analytic considerations (vs algebra), insensitive to source distribution (geometry).

FMM approach based on the following features

- A specified acceptable accuracy ϵ
- A hierarchical tree division of space
- a far field expansion of the kernel, in which the influence of the source and target points separates
- (optionally) the conversion of far field expansions into local expansions

Idea: Compress field in the far field as it's (relatively) smooth if it's well separated from evaluation point. How? Using a 'multipole expansion'. What are these?

Notes from [4]

page 152 develops the multipole expansion for the potential of an arbitrary charge distribution in 3D.

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{1}{d} \rho(\mathbf{r}') d\tau' \quad (1.9)$$

\mathbf{r} - vector from centre of expansion at charge distribution to the point of evaluation, d - the distance from volume element $d\tau'$ to the point of evaluation, $\rho(\mathbf{r}')$ - charge density, \mathbf{r}' - the vector from the centre of expansion to the volume element. α is the angle between r and r' .

From law of the cosines,

$$d^2 = r^2 + (r')^2 - 2rr' \cos \alpha = r^2 \left[1 + \left(\frac{r'}{r} \right)^2 - 2 \left(\frac{r'}{r} \right) \cos \alpha \right] \quad (1.10)$$

$$d = r \sqrt{1 + \epsilon} \quad (1.11)$$

Where,

$$\epsilon \equiv \left(\frac{r'}{r} \right) \left(\frac{r'}{r} - 2 \cos \alpha \right) \quad (1.12)$$

ϵ is small far away from charge dist. so can expand $1/d$ binomially

$$\frac{1}{d} = \frac{1}{r}(1 + \epsilon)^{-1/2} = \frac{1}{r} \left(1 - \frac{1}{2}\epsilon + \frac{3}{8}\epsilon^2 - \dots \right) \quad (1.13)$$

$$\frac{1}{d} = \frac{1}{r} \sum_{n=0}^{\infty} \left(\frac{r'}{r} \right)^n P_n(\cos \alpha) \quad (1.14)$$

So can write multipole expansion in terms of legendre polynomials coefficients exactly in 3D,

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{n=0}^{\infty} \frac{1}{r^{n+1}} \int (r')^n P_n(\cos \alpha) \rho(\mathbf{r}') d\tau' \quad (1.15)$$

Again from [3],

For discrete distributions of N charges q_i this goes to,

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^N \sum_{n=0}^{\infty} \frac{(r')^n q_i}{r^{n+1}} P_n(\cos \alpha) \quad (1.16)$$

Addition theorem for Legendre polynomials,

$$P_n(\cos \gamma) = \sum_{m=-n}^n Y_n^{-m}(\alpha, \beta) Y_n^m(\theta, \phi) \quad (1.17)$$

where two points P and Q with sph. coords. (r, θ, ϕ) and (ρ, α, β) γ is angle subtended between them,

From addition theorem, Multipole expansion goes to,

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^N \sum_{n=0}^{\infty} \frac{(r')^n q_i}{r^{n+1}} P_n(\cos \alpha) \quad (1.18)$$

$$= \frac{1}{4\pi\epsilon_0} \sum_{i=1}^N \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{(r')^n q_i Y_n^{-m}(\alpha_i, \beta_i)}{r^{n+1}} Y_n^m(\theta, \phi) \quad (1.19)$$

$$= \sum_{i=1}^N \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{M_n^m}{r^{n+1}} \cdot Y_n^m(\theta, \phi) \quad (1.20)$$

This is an exact expansion, can be truncated as required for tunable precision.

If instead expansion taken with centre at targets, at distance from sources, Can rewrite as Local Expansion.

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^N \sum_{j=0}^{\infty} \sum_{k=-j}^j L_j^k \cdot Y_j^k(\theta, \phi) \cdot r^j \quad (1.21)$$

Where the coefficients of the local expansion can be derived from the coefficients of the the multipole expansion.

Analytic expressions for shifting multipole and local expansions explained. Should probably specify shift operators in appendix for completeness... These shifts are exact.

1.1.2 Algorithm structure

Notes from [5]

FMM makes use of these representations in a recursive algorithm. computational domain is a box containing all particles, sources and targets. Hierarchically partitioned into a tree structure, called Octree in 3D. With each level l of the tree partitioned into 8^l geometric boxes. For each box, the potential induced by its source densities is represented by a multipole expansion centered around the box, while the potential induced by the sources from non-adjacent boxes is encoded in a local expansion.

Number of expansion terms p is chosen for a prescribed relative error ϵ , using $p = \log_c \epsilon$ where $c = \frac{4-\sqrt{3}}{\sqrt{3}}$ in 3D (numerically optimal?). The truncation error has rigorous bounds.

The availability of analytic translations enable the $\mathcal{O}(n)$ algorithm. In particular the following translations; M2M, L2L, M2L.

Two basic steps of FMM using tree structure.

