We present a modification of the Fast Multipole Method (FMM) in two dimensions. While previous implementations of the FMM have been designed for harmonic kernels, our algorithm works for a large class of kernels that satisfy fairly general conditions, amounting to the kernel being sufficiently smooth away from the diagonal. Our algorithm approximates appropriately chosen parts of the kernel with "tensor products" of Legendre expansions and uses the Singular Value Decomposition (SVD) to compress the resulting representations. The obtained singular function expansions replace the Taylor and Laurent expansions used in the original FMM. The algorithm requires $O(N)$ operations, and is stable and robust.The performance of the algorithm is illustrated with numerical examples.

A Generalized Fast Multipole Method for Non-Oscillatory Kernels

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1 Introduction

In this paper, we describe a fast algorithm for the evaluation of all pairwise interactions in large ensembles of particles in the plane, i.e., sums of the form

$$u(x_i) = \sum_{j=1}^{N} q_j K(x_i, x_j), \tag{1}$$

where $q_1, \ldots, q_N$ are arbitrary complex numbers, $x_1, \ldots, x_n$ are points in the plane, and $K : R^2 \rightarrow R^2$ is a non-oscillatory kernel. Such computations appear in a variety of numerical methods for the solution of problems of computational physics.

The algorithm of this paper is a version of the Fast Multipole Method (FMM) in two dimensions. The structure of the FMM algorithm is left virtually unchanged from the one described by in [3]. The version of the FMM algorithm used in this paper, however, replaces the Taylor and Laurent expansions with "tensor products" of Legendre expansions that are subsequently compressed via the Singular Value Decomposition (SVD). This approach leads to an algorithm that can be applied to a variety of non-oscillatory kernels that are sufficiently smooth away from the diagonal.

In two dimensions, the original Fast Multipole Method (FMM) relies on the Taylor and Laurent expansions (see [14], [7]) for the evaluation of Coulomb interactions in large ensembles of particles. During the last decade, several improvements of the original scheme have been suggested. A new version of the FMM, based on specially designed singular function expansions, was introduced in [10]. The approach taken in the latter paper, when used in combination with an intermediate representation consisting of complex exponentials, leads to an algorithm that is about five times as fast as the original FMM, due to the reduction of the number of parameters needed to represent far and near fields. A similar technique was used in one dimension in [18]. A version of the FMM for polynomial interpolation (see [5]) uses Chebyshev expansions that are compressed by a suitable change of basis obtained via Singular Value Decomposition (SVD). Finally, an analytical apparatus based on least squares approximation of integral operators was developed in [17]. This analytical apparatus leads to fast algorithms for a fairly large class of kernels in one dimension.

The plan of the paper is as follows. In Section 2, we introduce mathematical and numerical preliminaries. In Sections 3 and 4, we describe a generalized Fast Multipole Method in two dimensions and present the complexity analysis. Finally, in Section 5, we demonstrate the performance of the algorithm with several numerical examples.

2 Mathematical Preliminaries

2.1 Gaussian Integration and Interpolation

In what follows, we will denote by $P_n^{a,b}$ the n-th Legendre polynomial on the interval $[a, b] \subset R$. We will refer to the roots $x_1^{a,b}, \ldots, x_n^{a,b}$ of $P_n^{a,b}(x)$ as the Gaussian nodes of order n and will denote by $w_1^{a,b}, \ldots, w_n^{a,b}$ the weights of the corresponding Gaussian quadrature on the interval $[a, b]$. We will denote by L_n the projection from the space of continuous functions on the interval $[a, b]$ to the space of polynomials of order n, preserving the function values at

the Gaussian nodes. For a given continuous function $f : [a,b] \to C$, the function $L_n f(x)$ is the polynomial of order n such that $L_n f(x_m^{a,b}) = f(x_m^{a,b})$. As is well known, for all $x \in [a,b]$,

$$L_n f(x) = \sum_{k=0}^{n-1} a_k \cdot P_k^{a,b}(x), \tag{2}$$

and the coefficients a_k are given by the formula

$$a_k = \sum_{m=1}^{n} w_m^{a,b} \cdot f(x_m^{a,b}) \cdot P_k(x_m^{a,b}). \tag{3}$$

The polynomial $L_n f$ will be referred to as n-th order Legendre expansion of the function f. For any integer n we will denote by $||L_n||_\infty$ the L^∞-norm of the operator L_n, defined by the formula

$$||L_n||_\infty = \sup_{||f||_{L^\infty[a,b]}=1} ||L_n f||_{L^\infty[a,b]}. \tag{4}$$

We will denote by $\alpha_1(x), \ldots, \alpha_n(x)$ the set of polynomials of order n defined by the formulae

$$\alpha_i(x) = \prod_{k=1, k\neq i}^{n} \frac{x - x_k}{x_i - x_k}, \quad i = 1, 2, \ldots, n, \tag{5}$$

where $x_1, \ldots, x_k$ are the Gaussian nodes of order n on the interval $[a,b]$. It is readily seen from (5) that for any continuous function $f : [a,b] \to C$,

$$L_n f(x) = \sum_{k=0}^{n-1} a_k \cdot P_k(x) = \sum_{i=1}^{n} f(x_i) \cdot \alpha_i(x). \tag{6}$$

For any natural n and continuous function $f : [a,b] \to C$, we will denote by $E_n f$ the error of the best approximation to f among all polynomials of order n, i.e.,

$$E_n f = \min_P ||f - P||_{L^\infty[a,b]}. \tag{7}$$

Let $\rho > 0$ be an arbitrary positive real number. For any analytic function $f : C \to C$, we will denote by $M([a,b], f, \rho)$ the maximum of the absolute value of f in the ρ-neighborhood of the interval $[a,b]$, i.e.,

$$M([a,b], f, \rho) = \sup_{x\in[a,b]} \sup_{\theta\in[-\pi,\pi]} |f(x + \rho e^{i\theta})|. \tag{8}$$

The following five lemmas are well known. Their proofs can be found, for example, in [16], [12].

