A Multipole Based Treecode Using Spherical Harmonics for Potentials of the Form $r^{-\lambda}$*

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Abstract. In this paper we describe an efficient algorithm for computing the potentials of the form $r^{-\lambda}$ where $\lambda \geq 1$. This treecode algorithm uses spherical harmonics to compute multipole coefficients that are used to evaluate these potentials. The key idea in this algorithm is the use of Gegenbauer polynomials to represent $r^{-\lambda}$ in a manner analogous to the use of Legendre polynomials for the expansion of the Coulomb potential r^{-1}. We exploit the relationship between Gegenbauer and Legendre polynomials to come up with a natural generalization of the multipole expansion theorem used in the classical fast multipole algorithm [2]. This theorem is used with a hierarchical scheme to compute the potentials. The resulting algorithm has known error bounds and can be easily implemented with modification to the existing fast multipole algorithm. The complexity of the algorithm is $O(p^3 N \log N)$ and has several advantages over the existing Cartesian coordinates based expansion schemes.

1 Introduction

Computing the potentials of the form $r^{-\lambda}$ where $\lambda \geq 1$ is an important task in many fields like molecular dynamics [10], computational chemistry [9] and fluid mechanics [11]. Potentials such as Lennard-Jones, Van der Wall's forces and H-bonds require evaluation of functions of the form r^{-6}, r^{-10}, etc. The naive brute force algorithm based on particle-particle interaction takes $O(N^2)$, where N is the number of particles. There are various approximation algorithms with lower complexity that have been proposed for the potential evaluation problem. Appel's algorithm [12], Barnes-Hut algorithm [1] etc. reduce the complexity to $O(N \log N)$ by making use of the cluster-particle interactions. As opposed to brute force algorithm that evaluates the potential exactly, approximation algorithms estimate the potential to the desired accuracy that can be controlled by certain parameters. The fast multipole method (FMM), proposed by Greengard and Rokhlin [2], is the fastest contemporary approximation algorithm to

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solve the potential evaluation problem without losing much accuracy. FMM is based on cluster-cluster interaction of the particle system and has a complexity $O(N)$. Although FMM has complexity that is linear in the number of particles in the system, its applicability is limited to operators whose multipole expansions are available analytically. In absence of such expansions treecodes such as Barnes-Hut, Appel's algorithm may be used [3].

For potentials of the form $\Phi(r) = r^{-1}$, FMM exploits the separability of the Greens function kernel using spherical harmonics. However, for kernels of the form $r^{-\lambda}, \lambda \geq 1$, advances have been made by using Cartesian coordinates only. Duan et al. [3] propose a treecode which uses Gegenbauer polynomials and recurrence relations. Chowdhury et al. [5] recent approach generalizes single level fast multipole algorithm for these potentials using addition theorem for Gegenbauer polynomials. They develop necessary operators and error bounds based on these addition theorems. Although, their approach can be used for $r^{-\lambda}$ kernels, it is restricted to single level multipole expansions. The algorithm by Elliott et al. [4] uses multivariate Taylor expansions. Although, these methods are designed to compute such potentials, they strongly make use of Cartesian coordinates and special recurrence relations specific to their schemes.

In this paper we propose a multipole based treecode that uses spherical harmonics to evaluate potentials of the form $r^{-\lambda}$, where $\lambda \geq 1$. This treecode has several advantages over existing Cartesian coordinate based expansion schemes. First, the use of spherical harmonics gives an analytic formula to compute multipole coefficients efficiently. This analytic formula is a natural generalization of the multipole expansion theorem for r^{-1} potential. Second, any previous implementation of FMM can be modified to evaluate $r^{-\lambda}$ potentials using this approach. Third, our method allows precomputing certain vectors that significantly reduce the time to compute multipole coefficients. Finally, there is no need to use special recurrence relations or spherical harmonics other than the ones used in FMM.

