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A New Version of the Fast Multipole Method for Screened Coulomb Interactions in Three Dimensions

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We present a new version of the fast multipole method (FMM) for screened Coulomb interactions in three dimensions. Existing schemes can compute such interactions in $O(N)$ time, where N denotes the number of particles. The constant implicit in the $O(N)$ notation, however, is dominated by the expense of translating far-field spherical harmonic expansions to local ones. For each box in the FMM data structure, this requires $189p^4$ operations per box, where p is the order of the expansions used. The new formulation relies on an expansion in evanescent plane waves, with which the amount of work can be reduced to $40p^2 + 6p^3$ operations per box.

Key Words: translation operators; fast multipole method; screened Coulomb interaction.

1. INTRODUCTION

In the last few years, new versions of the fast multipole method (FMM) have been developed for the evaluation of harmonic potential fields in three dimensions. The schemes of [4, 10], for example, are extremely efficient in the evaluation of pairwise interactions in large ensembles of particles:

$$\Phi(\mathbf{x}_j) = \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{q_i}{\|\mathbf{x}_j - \mathbf{x}_i\|}, \tag{1}$$

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where $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ are points in $\mathbf{R}^3$ and $q_1, q_2, \ldots, q_N$ are the corresponding charge strengths. The algorithm of [4] requires $O(N)$ work and breaks even with the direct calculation at about $N = 750$ for three-digit precision, $N = 1500$ for six-digit precision, and $N = 2500$ for nine-digit precision.

While all fast multipole schemes require the repeated translation of far-field multipole expansions to local ones, the original method of [7, 9] required p^4 operations per translation, where harmonics up to order p^2 have been retained. In the new schemes, one first converts the multipole expansion to a plane wave expansion, then translates the plane wave expansion diagonally (at a cost of p^2 operations), and finally converts the plane wave expansion back to a local expansion.

In this paper, we extend the plane-wave approach to more general expressions of the form

$$\Phi(\mathbf{x}_j) = \sum_{\substack{i=1 \\ i \neq j}}^{N} q_i \cdot \frac{e^{-\lambda \|\mathbf{x}_j - \mathbf{x}_i\|}}{\|\mathbf{x}_j - \mathbf{x}_i\|}, \tag{2}$$

where $\lambda \in \mathbf{R}$. The governing interaction $e^{-\lambda r}/r$ is Green's function for the partial differential equation

$$\nabla^2 \Phi - \lambda^2 \Phi = f(\mathbf{x}) \tag{3}$$

in $\mathbf{R}^3$.

Such calculations arise in various problems in physics, chemistry, and biology when Coulomb forces are damped by screening effects. In nuclear physics, Green's function is referred to as the Yukawa potential. Equation (3) occurs in implicit marching schemes for the heat equation, in Debye–Huckel theory, and in linearization of the Poisson–Boltzmann equation [13, 14, 17]. Applications of the FMM in some of these settings will be reported at a later date. Here, we concentrate on describing the mathematical and algorithmic issues involved in evaluating the function $\Phi(\mathbf{x})$ in (2) as efficiently as possible.

The paper is organized as follows. In Section 2, we summarize the classical theory of multipole expansions for screened Coulomb potentials. In Section 3, we describe the plane wave representation of such potentials, and in Section 4, we describe a simple version of the FMM. In Section 5, we illustrate the performance of the method with several numerical examples. For a review of FMM-type methods and a more thorough discussion of the literature, we refer the reader to [10]. We should note here, however, the recent work of Boschitsch *et al.* [3], who give (to the best of our knowledge) the first detailed description of an FMM for (2). Their scheme, however, does not take into account the plane wave representation and relies on classical expansions. It should be noted that the FMM for high-frequency scattering [6, 16, 18] cannot be used for the case of interest in this paper. It relies on a very elegant diagonal form, but it is numerically unstable when applied to screened electrostatics.

2. MATHEMATICAL PRELIMINARIES

In this section, we describe the (classical) multipole and local representations for screened Coulomb potentials. For further details, see [1, 10, 12, 15].

Let $P_n(x)$ denote the usual Legendre polynomial of degree n. Then the spherical harmonics of degree n and order m can be defined according to the formula

$$Y_n^m(\theta,\phi) = \sqrt{\frac{2n+1}{4\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\cdot P_n^{|m|}(\cos\theta)e^{im\phi}, \tag{4}$$

where the associated Legendre functions P_n^m are defined by Rodrigues' formula

$$P_n^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x).$$

DEFINITION 2.1. The modified spherical Bessel and modified spherical Hankel functions $i_n(r)$, $k_n(r)$ are defined in terms of the usual Bessel function $J_\nu(z)$ via

$$\begin{aligned} I_\nu(r) &= i^{-\nu}J_\nu(ir) \quad (i=\sqrt{-1}),\\ K_\nu(r) &= \frac{\pi}{2\sin\nu\pi}[I_{-\nu}(r)-I_\nu r],\\ i_n(r) &= \sqrt{\frac{\pi}{2r}}I_{n+1/2}(r),\\ k_n(r) &= \sqrt{\frac{\pi}{2r}}K_{n+1/2}(r). \end{aligned}$$

In particular,

$$k_0(\lambda r) = \frac{\pi}{2}\frac{e^{-\lambda r}}{\lambda r}.$$

Using these special functions, we can conveniently describe the far field induced by a collection of point sources.