1. *Upward Pass* The tree is traversed, post-order. S2M at leaves - compute multipole expansion of leaf sources at leaf node. Shift multipole expansion to parent node, and sum together.
2. *Downward Pass* The tree is traversed pre-order. The local expansion for each box is the sum of two parts: (1) the L2L transformation collects the local expansion of B's parent (compressing the information for boxes non-adjacent to B's parent) (2) the M2L translation, for each multipole expansion of boxes which are the children of the neighbors of B's parent but not adjacent to B itself. At the end of the Downward Pass, the 'far' interaction which is evaluated using the local expansion at this box (L2T operation) at each target particle. Combined with the 'near' interaction by direct computation of potential over all source points in near field (within the box itself, and its direct neighbors).

1.1.3 Analysis

Begin with $O(N \log(N))$ algorithm variant; here post order traversal (from coarsest to finest level), compute multipole expansion for each box at each level, this has the Np^2 bound, at finest level assume $O(1)$ number of particles, so direct computation with nearest neighbour particles leads to $O(N)$ bound.

Full analysis defer to [3]. Enough to understand that the translation operators are what lead to the $\mathcal{O}(n)$ complexity. Beginning with upward pass, at leaf level each particle contributes to one expansion so S2M of the order $Np^2 - p^2$ is the order of operations for the multipole expansion, can see this from the equation. M2M/L2L/M2L shifts require p^4 operations, so all are bounded by $O(Np^4)$ (consider last level), precise bound dictated by number of boxes in interaction list. Evaluating the p^{th} degree local expansions at each target particle (L2T) bounded by $O(Np^2)$, small constant κ particles enforced at leaf level leads to $O(\kappa N)$ complexity for direct calculations at leaf level. We see that the whole algorithm is bounded by $O(N)$.

1.2 Overview of the Kernel-Independent FMM

1.2.1 Motivation

Analytic FMM implementation is Kernel specific, as we need to compute the multipole expansion coefficients. It's instead based solely on kernel evaluations, therefore can be programmed in an agnostic way.

1.2.2 Algorithm Structure

1.2.3 Analysis

Strategy for Practical Implementation

2.1 Bottleneck Analysis

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetur adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagittis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetur.

2.2 Space-Filling Curves

2.3 Operator Caching

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetur adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagittis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetur.

2.4 SVD Compression

2.5 Software Design

Experiments & Results

3.1 Section 1

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetur adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula. Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam

vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetur adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula. å

Conclusion

4.1 Section 1

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetur adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

Appendix

A.1 FMM Algorithm Specification

Notes from [3]

Initialisation: Choose refinement of $n \approx \log_8 N$ and precision ϵ , set $p = \lceil -\log_2(\epsilon) \rceil$.

Upward Pass

Step 1

From multipole expansions of potential field due to particles in each box at leaf level.

```
do  $ibox = 1, \dots, 8^n$   
  Form  $p^{th}$  degree multipole expansion  
end
```

Step 2

Translate Multipole expansion to coarser levels from the bottom up.

```
do  $l = n - 1, \dots, 0$   
  do  $ibox = 1, \dots, 8^l$   
    M2M shifting  
  end  
end
```

Downward Pass

Computations at the coarsest possible level. For a given box, done by including interactions with those boxes which are well separated, and whose interactions have not been accounted for at the parent level.

Step 3

Form local expansion about center of each box at each level $l \leq n - 1$, describes field due to all particles that are not contained in the current box, it's near neighbours or it's secondary near neighbors.

```
do  $l = 1, \dots, n - 1$   
  do  $ibox = 1, \dots, 8^l$   
    Do M2L OPERATIONS  
  end
```



```

do 1, ..., 8l
  Do L2L OPERATIONS
end
end

```

Step 4

After this step, leaf local expansions are available, can use this to evaluate potential at leaves from all particles in the far field.

```

do  $ibox = 1, \dots, 8^n$ 
  Find local expansion at leaf level, by doing M2L from interaction list.
end

```

Step 5

Evaluate local expansions at particle positions in all leaves

```

do  $ibox = 1, \dots, 8^n$ 
  For every particle in  $ibox$ 'th box, evaluate local expansion.
end

```

Step 6

Compute nearest neighbors directly,

```

do  $ibox = 1, \dots, 8^n$ 
  For every particle in  $ibox$ 'th box, compute potential directly with nearest neighbors.
end

```

Step 7

```

do  $ibox = 1, \dots, 8^n$ 
  Add direct and far field terms together for every particle in  $ibox$ 
end

```

A.2 Analytic FMM Operators for 3D Laplace Kernel

Expressions derived in [3]

For l charges of strengths q_1, \dots, q_l located inside sphere D of radius a center at $Q = (\rho, \alpha, \beta)$, and that for points $P = (r, \theta, \phi)$ outside D potential given by multipole expansion

Multipole Expansion,

$$\Phi(P) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{O_n^m}{r^{n+1}} \cdot Y_n^m(\theta', \phi') \quad (\text{A.1})$$