The paper is organized as follows: Section 2 discusses the multipole expansion theorem for r^{-1} functions. Section 3 describes the Gegenbauer polynomials and their relationship with Legendre polynomials. Section 4 describes a tree code based on the hierarchical multipole method. Section 5 discusses the complexity and implementation issues. Conclusions are presented in Section 6.

2 Multipole Expansion Theorem for r^{-1} Potential

This section describes the multipole expansion theorem from the classical FMM [2]. Let $P(r, \theta, \phi)$ and $Q(\rho, \alpha, \beta)$ be two points with spherical coordinates. Also let $P - Q = R(r', \theta', \phi')$ and γ be the angle between P and Q taken in anticlockwise direction. Then, if $\rho < r$, the potential $\Phi(P)$ at P due to a charge q at Q is given by

$$\Phi(P) = \frac{q}{r'} = \sum_{n=0}^{\infty} \frac{q \cdot \rho^n}{r^{n+1}} P_n(\cos\gamma), \tag{1}$$

where $P_n(\cos\gamma)$ is the Legendre polynomial of degree n. We also have the addition theorem for Legendre polynomials

$$P_n(\cos\gamma) = \sum_{m=-n}^{n} Y_n^{-m}(\alpha,\beta)Y_n^m(\theta,\phi), \tag{2}$$

where Y_n^m are the spherical harmonics given by

$$Y_n^m(x,y) = \sqrt{\frac{n-|m|}{n+|m|}}P_n^m(\cos x)e^{imy}, \tag{3}$$

in which P_n^m are the associated Legendre functions evaluated at $\cos x$. Using (1) and (2) we have the following theorem.

Theorem 1. *Suppose that a charge of strength q is located at $Q(\rho,\alpha,\beta)$ with $\rho < a$. At any point $P(r,\theta,\phi)$ with $r > a$, the potential $\Phi(P)$ is given by*

$$\Phi(P) = \frac{q}{r'} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{M_n^m}{r^{n+1}}Y_n^m(\theta,\phi), \tag{4}$$

where $M_n^m = q\rho^n Y_n^{-m}(\alpha,\beta)$.

If there are several charges $\{q_i : i = 0,1,\ldots k\}$ around Q with coordinates $\{(\rho_i,\alpha_i,\beta_i) : i = 1,2,\ldots k\}$ we can superpose them at Q and the resulting multipole moment at Q would be $M_n^m = \sum_{i=0}^{k} q_i\rho_i^n Y_n^{-m}(\alpha_i,\beta_i)$.

3 Gegenbauer Polynomials

Gegenbauer polynomials are *higher dimensional* generalization of Legendre polynomials [7,8]. Gegenbauer polynomials are eigenfunctions of the generalized angular momentum operator just as Legendre polynomials are eigenfunctions of the angular momentum operator in three dimensions. Gegenbauer polynomials allow addition theorem using hyperspherical harmonics similar to Legendre polynomials which allow addition theorem using spherical harmonics. One can refer to [7] for list of similarities between Gegenbauer and Legendre polynomials. Gegenbauer polynomials are also a generalization of Legendre polynomials in terms of the underlying generating function. Thus, if $x, y \in \Re$, then

$$\frac{1}{(1-2xy+y^2)^{\lambda/2}} = \sum_{n=0}^{\infty} C_n^{\lambda}(x)y^n, \tag{5}$$

where $C_n^{\lambda}(x)$ is a Gegenbauer polynomial of degree n. This generating function can be used to expand $r^{-\lambda}$ using Gegenbauer polynomials. Let $P(r,\theta,\phi)$ and $Q(\rho,\alpha,\beta)$ be points with spherical coordinates. Using (5) we have,

$$\frac{1}{(r')^{\lambda}} = \frac{1}{r^{\lambda}(1-2u\mu+\mu^2)^{\lambda/2}} = \sum_{n=0}^{\infty}\frac{\rho^n}{r^{n+\lambda}}C_n^{\lambda}(u) \tag{6}$$