THEOREM 2.1 (Multipole Expansion). *Suppose that N sources of strengths $q_1, q_2, \ldots, q_N$ are located at points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ with spherical coordinates $(\rho_1, \alpha_1, \beta_1)$, $(\rho_2, \alpha_2, \beta_2), \ldots, (\rho_N, \alpha_N, \beta_N)$, respectively. Suppose further that the points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ are located inside a sphere of radius a centered at the origin. Then, for any point $\mathbf{x} = (r,\theta,\phi) \in \mathbf{R}^3$ with $r > a$, the potential $\Phi(\mathbf{x})$, generated by the sources $q_1, q_2, \ldots, q_N$, is given by the formula*

$$\begin{aligned} \Phi(\mathbf{x}) &= \sum_{i=1}^N q_i\cdot\frac{e^{-\lambda\|\mathbf{x}_j-\mathbf{x}_i\|}}{\|\mathbf{x}_j-\mathbf{x}_i\|} = \frac{2\lambda}{\pi}\sum_{i=1}^N q_i\cdot k_0(\lambda\|\mathbf{x}_j-\mathbf{x}_i\|)\\ &= \sum_{n=0}^\infty\sum_{m=-n}^n M_n^m k_n(\lambda r)\cdot Y_n^m(\theta,\phi), \end{aligned} \tag{5}$$

where

$$M_n^m = 8\lambda\sum_{i=1}^N q_i\cdot i_n(\lambda\rho_i)\cdot Y_n^{-m}(\alpha_i,\beta_i). \tag{6}$$

Furthermore,

$$\left|\Phi(\mathbf{x}) - \sum_{n=0}^p\sum_{m=-n}^n M_n^m\, k_n(\lambda r)\cdot Y_n^m(\theta,\phi)\right| = O\left(\frac{a}{r}\right)^p. \tag{7}$$

In full implementations of the FMM, one also needs to be able to describe the field locally when the sources themselves are far away.

THEOREM 2.2 (Local Expansion). *Suppose that N sources of strengths $q_1, q_2, \ldots, q_N$ are located at the points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ in $\mathbf{R}^3$ with spherical coordinates $(\rho_1, \alpha_1, \beta_1)$, $(\rho_2, \alpha_2, \beta_2), \ldots, (\rho_N, \alpha_N, \beta_N)$, respectively. Suppose further that all the points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ are located outside the sphere S_a of radius a centered at the origin. Then, for any point $\mathbf{x} \in S_a$ with coordinates (r, θ, ϕ), the potential $\Phi(\mathbf{x})$ generated by the sources $q_1, q_2, \ldots, q_N$ is described by the local expansion*

$$\Phi(\mathbf{x}) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} L_j^k \, i_j(\lambda r) \cdot Y_j^k(\theta, \phi), \tag{8}$$

where

$$L_j^k = 8\lambda \sum_{l=1}^{N} q_l \, k_j(\lambda \rho_l) \cdot Y_j^{-k}(\alpha_l, \beta_l). \tag{9}$$

Furthermore,

$$\left| \Phi(\mathbf{x}) - \sum_{j=0}^{p} \sum_{k=-j}^{j} L_j^k i_j(\lambda r) \cdot Y_j^k(\theta, \phi) \right| = O\left(\frac{r}{a}\right)^p. \tag{10}$$

Theorems 2.1 and 2.2 follow easily from Graf's addition theorem [1].

Remark 2.1. An important aspect of working with modified Bessel function expansions concerns scaling. Since $K_n(\lambda r) \approx (\lambda r)^{-n}$ and $I_n(\lambda r) \approx (\lambda r)^n$, a naive use of such expansions is likely to encounter underflow and overflow issues. To avoid this, one must scale expansions, replacing M_n^m with M_n^m/σ^n and L_n^m with $L_n^m \cdot \sigma^n$. To compensate for this scaling, we replace k_n with $k_n \cdot \sigma^n$ and i_n with i_n/σ^n when evaluating expansions. The parameter σ is chosen to be approximately λr, and the evaluation of the scaled terms for small σ is based on asymptotic expansions. This scaling must be carried through the entire fast multipole analysis described below, but we omit the details—the formulas are involved enough as they are.

2.1. Multipole and Local Translation Operators

The FMM relies on a variety of translation operators, acting on either multipole (far field) or solid harmonic (local) expansions. For the Laplace equation, the analogous operators are described in [4, 7, 10]. The proofs are straightforward but tedious.

THEOREM 2.3 (Multipole Translation). *Suppose that N charges of strengths $q_1, q_2, \ldots, q_N$ are located inside the sphere D of radius a centered at $\mathbf{x}_0 = (\rho, \alpha, \beta)$. Suppose further that for any point $\mathbf{x} = (r, \theta, \phi) \in R^3 \backslash D$, the potential due to these charges is given by the multipole expansion*

$$\Phi(\mathbf{x}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} O_n^m \, k_n(\lambda r') \cdot Y_n^m(\theta', \phi'), \tag{11}$$

where (r', θ', ϕ') *are the spherical coordinates of the vector* $\mathbf{x} - \mathbf{x}_0$. *Then, for any point* $\mathbf{x} = (r, \theta, \phi)$ *outside the sphere* D_1 *of radius* $(a + \rho)$ *centered at the origin, the field can be described by a shifted multipole expansion*:

$$\Phi(\mathbf{x}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_n^m \, k_n(\lambda r) \cdot Y_n^m(\theta, \phi). \tag{12}$$

Moreover,

$$\left| \Phi(\mathbf{x}) - \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m \, k_n(\lambda r) \cdot Y_n^m(\theta, \phi) \right| = O\left(\frac{a+\rho}{r} \right)^p. \tag{13}$$

The linear operator mapping the old multipole coefficients $\{O_n^m\}$ *to the new multipole coefficients* $\{M_n^m\}$ *will be denoted* $\mathcal{T}_{MM}$.

THEOREM 2.4 (Conversion of a Multipole Expansion to a Local Expansion). *Suppose that* N *charges of strengths* $q_1, q_2, \ldots, q_N$ *are located inside the sphere* D_{X_0} *of radius* a *centered at the point* $X_0 = (\rho, \alpha, \beta)$, *and that* $\rho > (c + 1)a$ *for some* $c > 1$. *Then the corresponding multipole expansion* (11) *converges inside the sphere* D_0 *of radius* a *centered at the origin. Furthermore, for any point* $X \in D_0$ *with coordinates* (r, θ, ϕ), *the potential due to the charges* $q_1, q_2, \ldots, q_N$ *can be described by a local expansion of the form*

$$\Phi(\mathbf{x}) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} L_j^k i_j(\lambda r) \cdot Y_j^k(\theta, \phi). \tag{14}$$

Furthermore, for any $p \geq 1$,

$$\left| \Phi(\mathbf{x}) - \sum_{j=0}^{p} \sum_{k=-j}^{j} L_j^k i_j(\lambda r) \cdot Y_j^k(\theta, \phi) \right| = O\left(\frac{1}{c} \right)^{p+1}. \tag{15}$$

The linear operator mapping the multipole coefficients $\{M_n^m\}$ *to the local coefficients* $\{L_n^m\}$ *will be denoted* $\mathcal{T}_{ML}$.