Lemma 2.1. *If $n > 0$ is an integer, and $P : C \to C$ is a polynomial of order n, then for any interval $[a,b] \subset R$,*

$$\frac{1}{\sqrt{|b-a|}} ||P||_{L^2[a,b]} \leq ||P||_{L^\infty[a,b]} \leq \frac{n}{\sqrt{|b-a|}} ||P||_{L^2[a,b]}. \tag{9}$$

Lemma 2.2. *For any continuous function $f : [a, b] \to C$,*

$$||f - L_n f||_{L^\infty[a,b]} \leq (1 + ||L_n||_\infty) \cdot ||f - E_n f||_{L^\infty[a,b]}. \tag{10}$$

Lemma 2.3. *For any n times continuously differentiable function $f : [a, b] \to C$,*

$$||f - E_n f||_{L^\infty[a,b]} \leq \frac{2(b-a)^n}{4^n n!} \cdot ||f^{(n)}||_{L^\infty[a,b]}. \tag{11}$$

Lemma 2.4. *If $f : C \to C$ is an analytic function, then for any positive real $\rho > 0$,*

$$||f^{(n)}||_{L^\infty[a,b]} \leq n! \cdot \frac{M([a,b], f, \rho)}{\rho^n}. \tag{12}$$

Lemma 2.5. *For any natural n,*

$$||L_n||_\infty \leq n. \tag{13}$$

By combining (9), (10), (11), (12), and (13), we obtain the following theorem describing the rate of convergence of Legendre expansions of an analytic function on the interval $[a, b]$.

Lemma 2.6. *Suppose that $f : C \to C$ is an analytic function, and that for some positive $\rho > (b-a)/4$,*

$$M([a,b], f, \rho) < \infty. \tag{14}$$

Then

$$\lim_{n\to\infty} ||f - L_n f||_{L^\infty[a,b]} = 0. \tag{15}$$

Furthermore, for any $n \geq 1$,

$$||f - L_n f||_{L^\infty[a,b]} \leq 2(1+n) \cdot M([a,b], f, \rho) \cdot \left(\frac{b-a}{4\rho}\right)^n. \tag{16}$$

A standard approach to the construction of polynomial approximations of functions in higher dimensions is to expand them into "tensor products" of one-dimensional Legendre polynomials. For an m-dimensional cube $Q = [a_1, b_1] \times \ldots \times [a_m, b_m]$ and continuous function $f : Q \to C$, we will denote by $L_n f$ the (unique) polynomial of m variables having the form

$$L_n f(x_1, \ldots, x_m) = \sum_{k_1=0}^{n-1} \cdots \sum_{k_m=0}^{n-1} a_{k_1,\ldots,k_m} \cdot P_{k_1}^{a_1,b_1}(x_1) \cdot \ldots \cdot P_{k_m}^{a_m,b_m}(x_m), \tag{17}$$

and coinciding with f on the n^m "tensor product" Gaussian nodes

$$(x_{k_1}^{a_1,b_1}, \ldots, x_{k_m}^{a_m,b_m}), \quad k_1 = 1, \ldots, n; \ldots; k_m = 1, \ldots, n; \tag{18}$$

the coefficients $a_{k_1,\ldots,k_m}$ are given by the formula

$$a_{k_1,\ldots,k_m} = \sum_{k_1=0}^{n-1} \cdots \sum_{k_m=0}^{n-1} w_{k_1}^{a_1,b_1} \cdot \ldots \cdot w_{k_m}^{a_m,b_m} \cdot f(x_{k_1}^{a_1,b_1}, \ldots, x_{k_m}^{a_m,b_m}) \cdot P_{k_1}^{a_1,b_1}(x_{k_1}^{a_1,b_1}) \cdot \ldots \cdot P_{k_m}^{a_m,b_m}(x_{k_m}^{a_m,b_m}). \tag{19}$$

In a mild abuse of terminology, we will be referring to such polynomials as polynomials of order n in R^m and to expansions of the form (17) as Legendre expansions of order n in the cube $Q \in R^m$. For an analytic function $f : C^m \to C$, we will denote by $M(Q, f, \rho)$ the maximum of the absolute value of f in the ρ-neighborhood of the cube Q, i.e.,

$$M(Q, f, \rho) = \max_{k=1,\ldots,m} \sup_{x \in Q} \sup_{\theta \in [-\pi, \pi]} |f(x_1, \ldots, x_k + \rho e^{i\theta}, \ldots, x_m)|. \tag{20}$$

The following two lemmas are a simple consequence of Lemmas 2.1 and 2.6; they can be viewed as multidimensional analogues of the latter (see for example [17]).

Lemma 2.7. *If $n > 0$ is an integer and $P : C^m \to C$ is a polynomial of order n, then for any cube $Q = [a, b]^m \subset R^m$,*

$$\frac{1}{|b-a|^{m/2}} ||P||_{L^2(Q)} \leq ||P||_{L^\infty(Q)} \leq \frac{n^m}{|b-a|^{m/2}} ||P||_{L^2(Q)}. \tag{21}$$

Lemma 2.8. *Suppose that $f : C^m \to C$ is an analytic function on C^m, and that for some positive $\rho > (b-a)/4$,*

$$M([a, b]^m, f, \rho) < \infty. \tag{22}$$

Then, for any $n \geq 1$,

$$||f - L_n f||_{L^\infty[a,b]^m} \leq 2(1+n)^m \cdot M([a, b]^m, f, \rho) \cdot \left(\frac{b-a}{4\rho}\right)^n. \tag{23}$$

2.2 Singular Value Decomposition of Integral Operators

Let $T : L^2(Y) \to L^2(X)$ be integral operator given by the formula

$$(T \cdot f)(x) = \int_Y K(x, y) f(y)\, dy, \tag{24}$$

where K is a square integrable function on $X \times Y$, i.e.,

$$||K(x, y)||_{L^2(X \times Y)} = \left(\int \int_{X \times Y} |K(x, y)|^2\, dx\, dy \right)^{1/2} < +\infty. \tag{25}$$

The function $K : X \times Y \to R$ is usually referred to as the kernel of the integral operator T.