where $\mu = \rho/r$ and $u = \cos\gamma$. There are addition theorems for Gegenbauer polynomials using hyperspherical harmonics which allow us to separate $C_n^\lambda(u)$ in terms of the coordinates, but we require hyperspherical harmonics. Instead, we use a relation that exists between Gegenbauer and the Legendre polynomials [6] which allows us to use spherical harmonics in three dimensions. Let $P_n(x)$ and $C_n^\lambda(x)$ be Legendre and Gegenbauer polynomials, of degree n, respectively, Then

$$C_n^\lambda(x) = \sum_{s=0}^{\lfloor n/2 \rfloor} \frac{(\lambda)_{n-s}(\lambda - 1/2)_s}{(3/2)_{n-s}s!}(2n - 4s + 1)P_{n-2s}(x) \tag{7}$$

where $(p)_s$ is the Pochhammer symbol. We define

$$B_{n,s}^\lambda = \frac{(\lambda)_{n-s}(\lambda - 1/2)_s}{(3/2)_{n-s}s!}(2n - 4s + 1). \tag{8}$$

Using (2) and (7), we derive an addition theorem for Gegenbauer polynomials. The following lemma is found in abstract form in many places [7, 8]. A proof is omitted to conserve space.

Lemma 1. (Addition Theorem for Gegenbauer Polynomials) *Let P and Q be points with spherical coordinates (r, θ, ϕ) and (ρ, α, β), respectively, and let γ be the angle subtended by them at the origin. Then*

$$C_n^\lambda(\cos\gamma) = \sum_{m=0}^{\lfloor n/2 \rfloor} B_{n,m}^\lambda \mathbf{Y_{n,m}}(\theta, \phi) \cdot \overline{\mathbf{Y_{n,m}}}(\alpha, \beta) \tag{9}$$

where $\mathbf{Y_{n,m}^T}(x, y) = [Y_{n-2m}^{-(n-2m)}, Y_{n-2m}^{-(n-2m)+1}, \ldots, Y_{n-2m}^{(n-2m)}]$ is a vector of spherical harmonics of degree $n - 2m$.

Once we have an addition theorem for Gegenbauer polynomials we can prove the multipole expansion theorem for $r^{-\lambda}$ potentials.

Theorem 2. (Multipole Expansion) *Suppose that k charges of strengths $\{q_i, i = 1, \ldots k\}$ are located at the points $\{Q_i = (\rho_i, \alpha_i, \beta_i), i = 1, \ldots, k\}$, with $|\rho_i| < a$. Then for any point $P = (r, \theta, \phi)$ with $r > a$, the potential $\Phi(P)$ is given by*

$$\Phi(P) = \sum_{n=0}^{\infty} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{1}{r^{n+\lambda}} \mathbf{M_n^m} \cdot \mathbf{Y_{n,m}}(\theta, \phi) \tag{10}$$

where

$$\mathbf{M_n^m} = \sum_{i=1}^{k} q_i \rho_i^n B_{n,m}^\lambda \overline{\mathbf{Y_{n,m}}}(\alpha_i, \beta_i) \tag{11}$$

Furthermore, for any $p \geq 1$,

$$\left| \Phi(P) - \sum_{n=0}^{p} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{\mathbf{M_n^m}}{r^{n+\lambda}} \cdot \mathbf{Y_{n,m}}(\theta, \phi) \right| \leq \frac{AB}{r^{\lambda-1}(r-a)} \left(\frac{a}{r}\right)^{p+1} \tag{12}$$

where $A = \sum_{i=1}^{k} |q_i|$ and $B = \sum_{m=0}^{\lfloor n/2 \rfloor} \left|B_{n,m}^\lambda\right|$

Proof. From equation (6) and Lemma (1), for any q_i at Q_i we have

$$\begin{aligned}\Phi(P) &= \sum_{n=0}^{\infty} \frac{q_i \rho_i^n}{r^{n+\lambda}} C_n^{\lambda}(u) \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{\left[q_i \rho_i^n B_{n,m}^{\lambda} \overline{\mathbf{Y_{n,m}}}(\alpha_i, \beta_i)\right]}{r^{n+\lambda}} \mathbf{Y_{n,m}}(\theta, \phi)\end{aligned}$$

The moments in (11) are obtained by superposition.