THEOREM 2.5 (Local Translation). *Suppose that* N *charges of strengths* $q_1, q_2, \ldots, q_N$ *are located outside the sphere* D *of radius* a *centered at the origin. Suppose further that for any point* $\mathbf{x} = (r, \theta, \phi) \in D$, *the potential due to these charges is given by the local expansion*

$$\Phi(\mathbf{x}) = \sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m \, i_n(\lambda r) \cdot Y_n^m(\theta, \phi). \tag{16}$$

If $\mathbf{x}_0 = (\rho, \alpha, \beta) \in D$, *then the field in the neighborhood of* $\mathbf{x}_0$ *can be described by a local expansion of the form*

$$\Phi(\mathbf{x}) = \sum_{n=0}^{p} \sum_{m=-n}^{n} N_n^m \, i_n(\lambda r') \cdot Y_n^m(\theta', \phi'), \tag{17}$$

where (r', θ', ϕ') *are the spherical coordinates of the vector* $\mathbf{x} - \mathbf{x}_0$. *Assuming* $\rho + r' < a$, *we also have*

$$\left| \Phi(\mathbf{x}) - \sum_{n=0}^{p} \sum_{m=-n}^{n} N_n^m \, i_n(\lambda r') \cdot Y_n^m(\theta', \phi') \right| = O\left(\frac{r}{a}\right)^p. \tag{18}$$

The linear operator mapping the old local coefficients $\{L_n^m\}$ *to the new local coefficients* $\{N_n^m\}$ *will be denoted* $\mathcal{T}_{LL}$.

Remark 2.2. The explicit formulas for $\mathcal{T}_{MM}$, $\mathcal{T}_{ML}$, and $\mathcal{T}_{LL}$ are extremely complex and we omit them. Moreover, the matrices representing the operators are dense, so that applying them to truncated expansions with $O(p^2)$ coefficients costs $O(p^4)$ operations. For both ease of analysis and speed of computation, it is advantageous to apply $\mathcal{T}_{MM}$, $\mathcal{T}_{ML}$, and $\mathcal{T}_{LL}$ in factored form.

We require three lemmas.

LEMMA 2.1. *Consider the multipole expansion* (11) *with respect to the center* $\mathbf{x}_0 = (\rho, \alpha, \beta)$. *If we rotate the coordinate system so that the z-axis is aligned with the spherical angle* (α, β), *then there exist coefficients* $R(n, m, m', \alpha, \beta)$ *such that*

$$\Phi(\mathbf{x}) = \sum_{n=0}^{\infty} \sum_{m'=-n}^{n} \tilde{O}_n^{m'} \, k_n(\lambda r') \cdot Y_n^{m'}(\theta'', \phi''),$$

where (r', θ'', ϕ'') *are the new coordinates of* $\mathbf{x}$ *and*

$$\tilde{O}_n^{m'} = \sum_{m=-n}^{n} R(n, m, m', \alpha, \beta) O_n^m. \tag{19}$$

The operator defined in the preceding expression we denote $\mathcal{R}(\alpha, \beta)$. We refer the reader to [2] for a complete discussion of rotation matrices and for a variety of methods which can be used to compute the matrix entries $R(n, m, m', \alpha, \beta)$.

LEMMA 2.2. *Suppose the multipole expansion* (11) *is centered at a point* $\mathbf{x}_0$ *which lies along the z-axis at a distance* ρ *from the origin. Then the coefficients of the shifted expansion* (12) *are given by*

$$M_n^m = \sum_{n'=m}^{\infty} C_m^{n,n'} \cdot M_{n'}^m, \tag{20}$$

where

$$C_m^{n,n'} = \sum_{k=m}^{\min(n,n')} \left(\frac{1}{2}\right)^k (-1)^{n'+k} (2n'+1) \frac{(n'-m)!(n+m)!(2k)!(\lambda\rho)^{-k} i_{n'+n-k}(\lambda\rho)}{(k+m)!(k-m)!(n'-k)!(n-k)!k!}. \tag{21}$$

We denote the corresponding translation operator by $\mathcal{T}_{MM}^z(\rho)$.

LEMMA 2.3. *Suppose* $\mathbf{x}_0$ *lies along the z-axis at a distance* ρ *from the origin. Then the coefficients of the shifted expansion* (17) *are given by*

$$L_n^m = \sum_{n'=m}^{\infty} C_m^{n,n'} \cdot O_{n'}^m, \tag{22}$$

where

$$C_m^{n,n'} = \sum_{k=m}^{\min(n,n')} \left(\frac{1}{2}\right)^k (2n'+1) \frac{(n'-m)!(n+m)!(2k)!(\lambda\rho)^{-k} i_{n'+n-k}(\lambda\rho)}{(k+m)!(k-m)!(n'-k)!(n-k)!k!}. \tag{23}$$

We denote the corresponding translation operator by $\mathcal{T}_{LL}^z(\rho)$.

Proof of Lemmas 2.2 and 2.3. Formula (21) follows from Graf's addition theorem [1] and some algebraic manipulation. It can also be deduced from the analysis of partial wave expansions in [5].

Combining Lemmas 2.1, 2.2, and 2.3, we see that a multipole or local expansion can be translated for a cost proportional to p^3 by the following procedure. First, rotate the system of coordinates so that the new z-axis points to the desired translation center. Then, translate the expansion via (20) or (22). Finally, rotate the translated expansion back to the original system of coordinates. Each of the three stages requires $O(P^3)$ operations. Formally, the scheme we have outlined corresponds to the factorizations

$$\mathcal{T}_{MM} = [\mathcal{R}(\alpha, \beta)]^{-1} \circ \mathcal{T}_{MM}^z(\rho) \circ \mathcal{R}(\alpha, \beta), \tag{24}$$

$$\mathcal{T}_{LL} = [\mathcal{R}(\alpha, \beta)]^{-1} \circ \mathcal{T}_{LL}^z(\rho) \circ \mathcal{R}(\alpha, \beta), \tag{25}$$

where (ρ, α, β) is the desired shifting direction.