The following theorem can be found (in a more general form) in [15].

Theorem 2.9. *For any $K \in L^2(X \times Y)$, there exist two orthonormal systems of functions $\{u_k\} \in L^2(X)$, $\{v_k\} \in L^2(Y)$, and a sequence of nonnegative numbers $s_1 \geq s_2 \geq \ldots \geq 0$, for $k = 1, 2, \ldots$, such that*

$$K(x, y) = \sum_{k=1}^{\infty} u_k(x) s_k v_k(y), \tag{26}$$

in $L^2(X \times Y)$ sense,

$$\sum_{k=1}^{\infty} |s_k|^2 < +\infty, \tag{27}$$

and the sequence $\{s_k\}$ is uniquely determined by K.

Formula (26) is normally referred to as the singular value decomposition (SVD) of the operator T (or the kernel K). The functions u_k and v_k are usually referred to as the left and the right singular functions, respectively, and the numbers s_k are referred to as singular values of the operator K (or the kernel K).

The singular value decomposition can be used to construct finite-dimensional approximations to the operators of the form (24) and the corresponding kernels K. Specifically, given a positive real $\varepsilon > 0$, one can truncate the expression (26) after a finite number p of terms, leading to the expression

$$K(x,y) \approx \sum_{k=1}^{p} u_k(x) s_k v_k(y). \tag{28}$$

Now, if p has been chosen in such a manner that

$$\sqrt{\sum_{k=p+1}^{\infty} s_k^2} \leq \varepsilon, \tag{29}$$

then due to (26),

$$||K(x,y) - \sum_{k=1}^{p} u_k(x) s_k v_k(y)||_{L^2(X\times Y)} \leq \varepsilon. \tag{30}$$

Theorem 2.10 (Minimal property of the SVD). *Suppose that the SVD of the operator $T : L^2(Y) \to L^2(X)$ with the kernel $K : X \times Y \to R$ is given by the formula*

$$K(x,y) = \sum_{k=1}^{\infty} u_k(x) s_k v_k(y). \tag{31}$$

Then for any $f \in L^2(Y)$,

$$||(T \cdot f)(x) - \sum_{k=1}^{p} u_k(x) s_k b_k||_{L^2(X)} \leq s_{p+1} ||f||_{L^2(Y)}, \tag{32}$$

where the coefficients b_k are given by the formula

$$b_k = \int_Y f(y) v_k(y)\, dy. \tag{33}$$

2.3 Approximation of the SVD of Integrals Operators

The following theorem is a straightforward generalization of Theorem 2.10.

Theorem 2.11 (Approximation of the SVD). *Suppose that the operator $T : L^2(Y) \to L^2(X)$ is defined by (24), that there exist a positive number $\delta > 0$ and a square integrable function $\tilde{K} : X \times Y \to R$ such that*

$$||K(x,y) - \tilde{K}(x,y)||_{L^2(X\times Y)} \leq \delta, \tag{34}$$

and that the SVD of $\tilde{K}$ is given by the formula

$$\tilde{K}(x,y) = \sum_{k=1}^{\infty} \tilde{u}_k(x)\tilde{s}_k\tilde{v}_k(y). \tag{35}$$

Then for any $f \in L^2(Y)$,

$$||(T \cdot f)(x) - \sum_{k=1}^{p} \tilde{u}_k(x)\tilde{s}_k\tilde{b}_k||_{L^2(X)} \leq (\delta + \tilde{s}_{p+1})||f||_{L^2(Y)}, \tag{36}$$

where the coefficients $\tilde{b}_k$ are given by the formula

$$\tilde{b}_k = \int_Y f(y)\tilde{v}_k(y)\,dy. \tag{37}$$

Proof. Obviously, (34) implies

$$||\int_Y K(x,y)f(y)\,dy - \int_Y \tilde{K}(x,y)f(y)\,dy||_{L^2(X)} \leq \delta||f||_{L^2(Y)}, \tag{38}$$

and from Theorem 2.10, we obtain

$$||\int_Y \tilde{K}(x,y)f(y)\,dy - \sum_{k=1}^{p} \tilde{u}_k(x)\tilde{s}_k\tilde{b}_k||_{L^2(X)} \leq \tilde{s}_{p+1}||f||_{L^2(Y)}. \tag{39}$$

Now, (36) follows immediately from (38), (39), and the triangle inequality. □

3 Analytical Apparatus

In the remainder of this paper, we will be assuming that all charges are located in a unit square $[0,1] \times [0,1]$ in $\mathbf{R}^2$.

3.1 Notation

We will denote by $Y^{(l,k_1,k_2)}$ the square

$$Y^{(l,k_1,k_2)} = \left[\frac{k_1-1}{2^l}, \frac{k_1}{2^l}\right] \times \left[\frac{k_2-1}{2^l}, \frac{k_2}{2^l}\right], \tag{40}$$

where $l \geq 1$, $k_1 = 1, \ldots, 2^l$, $k_2 = 1, \ldots, 2^l$; l will be referred to as the level of the square $Y^{(l,k_1,k_2)}$, and (k_1, k_2) will be referred to as the coordinates of the square $Y^{(l,k_1,k_2)}$. We will denote by $Z^{(l,k_1,k_2)}$ the union of the square $Y^{(l,k_1,k_2)}$ and its immediate neighbors on the level l. We will denote the subset $X^{(l,k_1,k_2)}$ of $[0,1] \times [0,1]$ by the formula

$$X^{(l,k_1,k_2)} = [0,1] \times [0,1] \setminus Z^{(l,k_1,k_2)}, \tag{41}$$

and refer to $X^{(l,k_1,k_2)}$ as the interaction domain of the square $Y^{(l,k_1,k_2)}$. In other words, the interaction domain of the square $Y^{(l,k_1,k_2)}$ consists of all squares on level l that are

not immediate neighbors of $Y^{(l,k_1,k_2)}$ and not $Y^{(l,k_1,k_2)}$ itself. For consistency, we will also referring to the unit square $[0,1]\times[0,1]$ as $Y^{(0,1,1)}$.