We now prove the error bound. Note that for every $u \in \Re$ with $|u| \leq 1$, we have $|P_n(u)| \leq 1$. From (7), $\left|C_n^{\lambda}\right| \leq B$ where $B = \sum_{m=0}^{\lfloor n/2 \rfloor} \left|B_{n,m}^{\lambda}\right|$(using triangle inequality). Now, for each q_i located at Q_i having $|\rho_i| < a$, we have

$$\begin{aligned}\left|\Phi(P) - \sum_{n=0}^{p} \frac{q_i \rho_n^n}{r^{n+\lambda}} C_n^{\lambda}(u)\right| &= \left|\sum_{n=p+1}^{\infty} \frac{q_i \rho_i^n}{r^{n+\lambda}} C_n^{\lambda}(u)\right| \\ &\leq \frac{B}{r^{\lambda-1}} \frac{q_i}{r-a} \left(\frac{a}{r}\right)^{p+1}\end{aligned}$$

The error bound (12) is obtained by superposition of error bounds for all the k charges.

4 A Treecode for $r^{-\lambda}$ Potentials

The treecode can be viewed either as a variant of Barnes-Hut algorithm [1] or FMM [2] that uses only particle-cluster potential evaluations. The method works in two phases: The tree construction phase and the potential computation phase. In tree construction phase, a spatial tree representation of the domain is derived. At each step of this phase, if the domain contains more than s particles, where s is a preset constant, it is recursively divided into eight equal sub-domains. This process continues until each sub-domain has at most s elements. The resulting tree is an unstructured oct-tree. Each internal node in the tree computes and stores multipole series representation of the particles. Since we don't have any translations, at each level of the tree and for every sub-domain in that level we compute the multipole coefficients of all the particles contained in the sub-domain. These coefficients are obtained using the theorem given in the preceding section. Once the tree has been constructed, the potential at any point can be computed as follows: a *multipole acceptance criterion* is applied to the root of the tree to determine if an interaction can be computed; if not, the node is expanded and the process is repeated for each of its eight children. The multipole acceptance criterion computes the ratio of the distance of the point from the center of the box to the dimension of the box. If the ratio is greater than α, a specific constant, an interaction can be computed. In the following pseudo-code for computing the multipole coefficients and potential evaluation, p is the pre-specified multipole degree and s is the minimum number of particles contained in any leaf box and α, a constant.

```
Multipole_Calculation(p)

- For(each level in the Oct-tree)
    • For(each node in the level)
        * Find the multipole coefficients of all the particles in the
          node using Theorem 2 with respect to the box center of the
          node

Potential_Evaluation()

- For(each particle)
    • nodes = Alpha_Criteria(particle,root)
    • If(nodes = leaf)
        * Compute potentials directly
    • Else
        * Use the multipole expansion Theorem 2 to find the potential
    • Add direct and the computed potential

nodes = Alpha_Criteria(particle,node)

- ratio = distance of the particle from the box center/box length
- If(ratio > α)
    • return nodes;
- Else If(node = leaf)
    • return leafnodes;
- Else
    • For(each children nodes)
        * nodes = Alpha_Criteria(particle,node)
        * return nodes;
```

5 Complexity and Implementation

It can be seen from the multipole expansion theorem that the complexity for computing the multipole coefficients at each level of the tree is $O(p^3N)$, where N is the number of particles in the system and p is the multipole degree. Since there are $\log N$ levels in the tree, the total cost of computing the multipole cocoefficients is $O(p^3N \log N)$. Similarly, it can be seen that the complexity for the potential evaluation phase is $O(p^3N \log N)$. Thus, the overall complexity for the algorithm is $O(p^3N \log N)$.

We have experimentally verified the theorem for r^{-6} and r^{-10} potentials. The logarithmic plot (Fig 1 and Fig 2) shows the relative error and the error bound as multipole degree p varies from 1 to 10. For an efficient implementation of this algorithm, here are few pointers.