It is possible to factor $\mathcal{T}_{ML}$ in a similar manner, but the corresponding numerical scheme is only marginally more efficient than the (naive) unfactored one. Instead, we introduce a completely different representation.

2.2. The Plane Wave Representation

The new generation of FMMs is based on introducing an additional approximation tool: exponential, or "plane wave" expansions. Given a source point $P = (x_0, y_0, z_0)$ and a target location $Q = (x, y, z)$, with $z > z_0$ and $r = \|P - Q\|$, we begin with the formula [15]

$$k_0(\lambda r) = \frac{\pi}{2} \frac{e^{-\lambda r}}{\lambda r} = \frac{1}{4\lambda} \int_0^{\infty} e^{-(u+\lambda)(z-z_0)} \int_0^{2\pi} e^{i\sqrt{u^2+2u\lambda}((x-x_0)\cos\alpha + (y-y_0)\sin\alpha)} d\alpha\, du. \tag{26}$$

We approximate the integral in (26) via an appropriately chosen quadrature formula. For the outer u integral, we use the weights and nodes derived in [19] for the harmonic case ($\lambda = 0$). For the inner α integral, we use the trapezoidal rule.

LEMMA 2.4. *Suppose that* $Q = (x_0, y_0, z_0)$ *and* $P = (x, y, z)$ *are points in* $\mathbf{R}^3$, *and that* $r = \|P - Q\|$. *Suppose further that the coordinates* $(x - x_0, y - y_0, z - z_0)$ *of the vector* $P - Q$ *satisfy the conditions*

$$1 \le z - z_0 \le 4, \quad 0 \le \sqrt{(x-x_0)^2 + (y-y_0)^2} \le 4\sqrt{2}. \tag{27}$$

Then, for any desired precision ε, we can write

$$\lambda\left|k_0(\lambda r)-\sum_{k=1}^{s(\varepsilon)}\frac{w_k}{M_k}\sum_{j=1}^{M_k}e^{-(u_k+\lambda)\cdot(z-z_0)}\cdot e^{i\sqrt{u_k^2+2u_k\lambda}\cdot[(x-x_0)\cdot\cos(\alpha_{j,k})+(y-y_0)\cdot\sin(\alpha_j,k)]}\right|<\varepsilon, \quad (28)$$

where the integers $s(\varepsilon)$ and the triplets $\{M_k, w_k, u_k | k=1,\ldots,s(\varepsilon)\}$ all depend on ε, and where $\alpha_{j,k}=2\pi j/M_k$. The total number of exponential basis functions used in (28) *will be denoted*

$$S_{exp}=\sum_{k=1}^{s(\varepsilon)}M_k. \quad (29)$$

The conditions (27) appear to be rather special. They are, however, related to the geometric refinement of space introduced by the FMM and their use will become clear in the next section.

The actual weights and nodes used are available in [4, 10, 19]. We reproduce only those needed for three-digit accuracy here in the Appendix, which shows that 114 exponentials are required. For 6- and 11-digit accuracy, 454 and 1868 exponentials are required, respectively. In all cases, a factor of two savings can be obtained by making use of the fact that $k_0(\lambda r)$ is real; from obvious symmetry considerations, one need only use the nodes with α restricted to $[0, \pi]$.

The following corollary provides an expansion of the form (28) for the potential generated by a collection of charges. It is an immediate consequence of Lemma 2.4.

COROLLARY 2.1. *Suppose that N charges of strengths $q_1, q_2, \ldots, q_N$ are located at points $X_1, X_2, \ldots, X_N$ in $\mathbf{R}^3$ with Cartesian coordinates $(x_1, y_1, z_1), (x_2, y_2, z_2), \ldots, (x_N, y_N, z_N)$, respectively. Suppose further that all points $X_1, X_2, \ldots, X_N$ are inside a cubic box b with unit volume centered at the origin and that the vector $X=(x, y, z)\in\mathbf{R}^3$ satisfies the conditions* (27). *Let $\Phi(X)$ denote the potential generated by the charges $q_1, q_2, \ldots, q_N$ and let Ψ_ε be defined by the formula*

$$\Psi_\varepsilon(X)=\sum_{k=1}^{s(\varepsilon)}\sum_{j=1}^{M_k}W(k,j)\cdot e^{-(u_k+\lambda)z}\cdot e^{i\sqrt{u_k^2+2u_k\lambda}\cdot(x\cdot\cos(\alpha_{j,k})+y\cdot\sin(\alpha_{j,k}))}, \quad (30)$$

with the coefficients $W(k, j)$ given by the formula

$$W(k,j)=\frac{w_k}{M_k}\sum_{l=1}^{N}q_l\cdot e^{(u_k+\lambda)z_l}\cdot e^{-i\sqrt{u_k^2+2u_k\lambda}\cdot(x_l\cdot\cos(\alpha_{j,k})+y_l\cdot\sin(\alpha_j,k))}, \quad (31)$$

for all $k=1,\ldots,s(\varepsilon)$, $j=1,\ldots,M_k$. Then, if $A=\sum_{l=1}^{N}|q_l|$, we have the estimate

$$|\Phi(X)-\lambda\Psi_\varepsilon(X)|<A_\varepsilon. \quad (32)$$

3. DATA STRUCTURES AND DIAGONAL TRANSLATION OPERATORS

For the sake of completeness, we briefly summarize the data structures used by the FMM, following the discussion of [4, 10].

The *computational domain* is defined to be the smallest cube in $\mathbf{R}^3$ containing all sources. We refer to this box as refinement level 0 and build a hierarchy of boxes recursively. Refinement level $l+1$ is obtained from level l by the subdivision of each box at level l into eight cubic boxes of equal size. In the nonadaptive case, this process is halted after roughly $\log_8 N$ levels, where N is the total number of sources under consideration.