Suppose now that the function $K : Y^{(0,1,1)} \times Y^{(0,1,1)} \rightarrow C$ is such that

$$\int_{X^{(l,k_1,k_2)}} \left(\int_{Y^{(l,k_1,k_2)}} |K(x,y)|^2 \, dy \right) dx < +\infty, \tag{42}$$

and

$$\int_{Y^{(l,k_1,k_2)}} \left(\int_{X^{(l,k_1,k_2)}} |K(y,x)|^2 \, dx \right) dy < +\infty, \tag{43}$$

for all $l \geq 1$, $k_1 = 1,\ldots,2^l$, $k_2 = 1,\ldots,2^l$. For any square $Y^{(l,k_1,k_2)}$, we will define the integral operators

$$P^{(l,k_1,k_2)} \;:\; L^2(Y^{(l,k_1,k_2)}) \rightarrow L^2(X^{(l,k_1,k_2)}), \tag{44}$$

$$R^{(l,k_1,k_2)} \;:\; L^2(X^{(l,k_1,k_2)}) \rightarrow L^2(Y^{(l,k_1,k_2)}), \tag{45}$$

by the formulae

$$(P^{(l,k_1,k_2)} \cdot \sigma)(x) = \int_{Y^{(l,k_1,k_2)}} K(x,y)\sigma(y)\, dy, \tag{46}$$

$$(R^{(l,k_1,k_2)} \cdot \sigma)(y) = \int_{X^{(l,k_1,k_2)}} K(y,x)\sigma(x)\, dx. \tag{47}$$

The function $(P^{(l,k_1,k_2)} \cdot \sigma) \in L^2(X^{(l,k_1,k_2)})$ with $\sigma \in L^2(Y^{(l,k_1,k_2)})$ will be referred to as the potential due to the charge distribution σ on the square $Y^{(l,k_1,k_2)}$. Similarly, the function $(R_{r_1}^{(l,k_1,k_2)} \cdot \sigma) \in L^2(Y^{(l,k_1,k_2)})$ with $\sigma \in L^2(X^{(l,k_1,k_2)})$ will be referred to as the incoming potential due to some charge distribution σ on $X^{(l,k_1,k_2)}$.

Due to (42), (43), and Theorem 2.9, there exist functions

$$\{u_k^{in,(l,k_1,k_2)}\} \in L^2(Y^{(l,k_1,k_2)}), \quad \{v_k^{out,(l,k_1,k_2)}\} \in L^2(Y^{(l,k_1,k_2)}), \tag{48}$$

$$\{u_k^{out,(l,k_1,k_2)}\} \in L^2(X^{(l,k_1,k_2)}), \quad \{v_k^{in,(l,k_1,k_2)}\} \in L^2(X^{(l,k_1,k_2)}), \tag{49}$$

and positive real numbers

$$\{s_k^{in,(l,k_1,k_2)}\}, \quad \{s_k^{out,(l,k_1,k_2)}\}, \tag{50}$$

such that

$$K(x,y) = \sum_{k=1}^{\infty} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} v_k^{out,(l,k_1,k_2)}(y), \tag{51}$$

$$K(y,x) = \sum_{k=1}^{\infty} u_k^{in,(l,k_1,k_2)}(y) s_k^{in,(l,k_1,k_2)} v_k^{in,(l,k_1,k_2)}(x). \tag{52}$$

We will refer to (51), (52) as the outgoing and incoming singular value decompositions for the square $Y^{(l,k_1,k_2)}$, respectively.

We will be using finite-dimensional approximations to the operators (44), (45) obtained by truncating expressions (51), (52) after a finite number of terms. Specifically, given two natural numbers p_1 and r_1, we will define the operators

$$P_{p_1}^{(l,k_1,k_2)} \;:\; L^2(Y^{(l,k_1,k_2)}) \rightarrow L^2(X^{(l,k_1,k_2)}), \tag{53}$$

$$R_{r_1}^{(l,k_1,k_2)} \;:\; L^2(X^{(l,k_1,k_2)}) \rightarrow L^2(Y^{(l,k_1,k_2)}) \tag{54}$$

by the formulae

$$(P_{p_1}^{(l,k_1,k_2)} \cdot \sigma)(x) = \int_{Y^{(l,k_1,k_2)}} K_{p_1}(x,y)\sigma(y)\,dy, \tag{55}$$

$$(R_{r_1}^{(l,k_1,k_2)} \cdot \sigma)(y) = \int_{X^{(l,k_1,k_2)}} K_{r_1}(y,x)\sigma(x)\,dx, \tag{56}$$

with

$$K_{p_1}(x,y) = \sum_{k=1}^{p_1} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} v_k^{out,(l,k_1,k_2)}(y), \tag{57}$$

$$K_{r_1}(y,x) = \sum_{k=1}^{r_1} u_k^{in,(l,k_1,k_2)}(y) s_k^{in,(l,k_1,k_2)} v_k^{in,(l,k_1,k_2)}(x). \tag{58}$$

