Accelerating the Kernel-Independent Fast Multipole Method

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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. 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 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 implementations 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 usage 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 can compete in terms of performance with a C++ equivalent. This thesis presents a systematic performance analysis of a naive implementation of the KIFMM algorithm, before proceeding to examine and implement acceleration techniques. The speed and accuracy of the implementation is tested for some simple Green's functions, and it concludes with a discussion on future avenues for investigation.

Contents

Glossary

latex Is a mark up language specially suited for scientific documents. 8

near neighbours Two boxes in computational tree are near neighbours if they are at the same level of refinement, and share a boundary point. . 13

well separated Two boxes in computational tree are near neighbours if they are at the same level of refinement, and are not near neighbours. . 13

Introduction

1.1 Overview of the Analytic FMM

1.1.1 Motivation

Notes from [2]

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

$$\Phi = \Phi_{\text{near}} + \Phi_{\text{external}} + \Phi_{\text{far}} \tag{1.1}$$

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

$$\phi(x_j) = \sum_{i=1,\, i\neq j}^{N} \frac{m_i}{r_{i,j}} \tag{1.2}$$

Gravitational field 3D.

$$\mathbf{E}(\mathbf{x_j}) = \sum_{i=1,\, i\neq j}^{N} m_i \frac{\mathbf{x_j} - \mathbf{x_i}}{r_{i,j}^3} \tag{1.3}$$

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,

$$u(\mathbf{x}) = \int K(\mathbf{x}, \mathbf{y}) w(\mathbf{y}) d\mathbf{y} \tag{1.4}$$

Discrete case,

$$u(\mathbf{x}) = \sum_{i=1}^{N} w_i K(\mathbf{x}, \mathbf{y}_i) \tag{1.5}$$

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.

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{1}{d} \rho(\mathbf{r}') d\tau' \tag{1.6}$$

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. *alpha* is the angle between r and r'.

From law of the cosines,

$$d^2 = r^2 + (r')^2 - 2rr'\cos\alpha = r^2\left[1 + \left(\frac{r'}{r}\right)^2 - 2\left(\frac{r'}{r}\right)\cos\alpha\right] \tag{1.7}$$

$$d = r\sqrt{1+\epsilon} \tag{1.8}$$

Where,

$$\epsilon \equiv \left(\frac{r'}{r}\right)\left(\frac{r'}{r} - 2\cos\alpha\right) \tag{1.9}$$

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

$$\frac{1}{d} = \frac{1}{r}(1+\epsilon)^{-1/2} = \frac{1}{r}\left(1 - \frac{1}{2}\epsilon + \frac{3}{8}\epsilon^2 - ...\right) \tag{1.10}$$

$$\frac{1}{d} = \frac{1}{r}\sum_{n=0}^{\infty}\left(\frac{r'}{r}\right)^n P_n(\cos\alpha) \tag{1.11}$$

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

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\sum_{n=0}^{\infty}\frac{1}{r^{n+1}}\int (r')^n P_n(\cos\alpha)\rho(\mathbf{r}')d\tau' \tag{1.12}$$

Again from [3],
For discrete distributions of N charges q_i this goes to,

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\sum_{i=1}^{N}\sum_{n=0}^{\infty}\frac{(r')^n q_i}{r^{n+1}}P_n(\cos\alpha) \tag{1.13}$$

Addition theorem for Legendre polynomials,

$$P_n(\cos\gamma) = \sum_{m=-n}^{n} Y_n^{-m}(\alpha,\beta)Y_n^m(\theta,\phi) \tag{1.14}$$

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,

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\sum_{i=1}^{N}\sum_{n=0}^{\infty}\frac{(r')^n q_i}{r^{n+1}}P_n(\cos\alpha) \tag{1.15}$$

$$= \frac{1}{4\pi\epsilon_0}\sum_{i=1}^{N}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{(r')^n q_i Y_n^{-m}(\alpha_i,\beta_i)}{r^{n+1}}Y_n^m(\theta,\phi) \tag{1.16}$$

$$= \sum_{i=1}^{N}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{M_n^m}{r^{n+1}}\cdot Y_n^m(\theta,\phi) \tag{1.17}$$

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

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

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\sum_{i=1}^{N}\sum_{j=0}^{\infty}\sum_{k=-j}^{j}L_j^k\cdot Y_j^k(\theta,\phi)\cdot r^j \tag{1.18}$$

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 it's 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 trucation 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 it's 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

1.2.2 Algorithm structure

1.2.3 Analysis

Latex

Strategy for Practical Implementation

2.1 Bottleneck Analysis

2.2 Space-Filling Curves

2.3 Operator Caching

2.4 SVD Compression

Experiments & Results

3.1 Section 1

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Conclusion

4.1 Section 1

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Appendix

A.1 FMM Algorithm Specification

textbfNotes 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 $ibox = 1, .., 8^n$
Form p^{th} degree multipole expansion
end

Step 2

Translate Multipole expansion to coarser levels from the bottom up.

do $l = n - 1, .., 0$
do $ibox = 1, .., 8^l$
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 $l = 1, ..., n - 1$
do $ibox = 1, ..., 8^l$
Do M2L OPERATIONS
end

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

Step 6

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

Step 7

do $ibox = 1, ..., 8^n$
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 $q_1, ..., q_l$ 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,

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

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

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

Defined,

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

and,

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

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

M2L shifted

For l charges of strengths $q_1, ..., q_l$ 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,

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

where,

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

where A_n^m same as above,
but,

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

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,

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

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

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

where,

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

where A_n^m same as above,

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

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