DEFINITION 3.1. A box c is said to be a *child* of box b if box c is obtained by a single subdivision of box b. Box b is said to be the *parent* of box c.

Two boxes are said to be *colleagues* if they are at the same refinement level and share a boundary point. (A box is considered to be a colleague of itself.) The set of colleagues of a box b will be denoted *Coll*(b).

Two boxes are said to be *well separated* if they are at the same refinement level and are not colleagues.

With each box b is associated an *interaction list*, consisting of the children of the colleagues of b's parent, which are well separated from box b (Fig. 1).

Note that a box can have up to 27 colleagues and that its interaction list contains up to 189 boxes. Figure 1 depicts the colleagues and interaction list of a box in a two-dimensional setting.

The interaction list for each box will be further subdivided into six lists, associated with the six coordinate directions $(+z,\ -z,\ +y,\ -y,\ +x,\ -x)$. We will refer to the $+z$ direction as *up*, the $-z$ direction as *down*, the $+y$ direction as *north*, the $-y$ direction as *south*, the $+x$ direction as *east*, and the $-x$ direction as *west*.

DEFINITION 3.2 (Direction Lists). The *Uplist* for a box b consists of those elements of the interaction list which lie *above* b and are separated by at least one box in the $+z$-direction (Fig. 2).

The *Downlist* for a box b consists of those elements of the interaction list which lie *below* b and are separated by at least one box in the $-z$-direction.

The *Northlist* for a box b consists of those elements of the interaction list which lie *north* of b, are separated by at least one box in the $+y$-direction, and are not contained in the *Up-* or *Downlists*.

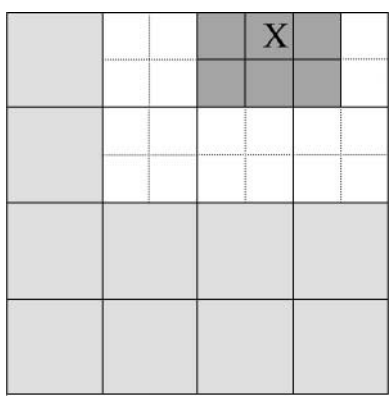

FIG. 1. The colleagues of a (two dimensional) box b are darkly shaded, while its interaction list is indicated in white. In three dimensions, a box b has up to 27 colleagues and its interaction list contains up to 189 boxes.

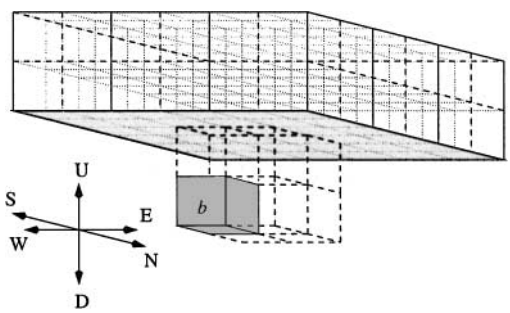

FIG. 2. The *Uplist* for the box b (see Definition 3.2).

The *Southlist* for a box b consists of those elements of the interaction list which lie *south* of b, are separated by at least one box in the $-y$-direction, and are not contained in the *Up-* or *Downlists*.

The *Eastlist* for a box b consists of those elements of the interaction list which lie *east* of b, are separated by at least one box in the $+x$-direction, and are not contained in the *Up-*, *Down-*, *North-*, or *Southlists*.

The *Westlist* for a box b consists of those elements of the interaction list which lie west of b, are separated by at least one box in the $-x$-direction, and are not contained in the *Up-*, *Down-*, *North-*, or *Southlists*.

For any box b, we will denote the number of elements in its *Uplist* by $N(Uplist(b))$ and adopt a similar convention for each of the remaining five lists.

It is easy to verify that the original interaction list is equal to the union of the *Up-*, *Down-*, *North-*, *South-*, *East-*, and *Westlists*. It is also easy to verify for two boxes, b, c, that

$$\begin{aligned} c \in Uplist(b) &\Leftrightarrow b \in Downlist(c), \\ c \in Northlist(b) &\Leftrightarrow b \in Southlist(c), \\ c \in Eastlist(b) &\Leftrightarrow b \in Westlist(c). \end{aligned} \tag{33}$$

Furthermore, suppose that two boxes, b and c, are of unit volume and that $c \in Uplist(b)$. Then for any point $X_0 = (x_0, y_0, z_0) \in b$ and any point $X = (x, y, z) \in c$, the vector $X - X_0 = (x - x_0, y - y_0, z - z_0)$ satisfies the inequality

$$1 \le z - z_0 \le 4, \quad 0 \le \sqrt{(x - x_0)^2 + (y - y_0)^2} \le 4\sqrt{2}. \tag{34}$$

This is precisely the condition (27) in Lemma 2.4.

3.1. Plane-Wave-Based Translation Operators

In three-dimensional fast multipole schemes, the operator $\mathcal{T}_{ML}$ (converting multipole expansions into local ones) is applied much more frequently then the operators $\mathcal{T}_{MM}$, $\mathcal{T}_{LL}$, which shift multipole and local expansions. Ignoring boundary effects, one ends up applying $\mathcal{T}_{ML}$ to the multipole expansion for each box in the interaction list—about 189 times when the charge distribution is uniform. The operators $\mathcal{T}_{MM}$, $\mathcal{T}_{LL}$, on the other hand, are applied roughly once per box. In the algorithm of this paper, the operators $\mathcal{T}_{MM}$, $\mathcal{T}_{LL}$ are applied via the order p^3 scheme described in Section 2.1; $\mathcal{T}_{ML}$ is applied by means of a much more complicated procedure, involving the plane wave representation introduced in Lemma 2.4.

Remark 3.1. A somewhat involved analysis shows that under the conditions of Lemma 2.4, $s(\varepsilon) \sim p$, where p is chosen according to (7) to achieve the same accuracy using a multipole expansion. Likewise, the total number of exponential basis functions S_{exp} in (30) is approximately the same as the total number of multipole moments (p^2) in order that the two expansions provide the same precision ε.