Substituting (57), (58) into (55), (56), we obtain

$$(P_{p_1}^{(l,k_1,k_2)} \cdot f)(x) = \sum_{k=1}^{p_1} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{59}$$

with the coefficients $a_k^{out,(l,k_1,k_2)}$ given by the formula

$$a_k^{out,(l,k_1,k_2)} = \int_{Y^{(l,k_1,k_2)}} v_k^{out,(l,k_1,k_2)}(y)\sigma(y)\,dy, \tag{60}$$

and

$$(R_{r_1}^{(l,k_1,k_2)} \cdot \sigma)(y) = \sum_{k=1}^{r_1} u_k^{in,(l,k_1,k_2)}(y) s_k^{in,(l,k_1,k_2)} a_k^{in,(l,k_1,k_2)}, \tag{61}$$

with the coefficients $a_k^{in,(l,k_1,k_2)}$ given by the formula

$$a_k^{in,(l,k_1,k_2)} = \int_{X^{(l,k_1,k_2)}} v_k^{in,(l,k_1,k_2)}(x)\sigma(x)\,dx. \tag{62}$$

The function $(P_{p_1}^{(l,k_1,k_2)} \cdot \sigma) \in L^2(X^{(l,k_1,k_2)})$ with $\sigma \in L^2(Y^{(l,k_1,k_2)})$ will be referred to as the outgoing singular function expansion due to the charge distribution σ on the square $Y^{(l,k_1,k_2)}$. Similarly, the function $(R_{r_1}^{(l,k_1,k_2)} \cdot \sigma) \in L^2(X^{(l,k_1,k_2)})$ with $\sigma \in L^2(Y^{(l,k_1,k_2)})$ will be referred to as the incoming singular function expansion due to some charge distribution σ on $X^{(l,k_1,k_2)}$.

3.2 Singular Function Expansions of the Potentials

The following theorem provides a tool for approximating potentials produced by arbitrary charge distributions.

Theorem 3.1. *Suppose that the outgoing potential $g^{(l,k_1,k_2)} \in L^2(X^{(l,k_1,k_2)})$ is induced by the charge distribution $\sigma^{(l,k_1,k_2)} : L^2(Y^{(l,k_1,k_2)}) \to R$, i.e.*

$$g^{(l,k_1,k_2)}(x) = (P^{(l,k_1,k_2)} \cdot \sigma^{(l,k_1,k_2)})(x) = \int_{Y^{(l,k_1,k_2)}} K(x,y)\sigma^{(l,k_1,k_2)}(y)\,dy. \tag{63}$$

Then

$$g^{(l,k_1,k_2)}(x) = \sum_{k=1}^{\infty} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{64}$$

with the coefficients $a_k^{out,(l,k_1,k_2)}$ *given by the formula*

$$a_k^{out,(l,k_1,k_2)} = \int_{Y^{(l,k_1,k_2)}} \sigma^{(l,k_1,k_2)}(y) v_k^{out,(l,k_1,k_2)}(y)\, dy. \tag{65}$$

Furthermore, for any $p \geq 1$,

$$\begin{aligned} &||g^{(l,k_1,k_2)}(x) - \sum_{k=1}^{p} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}||_{L^2(X^{(l,k_1,k_2)})} \leq \\ &\leq s_{p+1}^{out,(l,k_1,k_2)} ||\sigma^{(l,k_1,k_2)}||_{L^2(Y^{(l,k_1,k_2)})}, \end{aligned} \tag{66}$$

and

$$\sum_{k=1}^{p} |a_k^{out,(l,k_1,k_2)}|^2 \leq ||\sigma^{(l,k_1,k_2)}||^2_{L^2(Y^{(l,k_1,k_2)})}. \tag{67}$$

Proof. (66) follows immediately from Theorem 2.10. Singular values $s_k^{out,(l,k_1,k_2)}$ converge to zero as $k \to \infty$; therefore, (66) implies (64). Finally, due to (65), $a_k^{out,(l,k_1,k_2)}$ are the coefficients in the orthonormal basis $\{v_k^{out,(l,k_1,k_2)}\}$, from which (67) follows immediately. □

3.3 Translation Operators and Error Bounds

The following three theorems constitute the principal analytical tool for manipulating outgoing and incoming singular function expansions. Theorems 3.2, 3.4 provide formulae for the translation of outgoing and incoming singular function expansions, respectively. Theorem 3.3 describes a mechanism for converting an outgoing singular function expansion into an incoming singular function expansion.

Theorem 3.2 (Outgoing to Outgoing). *Suppose that the outgoing singular function expansion* $g^{out,(l,k_1,k_2)} : L^2(X^{(l,k_1,k_2)}) \to R$ *is given by the formula*

$$g^{out,(l,k_1,k_2)}(x) = \sum_{k=1}^{\infty} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{68}$$

with the coefficients $a_k^{out,(l,k_1,k_2)}$ *such that*

$$\sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2 < +\infty, \tag{69}$$

and that $Y^{(l,k_1,k_2)} \subset Y^{(l-1,m_1,m_2)}$.