- An existing FMM code can be appropriately modified to compute the multipole coefficients in this algorithm.
- The Gegenbauer constants can be precomputed and used in the potential evaluation phase to reduce computation time of the multipole coefficients.

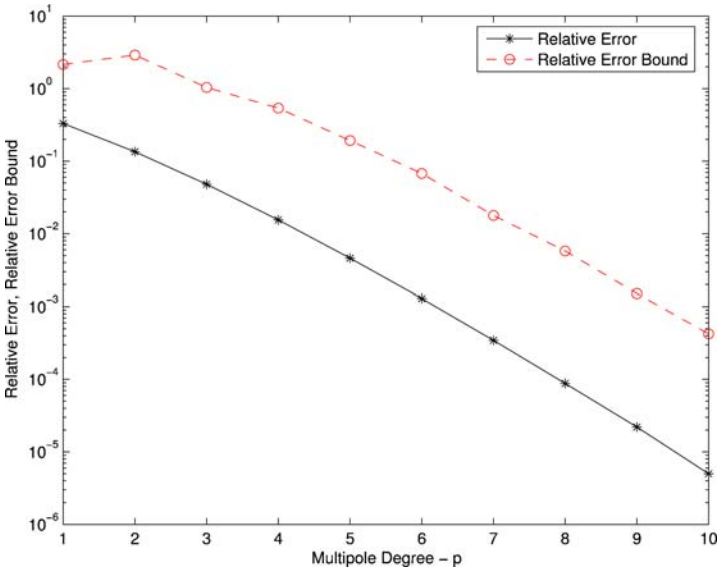

Fig. 1. Relative error and error bound for the potential $\Phi(r) = r^{-6}$

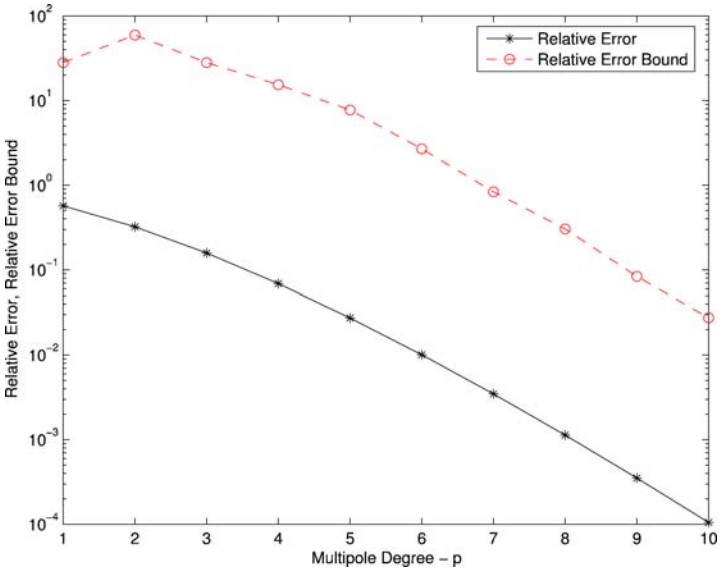

Fig. 2. Relative error and error bound for the potential $\Phi(r) = r^{-10}$

– Due to the decreasing nature of the indices in the Legendre polynomial's relation with the Gegenbauer polynomial (Equation 7), only the spherical harmonics for r^{-1} potential is needed. They can be used to the compute multipole coefficients for the $r^{-\lambda}$ potentials. It should be noted that the set spherical harmonics for $r^{-\lambda}$ potentials are the same as the set of spherical harmonics for r^{-1}, but with the shift $n-2m$ for $m = 0, 1, ...\lfloor n/2 \rfloor$ as Lemma 1 shows.

6 Conclusion

An efficient algorithm for the computation of $r^{-\lambda}$ potentials using spherical harmonics is presented. This algorithm has advantages over existing Cartesian coordinate based expansion schemes. Since, there are no special recurrence relations or spherical harmonics required, an FMM code can be appropriately modified to implement the proposed algorithm.

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