Expansions of the form (30) will be referred to as *exponential expansions*. Their main utility is that translation takes a particularly simple form.

THEOREM 3.1 (Diagonal Translation). *Suppose that a function* $\Psi_\varepsilon(X) : \mathbf{R}^3 \mapsto \mathbf{C}$ *is defined by the formula* (30), *which we view as an expansion centered at the origin for* $X = (x, y, z)$. *Then, for any vector* $X_0 = (x_0, y_0, z_0) \in \mathbf{R}^3$, *we have the shifted expansion*

$$\Psi_\varepsilon(X) = \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} V(k, j) \cdot e^{-(u_k+\lambda)(z-z_0)} \cdot e^{i\sqrt{u_k^2+2u_k\lambda}\cdot((x-x_0)\cdot\cos(\alpha_{j,k})+(y-y_0)\cdot\sin(\alpha_{j,k}))}, \quad (35)$$

where

$$V(k, j) = W(k, j) \cdot e^{-(u_k+\lambda)z_0} \cdot e^{i\sqrt{u_k^2+2u_k\lambda}\cdot(x_0\cdot\cos(\alpha_{j,k})+y_0\cdot\sin(\alpha_{j,k}))} \quad (36)$$

for $k = 1\ldots, s(\varepsilon)$, $j = 1, \ldots, M_k$.

DEFINITION 3.3. Formula (36) defines a linear operator mapping the coefficients $\{W(k, j)\}$ to the coefficients $\{V(k, j)\}$. This linear operator will be denoted $\mathcal{D}_{exp}$.

The operator $\mathcal{D}_{exp}$ provides a tool for translating expansions of the form (30) at a cost of $O(S_{exp}) \sim O(p^2)$ operations. In FMM algorithms, however, it is more efficient to use multipole and local expansions for communication between levels. Thus, to be able to use the diagonal translation operator $\mathcal{D}_{exp}$, linear operators converting multipole expansions into exponential expansions and exponential expansions into local expansions have to be constructed. The following two theorems provide such operators.

THEOREM 3.2. *Suppose that* N *charges of strengths* $q_1, q_2, \ldots, q_N$ *are located inside a box* b *of volume* d^3 *centered at the origin, that* ε *is a positive real number, and that* p *is an integer such that for any point* $X \in Uplist(b)$ *with spherical coordinates* (r, θ, ϕ), *the potential* $\Phi(X)$ *generated by the charges* $q_1, q_2, \ldots, q_N$ *satisfies the inequality*

$$\left| \Phi(X) - \sum_{n=0}^{p} \sum_{m=-n}^{n} \mathcal{O}_n^m \cdot Y_n^m(\theta, \phi) k_n(\lambda r) \right| < \varepsilon. \quad (37)$$

Then

$$\left| \Phi(X) - \lambda \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} W(k, j) \cdot e^{-(u_k+\lambda)\cdot(z/d)} \cdot e^{i\sqrt{u_k+2u_k\lambda}\cdot((x/d)\cdot\cos(\alpha_{j,k})+(y/d)\cdot\sin(\alpha_{j,k}))} \right| = O(\varepsilon), \quad (38)$$

where (x, y, z) *are the Cartesian coordinates of* X *and*

$$W(k, j) = \frac{\pi w_k}{2d\lambda M_k} \sum_{m=-p}^{p} i^{|m|} \cdot e^{im\cdot\alpha_{j,k}} \sum_{n=|m|}^{p} O_n^m \sqrt{\frac{2n+1}{4\pi}} \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}\left(\frac{\lambda+u_k}{\lambda}\right) \quad (39)$$

for $k = 1, \ldots, s(\varepsilon)$, $j = 1, \ldots, M_k$.

Proof. Suppose that $f_n(x_1, \ldots, x_p)$ is a homogeneous rational algebraic function of degree n, and that $F(x)$ is a smooth function of one variable. If we let $r^2 = x_1^2 + x_2^2 + \cdots + x_p^2$, then ([11], p. 126)

$$f_n\left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_p}\right) F(r^2) = \left\{ 2^n \frac{d^n F}{d(r^2)^n} + \frac{2^{n-2}}{1!} \frac{d^{n-1} F}{d(r^2)^{n-1}} \nabla^2 + \cdots \right.$$
$$\left. + \frac{2^{n-2m}}{m!} \frac{d^{n-m} F}{d(r^2)^{n-m}} \nabla^{2m} + \cdots \right\} f_n(x_1, x_2, \ldots, x_p), \quad (40)$$

where $\nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2}$. The result now follows by choosing $\{F(r^2) = k_0(\omega r), f_n = r^n P_n^{|m|}(\cos\theta) e^{im\phi}\}$, and a lot of algebra.

DEFINITION 3.4. Formula (39) defines a linear operator converting the coefficients $\{O_n^m\}$ into the coefficients $\{W(k, j)\}$. This linear mapping will be denoted $\mathcal{C}_{MX}$.

THEOREM 3.3. *Suppose that N charges of strengths $q_1, q_2, \ldots, q_N$ are located inside a box b of volume d^3 centered at the origin, that ε is a positive real number, and that for any point $X = (x, y, z) \in Uplist(b)$, the potential $\Phi(X)$ generated by the charges $q_1, q_2, \ldots, q_N$ satisfies the inequality*

$$\left| \Phi(X) - \lambda \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} W(k, j) \cdot e^{-(u_k+\lambda)\cdot(z/d)} \cdot e^{i\sqrt{u_k^2+2u_k\lambda}\cdot((x/d)\cdot\cos(\alpha_{j,k})+(y/d)\cdot\sin(\alpha_{j,k}))} \right| < \varepsilon. \quad (41)$$

Then there exists an integer p such that

$$\left| \Phi(X) - \sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m \cdot i_n(\lambda r) \cdot Y_n^m(\theta, \phi) \right| = O(\varepsilon), \quad (42)$$

where (r, θ, ϕ) are the spherical coordinates of X with respect to the box center and

$$L_n^m = (-1)^n i^{|m|} \sqrt{4\pi} \sqrt{2n+1} \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} \sum_{k=1}^{s(\varepsilon)} P_n^{|m|}\left(\frac{u_k+\lambda}{\lambda}\right) \sum_{j=1}^{M_k} W(k, j) \cdot e^{im\cdot\alpha_{j,k}}, \quad (43)$$

for $n = 0, \ldots, p$, $m = -n, \ldots, n$.