Then there exists a linear mapping

$$A^{(l-1,m_1,m_2),(l,k_1,k_2)} : l^2(N) \to l^2(N) \tag{70}$$

converting the sequence of coefficients $\{a_k^{out,(l,k_1,k_2)}\}$, $k = 1, 2, \ldots$ *into the sequence* $\{a_m^{out,(l-1,m_1,m_2)}\}$, $m = 1, 2, \ldots$, *defined by the formulae*

$$a_m^{out,(l-1,m_1,m_2)} = \sum_{k=1}^{\infty} A_{mk}^{(l-1,m_1,m_2),(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{71}$$

$$A_{mk}^{(l-1,m_1,m_2),(l,k_1,k_2)} = \int_{Y^{(l,k_1,k_2)}} v_k^{out,(l,k_1,k_2)}(y) v_m^{out,(l-1,m_1,m_2)}(y)\, dy, \tag{72}$$

such that for all x *inside* $X^{(l-1,m_1,m_2)}$,

$$g^{out,(l,k_1,k_2)}(x) = \sum_{m=1}^{\infty} u_m^{out,(l-1,m_1,m_2)}(x) s_m^{out,(l-1,m_1,m_2)} a_m^{out,(l-1,m_1,m_2)}. \tag{73}$$

Furthermore, for any $p \geq 1$,

$$||g^{out,(l,k_1,k_2)}(x) - \sum_{m=1}^{p} u_m^{out,(l-1,m_1,m_2)}(x) s_m^{out,(l-1,m_1,m_2)} a_m^{out,(l-1,m_1,m_2)}||_{L^2(X^{(l-1,m_1,m_2)})} \leq$$

$$\leq s_{p+1}^{out,(l-1,m_1,m_2)} \sqrt{\sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2}. \tag{74}$$

Proof. We observe that $g^{out,(l,k_1,k_2)}$ can be viewed as the potential

$$g^{out,(l,k_1,k_2)}(x) = \int_{Y^{(l,k_1,k_2)}} K(x,y) \sigma^{(l,k_1,k_2)}(y)\, dy \tag{75}$$

induced by the charge distribution $\sigma^{(l,k_1,k_2)} : L^2(Y^{(l,k_1,k_2)}) \to R$, defined by the formula

$$\sigma^{(l,k_1,k_2)}(y) = \sum_{k=1}^{\infty} a_k^{out,(l,k_1,k_2)} v_k^{out,(l,k_1,k_2)}(y). \tag{76}$$

We will denote by $\sigma^{(l-1,m_1,m_2)}$ the charge distribution on the square $Y^{(l-1,m_1,m_2)}$ given by the formula

$$\sigma^{(l-1,m_1,m_2)}(y) = \begin{cases} \sigma^{(l,k_1,k_2)}(y), & \text{if } y \in Y^{(l,k_1,k_2)}, \\ 0, & \text{if } y \in Y^{(l-1,m_1,m_2)} \backslash Y^{(l,k_1,k_2)}, \end{cases} \tag{77}$$

and by $g^{(l-1,m_1,m_2)}$ the outgoing potential on $X^{(l-1,m_1,m_2)}$ due to the distribution $\sigma^{(l-1,m_1,m_2)}$ on the square $Y^{(l-1,m_1,m_2)}$, i.e.,

$$g^{(l-1,m_1,m_2)}(x) = (P^{(l-1,m_1,m_2)} \cdot \sigma^{(l-1,m_1,m_2)})(x) =$$

$$= \int_{Y^{(l-1,m_1,m_2)}} K(x,y) \sigma^{(l-1,m_1,m_2)}(y)\, dy. \tag{78}$$

Due to Theorem 3.1,

$$g^{(l-1,m_1,m_2)}(x) = \sum_{m=1}^{\infty} u_m^{out,(l-1,m_1,m_2)}(x) s_m^{out,(l-1,m_1,m_2)} a_m^{out,(l-1,m_1,m_2)}, \tag{79}$$

with the coefficients $a_m^{out,(l-1,m_1,m_2)}$ defined by the formula

$$a_m^{out,(l-1,m_1,m_2)} = \int_{Y^{(l-1,m_1,m_2)}} \sigma^{(l-1,m_1,m_2)}(y) v_m^{out,(l-1,m_1,m_2)}(y)\, dy. \tag{80}$$

Now, using (77), we have

$$a_m^{out,(l-1,m_1,m_2)} = \int_{Y^{(l,k_1,k_2)}} \sigma^{(l,k_1,k_2)}(y) v_m^{out,(l-1,m_1,m_2)}(y)\, dy. \tag{81}$$

Substituting (76) into (81), we arrive at

$$a_m^{out,(l-1,m_1,m_2)} = \sum_{k=1}^{\infty} a_k^{out,(l,k_1,k_2)} \left(\int_{Y^{(l,k_1,k_2)}} v_k^{out,(l,k_1,k_2)}(y) v_m^{out,(l-1,m_1,m_2)}(y)\, dy \right) =$$

$$= \sum_{k=1}^{\infty} a_k^{out,(l,k_1,k_2)} A_{mk}^{(l,k_1,k_2),(l-1,m_1,m_2)}, \tag{82}$$

where

$$A_{mk}^{(l,k_1,k_2),(l-1,m_1,m_2)} = \int_{Y^{(l,k_1,k_2)}} v_k^{out,(l,k_1,k_2)}(y) v_m^{out,(l-1,m_1,m_2)}(y)\, dy. \tag{83}$$

Now, from the combination of (78) and Theorem 2.10, we obtain

$$\| \int_{Y^{(l-1,m_1,m_2)}} K(x,y)\sigma^{(l-1,m_1,m_2)}(y)\, dy -$$

$$\sum_{m=1}^{p} u_m^{out,(l-1,m_1,m_2)}(x) s_m^{out,(l-1,m_1,m_2)} a_m^{out,(l-1,m_1,m_2)} \|_{L^2(X^{(l-1,m_1,m_2)})} \leq$$

$$\leq s_{p+1}^{out,(l-1,m_1,m_2)} \|\sigma^{(l-1,m_1,m_2)}\|_{L^2(Y^{(l-1,m_1,m_2)})}. \tag{84}$$

Due to (77), we have

$$\| \int_{Y^{(l,k_1,k_2)}} K(x,y)\sigma^{(l,k_1,k_2)}(y)\, dy -$$

$$\sum_{m=1}^{p} u_m^{out,(l-1,m_1,m_2)}(x) s_m^{out,(l-1,m_1,m_2)} a_m^{out,(l-1,m_1,m_2)} \|_{L^2(X^{(l-1,m_1,m_2)})} \leq$$

$$\leq s_{p+1}^{out,(l-1,m_1,m_2)} \|\sigma^{(l,k_1,k_2)}\|_{L^2(Y^{(l,k_1,k_2)})}. \tag{85}$$