$P - Q = (r', \theta', \phi')$. Then for any point P outside sphere D_1 of radius $a + \rho$, M2M shifted

$$\Phi(P) = \sum_{j=0}^{\infty} \sum_{k=-j}^j \frac{M_j^k}{r^{j+1}} \cdot Y_j^k(\theta, \phi) \quad (\text{A.2})$$

Defined,

$$M_j^k = \sum_{n=0}^j \sum_{m=-n}^n \frac{O_{j-n}^{k-m} \cdot J_m^{k-m} \cdot A_n^m \cdot A_{j-n}^{k-m} \cdot \rho^n \cdot Y_n^{-m}(\alpha, \beta)}{A_j^k} \quad (\text{A.3})$$

and,

$$J_m^{m'} = \begin{cases} (-1)^{\min(|m'|, |m|)} & \text{if } m \cdot m' < 0 \\ 1 & \text{otherwise} \end{cases} \quad (\text{A.4})$$

$$A_n^m = \frac{(-1)^n}{\sqrt{(n-m)! \cdot (n+1)!}} \quad (\text{A.5})$$

M2L shifted

For l charges of strengths q_1, \dots, q_l located inside sphere D_Q of radius a center at $Q = (\rho, \alpha, \beta)$, and that $\rho > (c+1)a$ with $c > 1$. The corresponding multipole expansion, converges inside sphere D_0 of radius a centered at origin. Inside D_0 the potential due to charges has the local expansion,

$$\Phi(P) = \sum_{j=0}^{\infty} \sum_{k=-j}^j L_j^k \cdot Y_j^k(\theta, \phi) \cdot r^j \quad (\text{A.6})$$

where,

$$L_j^k = \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{O_n^m \cdot J_m^k \cdot A_n^m \cdot A_j^k \cdot Y_{j+n}^{m-k}(\alpha, \beta)}{A_{j+n}^{m-k} \cdot \rho^{j+n+1}} \quad (\text{A.7})$$

where A_n^m same as above,
but,

$$J_m^{m'} = \begin{cases} (-1)^{n'} (-1)^{\min(|m'|, |m|)} & \text{if } m \cdot m' < 0 \\ (-1)^{n'} & \text{otherwise} \end{cases} \quad (\text{A.8})$$

n' refers to j , m' refers to k

and that for points $P = (r, \theta, \phi)$ outside D potential given by multipole expansion

L2L shifted

Let $Q = (\rho, \alpha, \beta)$ be the origin of a local expansion,

$$\Phi(P) = \sum_{n=0}^p \sum_{m=-n}^n O_n^m \cdot Y_n^m(\theta', \phi') \cdot r'^m \quad (\text{A.9})$$

Where $P = (r, \theta, \phi)$ and $P - Q = (r', \theta', \phi')$.

$$\Phi(P) = \sum_{j=0}^p \sum_{k=-j}^j L_j^k \cdot Y_j^k(\theta, \phi) \cdot r^j \quad (\text{A.10})$$

where,

$$L_j^k = \sum_{n=j}^p \sum_{m=-n}^n \frac{O_n^m \cdot J_{n-j, m-k}^m \cdot A_{n-j}^{m-k} \cdot A_j^k \cdot Y_{n-j}^{m-k}(\alpha, \beta) \cdot \rho^{n-j}}{A_j^k} \quad (\text{A.11})$$

where A_n^m same as above,

$$J_{n,m}^{m'} = \begin{cases} (-1)^n (-1)^m & \text{if } m \cdot m' < 0 \\ (-1)^n (-1)^{m'-m} & \text{if } m \cdot m' > 0 \text{ and } |m'| < |m| \\ (-1)^n & \text{otherwise} \end{cases} \quad (\text{A.12})$$

Bibliography

- [1] Rick Beatson and Leslie Greengard. “A Short Course on Fast Multipole Methods”. In: *Wavelets, Multilevel Methods, and Elliptic PDEs*. Clarendon Press, 1997.
- [2] Barry A. Cipra. “The Best of the 20th Century: Editors Name Top 10 Algorithms”. In: *SIAM News* 33.4 (2000).
- [3] Leslie Greengard. “The Rapid Evaluation of Potential Fields in Particle Systems”. PhD thesis. Yale University, 1987.
- [4] David J. Griffiths. *Introduction to Electrodynamics*. 4th ed. Cambridge University Press, 2017. DOI: 10.1017/9781108333511.
- [5] Denis Zorin Lexing Ying George Biros. “A kernel-independent adaptive fast multipole algorithm in two and three dimensions”. In: *Journal of Computational Physics* 196.2 (2004), pp. 591–626. DOI: <http://dx.doi.org/10.1016/j.jcp.2003.11.021>.
- [6] Lorena A. Barba Rio Yokota. *ExaFMM User’s Manual*. 2011. URL: <http://www.bu.edu/exafmm/files/2011/06/ExaFMM-UserManual1.pdf>.