Proof. The desired formula (43) is obtained from a Taylor expansion of each exponential term in (41) and some algebraic manipulation.

DEFINITION 3.5. Formula (43) defines a linear operator converting the coefficients $\{W(k, j)\}$ into the coefficients $\{L_n^m\}$. This linear mapping will be denoted $\mathcal{C}_{XL}$.

Remark 3.2. It is easy to see that (39) can be evaluated numerically for $k = 1, \ldots, s(\varepsilon)$, $j = 1, \ldots, M_k$, at a cost proportional to p^3. Indeed, we first calculate $(2p+1) \cdot s(\varepsilon)$ quantities $F_{k,m}$ defined by the formula

$$F_{k,m} = \sum_{n=|m|}^{p} O_n^m \sqrt{\frac{2n+1}{4\pi}} \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}\left(\frac{\lambda d + u_k}{\lambda d}\right), \quad (44)$$

for $k = 1, \ldots, s(\varepsilon)$, $m = -p, \ldots, p$. This step requires $O(s(\varepsilon) \cdot p^2)$ operations. We then evaluate the coefficients $W(k, j)$ via the formula

$$W(k, j) = \frac{\pi w_k}{2\lambda d M_k} \sum_{m=-p}^{p} i^{|m|} \cdot e^{im \cdot \alpha_{j,k}} \cdot F_{k,m}, \tag{45}$$

for $k = 1, \ldots, s(\varepsilon)$, $j = 1, \ldots, M_k$, at a cost of $O(S_{exp} \cdot p)$ operations. Thus, the total cost of applying the operator $\mathcal{C}_{MX}$ to a pth-order multipole expansion is

$$Cost(\mathcal{C}_{MX}) \sim O(p^2 s(\varepsilon) + p S_{exp}) \sim O(p^3), \tag{46}$$

making use of Remark 3.1. A similar argument shows that the operator $\mathcal{C}_{XL}$ can also be evaluated numerically for a cost proportional to p^3.

Remark 3.3 (Multipole to Local Translation for the Uplist). Suppose that b, c are two boxes such that c is in the Uplist of b. Then the translation operator $\mathcal{T}_{ML}$ which converts a multipole expansion centered in b to a local expansion centered in c can be factored as

$$\mathcal{T}_{ML} = \mathcal{C}_{XL} \circ \mathcal{D}_{exp} \circ \mathcal{C}_{MX}. \tag{47}$$

Remark 3.4 (Multipole to Local Translation: General Case). The decomposition (47) of the operator $\mathcal{T}_{ML}$ is valid only when box c is in the Uplist of box b. When box c is not in the Uplist of box b, the operator $\mathcal{T}_{ML}$ can easily be applied by first rotating the system of coordinates, so that in the new coordinate system, box c lies in the Uplist of box b. This corresponds to the factorization

$$\mathcal{T}_{ML} = \mathcal{R}(\alpha, \beta)^{-1} \circ \mathcal{C}_{XL} \circ \mathcal{D}_{exp} \circ \mathcal{C}_{MX} \circ \mathcal{R}(\alpha, \beta), \tag{48}$$

where (α, β) describes the spherical angle of rotation.

4. THE FAST MULTIPOLE ALGORITHM

Remark 4.1. The procedure of the preceding section has been further accelerated. Symmetry considerations can be used to reduce the number of translations per box from 189 to 40 without any loss of precision. We refer the reader to [10] for details.

ALGORITHM.

[**Comment** The parent of a box j will be denoted $p(j)$. The list of children of a box j will be denoted $c(j)$. For each box j, the "outgoing" exponential expansion with coefficients $\{W(n, m)\}$, $n = 1, \ldots, s(\varepsilon)$; $m = 1, \ldots, M(n)$, will be denoted W_j. We will also associate an "incoming" exponential expansion with each box, denoted V_j.]

Upward Pass

Initialization

[**Comment** Choose the number of refinement levels $n \approx \log_8 N$, and the desired order p of the multipole expansion. The number of boxes at the finest level is then 8^n, and the average number of particles per box is $s = N/(8^n)$.]

Step 1

Form the multipole expansions $\Phi_{n,i}$ of the potential field due to particles in each box about the box center at the finest mesh level, via Theorem 2.1.

Step 2

Do for levels $l = n-1, \ldots, 2$,

Form multipole expansions $\Phi_{l,j}$ about the center of each box at level l by merging expansions from its eight children via Theorem 2.3.

$$\Phi_{l,j} = \sum_{k \in child(j)} \mathcal{T}_{MM} \Phi_{l+1,k}.$$

(In applying $\mathcal{T}_{MM}$, use the factorization of equation (25).)

End do

Downward Pass

Initialization

Set $\Psi_{1,1} = \Psi_{1,2} = \cdots = \Psi_{1,8} = (0, 0, \ldots, 0)$.

Step 3A

Do for levels $l = 2, \ldots, n$,

Form the expansion $\tilde{\Psi}_{l,j}$ for each box j at level l by using Theorem 2.5 to shift the local Ψ expansion of j's parent to j itself.

$$\tilde{\Psi}_{l,j} = \mathcal{T}_{LL} \Psi_{l-1,p(j)}.$$

(In applying $\mathcal{T}_{LL}$, use the factorization of equation (25).)

Set $\Psi_{l,j} = \tilde{\Psi}_{l,j}$.

Step 3B

[**Comment** For each direction $Dir = Up, Down, North, South, East, West$, the opposite direction will be denoted $-Dir$, so that $-Up = Down$, $-Down = Up$, etc. Thus, if a box B sends an outgoing expansion in direction Dir to box C on its $Dirlist$, then C can be viewed as receiving the expansion from B which is an element of its $-Dirlist$ (see Eq. (32)).]