Thus,

$$\|g^{out,(l,k_1,k_2)}(x) - \sum_{m=1}^{p} u_m^{out,(l-1,m_1,m_2)}(x) s_m^{out,(l-1,m_1,m_2)} a_m^{out,(l-1,m_1,m_2)} \|_{L^2(X^{(l-1,m_1,m_2)})} \leq$$

$$\leq s_{p+1}^{out,(l-1,m_1,m_2)} \sqrt{\sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2}. \tag{86}$$

Finally, the singular values $s_k^{out,(l,k_1,k_2)}$ converge to zero as $k \to \infty$; therefore, (86) implies (73), and from the combination of (76), (77), (80), we have

$$\sum_{m=1}^{p} |a_m^{out,(l-1,m_1,m_2)}|^2 \leq \|\sigma^{(l-1,m_1,m_2)}\|^2_{L^2(Y^{(l-1,m_1,m_2)})} =$$

$$= \|\sigma^{(l,k_1,k_2)}\|^2_{L^2(Y^{(l,k_1,k_2)})} = \sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2. \tag{87}$$

□

The proof of the following two theorems is virtually identical to that of Theorem 3.2, and is omitted.

Theorem 3.3 (Outgoing to Incoming). *Suppose that the outgoing singular function expansion* $g^{out,(l,k_1,k_2)} : L^2(X^{(l,k_1,k_2)}) \to R$ *is given by the formula*

$$g^{out,(l,k_1,k_2)}(x) = \sum_{k=1}^{\infty} u_k^{out,(l,k_1,k_2)}(x) s_k^{out,(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{88}$$

with the real coefficients $a_k^{out,(l,k_1,k_2)}$ *such that*

$$\sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2 < +\infty, \tag{89}$$

and that $Y^{(l,m_1,m_2)} \subset X^{(l,k_1,k_2)}$.

Then there exists a linear mapping

$$B^{(l,m_1,m_2),(l,k_1,k_2)} : l^2(N) \to l^2(N) \tag{90}$$

converting the sequence of coefficients $\{a_k^{out,(l,k_1,k_2)}\}$, $k = 1, 2, \ldots$ *into the sequence* $\{a_m^{in,(l,m_1,m_2)}\}$, $m = 1, 2, \ldots$, *defined by the formulae*

$$a_m^{in,(l,m_1,m_2)} = \sum_{k=1}^{\infty} B_{mk}^{(l,m_1,m_2),(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{91}$$

$$B_{mk}^{(l,m_1,m_2),(l,k_1,k_2)} = \int_{Y^{(l,k_1,k_2)}} v_k^{out,(l,k_1,k_2)}(y) v_m^{in,(l,m_1,m_2)}(y)\, dy, \tag{92}$$

such that for all x *inside* $Y^{(l,m_1,m_2)}$,

$$g^{out,(l,k_1,k_2)}(x) = \sum_{m=1}^{\infty} u_m^{in,(l,m_1,m_2)}(x) s_m^{in,(l,m_1,m_2)} a_m^{in,(l,m_1,m_2)} \tag{93}$$

and

$$\sum_{m=1}^{\infty} |a_m^{in,(l,m_1,m_2)}|^2 \le \sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2. \tag{94}$$

Furthermore, for any $p \ge 1$,

$$||g^{out,(l,k_1,k_2)}(x) - \sum_{m=1}^{p} u_m^{in,(l,m_1,m_2)}(x) s_m^{in,(l,m_1,m_2)} a_m^{in,(l,m_1,m_2)}||_{L^2(Y^{(l,m_1,m_2)})} \le$$

$$\le s_{p+1}^{in,(l,m_1,m_2)} \sqrt{\sum_{k=1}^{\infty} |a_k^{out,(l,k_1,k_2)}|^2}. \tag{95}$$

Theorem 3.4 (Incoming to Incoming). *Suppose that the incoming singular function expansion* $g^{in,(l,k_1,k_2)} : L^2(Y^{(l,k_1,k_2)}) \to R$ *is given by the formula*

$$g^{in,(l,k_1,k_2)}(x) = \sum_{k=1}^{\infty} u_k^{in,(l,k_1,k_2)}(x) s_k^{in,(l,k_1,k_2)} a_k^{in,(l,k_1,k_2)}, \tag{96}$$

with the coefficients $a_k^{in,(l,k_1,k_2)}$ *such that*

$$\sum_{k=1}^{\infty} |a_k^{in,(l,k_1,k_2)}|^2 < +\infty, \tag{97}$$

and that $Y^{(l+1,m_1,m_2)} \subset Y^{(l,k_1,k_2)}$.

Then there exists a linear mapping

$$C^{(l+1,m_1,m_2),(l,k_1,k_2)} : l^2(N) \to l^2(N) \tag{98}$$

converting the sequence of coefficients $\{a_k^{in,(l,k_1,k_2)}\}$, $k = 1, 2, \ldots$ *into the sequence* $\{a_m^{in,(l+1,m_1,m_2)}\}$, $m = 1, 2, \ldots$, *defined by the formulae*

$$a_m^{in,(l,m_1,m_2)} = \sum_{k=1}^{\infty} C_{mk}^{(l+1,m_1,m_2),(l,k_1,k_2)} a_k^{out,(l,k_1,k_2)}, \tag{99}$$

where

$$C_{mk}^{(l+1,m_1,m_2),(l,k_1,k_2)} = \int_{X^{(l,k_1,k_2)}} v_k^{in,(l,k_1,k_2)}(y) v_m^{in,(l+1,m_1,m_2)}(y)\, dy, \tag{100}$$

such that for all y *inside* $Y^{(l+1,m_1,m_2)}$,

$$g^{in,(l,k_1,k_2)}(x) = \sum_{m=1}^{\infty} u_m^{in,(l+1,m_1,m_2)}(x) s_m^{in,(l+1,m_1,m_2)} a_m^{in,(l+1,m_1,m_2)} \tag{101}$$

and

$$\sum_{m=1}^{\infty} |a_m^{in,(l+1,m_1,m_2)}|^2 \le \sum_{k=1}^{\infty} |a_k^{in,(l,k_1,k_2)}|^2. \tag{102}$$

