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

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...

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,

1.1.3 Analysis

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 Section 1

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Glossary

latex Is a mark up language specially suited for scientific documents. 6

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