Do for $Dir = Up, Down, North, South, East, West$,

For each box j at level l, convert the multipole expansion $\Phi_{l,j}$ into the "outgoing" exponential expansion for direction Dir.

$$W_j = C_{MX}^{Dir} \Phi_{l,j}.$$

For each box j at level l, collect the "outgoing" exponential expansions from the $-Dirlist$ of box j as an "incoming" exponential expansion

$$V_j = \sum_{k \in -Dirlist} \mathcal{D}_{\vec{kj}} W_k,$$

where $\mathcal{D}_{\vec{kj}}$ is the appropriately scaled vector from the center of box k to the center of box j in the rotated coordinate system.

For each box j at level l, convert the accumulated "incoming" exponential expansion V_j into a local harmonic expansion and add result to $\Psi_{l,j}$.

$$\Psi_{l,j} = \Psi_{l,j} + C_{XL}^{Dir} V_j.$$

End do

End do

Step 4

For each particle in each box j at the finest level n,
evaluate $\Psi_{n,j}$ at the particle position.

Step 5

For each particle in each box j at the finest level n,
compute interactions with particles in near neighbor boxes directly.

Remark 4.2. Step 1 requires approximately Np^2 work. Steps 2 and 3A require $(N/s)3p^3$ work. In Step 3B, the applications of the multipole to exponential operators $\mathcal{C}_{MX}^{Dir}$ and the exponential-to-local-operators $\mathcal{C}_{XL}^{Dir}$ require a total of approximately $20p^3(N/s)$ work, while the exponential translations require approximately $40p^2(N/s)$ work. Step 4 requires Np^2 work, and Step 5 requires $27Np$ work. Thus, a reasonable estimate for the total operation count (where we set the parameter $s = p$) is

$$67Np + 25Np^2. \tag{49}$$

With naive translation operators (requiring $O(p^4)$ work), the optimized estimate would be $216Np^2$, having set the parameter $s = p^2$.

Remark 4.3. The reader may have noticed that we have disregarded one vital issue, namely that the plane wave quadratures are designed for a box of unit dimensions. This requires an appropriate rescaling at every level of the FMM hierarchy. This is done on the fly, in the application of the "interlevel" translation operators $\mathcal{T}_{MM}$ and $\mathcal{T}_{LL}$. For optimal performance, we also precompute and store all of the exponentials needed at each level of the hierarchy.

5. NUMERICAL RESULTS

The algorithm described in Section 4 has been implemented in Fortran 77, and numerical experiments have been carried out for charges distributed randomly but uniformly in the cube $[-0.5, 0.5]^3$ using a 440 MHz Sun Ultra 10 workstation. The results of our experiments are summarized in Table I, with all timings given in seconds.

TABLE I
Timing Results for the FMM with Charges Uniformly Distributed in a Cube and $\lambda = 1$

N	Levels	p	S_{exp}	T_{fmm}	T_{dir}	Error
1,000	3	9	57	0.23	0.4	2.3×10^{-4}
8,000	4	9	57	1.9	26	3.5×10^{-4}
64,000	5	9	57	24	(1660)	1.6×10^{-4}
1,000	3	16	227	0.57	0.4	6.7×10^{-7}
10,000	4	16	227	5.4	48	7.3×10^{-7}
100,000	5	16	227	83	(4800)	6.8×10^{-7}
1,000	3	30	934	2.7	0.4	8.5×10^{-12}
10,000	3	30	934	13.8	48	6.3×10^{-12}
50,000	4	30	934	84	(1200)	7.1×10^{-12}

Numerical tests were performed with 3-, 6-, and 11-digit accuracy and the timings produced by the FMM were compared with those obtained by direct calculation. Because of obvious CPU considerations, it was not practical to apply the direct scheme to large-scale ensembles of particles. Thus, the direct algorithm was used to evaluate the potentials at 100 elements of the ensemble, and the resulting CPU time was extrapolated. Similarly, the accuracy of the algorithm was calculated at those 100 locations via the formula

$$E = \left(\frac{\sum_{i=1}^{N} |\Phi(x_i) - \tilde{\Phi}(x_i)|^2}{\sum_{i=1}^{N} |\Phi(x_i)|^2} \right)^{1/2}. \tag{50}$$

The following observations can be made from these tables.

1. The algorithm breaks even with the direct calculation at about $N = 750$ for three-digit precision, $N = 1500$ for six-digit precision, and $N = 5000$ for 11-digit precision.

2. The actual CPU time required by the nonadaptive FMM algorithm grows approximately linearly with the number of particles N. Because we are computing free-space interactions, there is a mild boundary effect at play; particles at the periphery of the unit cube are involved in fewer direct interactions than those near the center. As the number of levels increases, the relative number of such particles decreases, giving the (false) impression of slightly superlinear growth.

We have carried out similar studies for λ in the range $[10^{-9}, 10^{3}]$. The timing results vary by at most 20% from those listed in Table I. Larger values of λ involve such rapid decay that interactions can be effectively ignored.

6. CONCLUSIONS

We have described an FMM for screened Coulomb interactions based on a new diagonal form for translation operators. It is an extension of the "modern" FMM for the Laplace equation [4, 10]. Applications in biophysical simulations will be reported at a later date. An analogous procedure can be carried out for the Helmholtz equation at low frequency. The relevant plane–wave representation can be found in [8].

TABLE II
Nodes, Weights, and M_k^3 for Three-Digit Accuracy

k	Node	Weight	M_k^3
1	0.09927399673971	0.24776441819008	4
2	0.47725674637049	0.49188566500464	8
3	1.05533661382183	0.65378749137677	12
4	1.76759343354008	0.76433038408784	16
5	2.57342629351471	0.84376180565628	20
6	3.44824339201583	0.90445883985098	20
7	4.37680983554726	0.95378613136833	24
8	5.34895757205460	0.99670261613218	8
9	6.35765785313375	1.10429422730252	2

APPENDIX

The nodes and weights needed for discretization of the outer integral in Lemma 2.4 with three-digit accuracy are presented in Table II. Column 4 contains the number of discretization points needed in the inner integral, which we denote M_k^d. Tables for higher accuracy can be found in [4, 19].

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