Furthermore, for any $p \ge 1$,

$$\| g^{in,(l,k_1,k_2)}(x) - \sum_{m=1}^{p} u_m^{in,(l+1,m_1,m_2)}(x) s_m^{in,(l+1,m_1,m_2)} a_m^{in,(l+1,m_1,m_2)} \|_{L^2(Y^{(l+1,m_1,m_2)})} \le$$

$$\le s_{p+1}^{in,(l+1,m_1,m_2)} \sqrt{\sum_{k=1}^{\infty} |a_k^{in,(l,k_1,k_2)}|^2}. \tag{103}$$

3.4 Singular Value Decompositions of Translation Operators

The algorithm of the following section (like its counterpart for harmonic fields described, for example, in [3]) depends on the efficient application of the translation operators (70), (90), (98) to arbitrary vectors. Clearly, these operators convert functions on the square

into functions on the square, and could be extremely expensive to deal with numerically. Fortunately, Theorems 2.7, 2.8 of Section 2 guarantee that (asymptotically speaking) the cost of applying each of the operators (70), (90), (98) to an arbitrary vector is of the order

$$c + d \cdot \log(\varepsilon)^4, \tag{104}$$

with the constants c, d independent of the operator to be applied (as long as the conditions of Theorem 2.8 are satisfied). We will discuss the procedure for the efficient numerical evaluation of the operator (90) in some detail; the operators (70), (98) are in this respect identical to the operator (90).

Let us consider the operator (90) with some m_1, m_2, k_1, k_2. Choosing some natural n, we construct an $n \times n$ tensor-product Gaussian discretization of each of the squares $Y^{(l,m_1,m_2)}$, $Y^{(l,k_1,k_2)}$, and expand the kernel K on $Y^{(l,m_1,m_2)} \times Y^{(l,k_1,k_2)}$ into a 4-dimensional tensor product Legendre series. Due to Theorem 2.8, the error of such an expansion is bounded by

$$b(1+n)^4 \cdot q^n, \tag{105}$$

where b is a positive constant and $|q| < 1$. Choosing $n = c + d \cdot \log(\varepsilon)$, we guarantee that the error of our expansion is less than any arbitrary a-priori prescribed ε. An examination of (105) shows that the length of the expansion required to obtain reasonable accuracy is not excessive, though it is considerably greater than the lengths expansions required for harmonic kernels (see, for example, [3]). An additional improvement in the required lengths of expansions is obtained by replacing the tensor-product Legendre expansions of the operators (70), (90), (98) with their Singular Value Decompositions via Theorems 2.9, 2.10, 2.11. The cost of this latter step (in terms of CPU time requirements) is of the order p^3, and would be excessive, except for the fact that this procedure has to be performed only once for each kernel, since the necessary SVDs can be precomputed and stored; needless to say, this requires an amount of storage proportional to $p \cdot n^2$.

Remark 3.5. *The situation is simplified when the kernel K is convolutional, i.e depends only on the difference between its arguments. Indeed, in this case, the SDVs of the translation operators* $A^{(l-1,m_1,m_2),(l,k_1,k_2)}$, $B^{(l,m_1,m_2),(l,k_1,k_2)}$, $C^{(l+1,m_1,m_2),(l,k_1,k_2)}$ *do not have to be calculated for all interacting pairs of squares on all levels, but only for all interactions of a single square on each level. In this case, the construction of the SVDs requires trivial amounts of both CPU time and disk space. When the kernel K is not only convolutional but possesses additional symmetry (rotational, up-down, etc.) the situation is further simplified.*

4 Generalized Fast Multipole Method in Two Dimensions

4.1 Notation

In this section we will introduce the notation to be used in the description of the algorithm.

For any subset A of the computational box, $T(A)$ will denote the set of particles inside A.

B_l is the set of all nonempty boxes at the level l. B_0 will denote the computational box itself.

If box contains more than s particles, it is called a *parent* box. Otherwise, the box is said to be *childless*. Note that s is the maximum number of points in a childless box.

A *child* box is nonempty box obtained from the division of a parent box into four.

Colleagues are adjacent boxes of the same size at the same level. A given box has at most eight colleagues.

Two boxes b and c are said to be *well separated* if they are separated a distance greater or equal to the length of the size of the smallest box.

With each box b at the level l, we will associate five lists of other boxes.

List 1 of a box b will be denoted by U_b. It is empty if b is a parent box. If b is childless, it consists of b and of all childless boxes c that are adjacent to b.

List 2 of a box b will be denoted by V_b. It consists of all boxes c that are children of the colleagues of the b's parent and that are well separated from b.

List 3 of a box b will be denoted by W_b. It is empty if b is a parent box. If b is childless, it consists of all descendants of b's colleagues whose parent are adjacent to b but who are not adjacent to b themselves. Note that b is separated from each box c in W_b by a distance greater or equal to the length of the size of c.

List 4 of a box b will be denoted by X_b. It consists of all boxes c such that $b \in W_c$. Note that all boxes in List 4 are childless and larger that b.

List 5 of a box b will be denoted by Y_b. It consists of all boxes c that are well separated from b's parent.

Φ_b will denote the p-term outgoing singular function expansion for the box b.

Ψ_b will denote the p-term incoming singular function expansion for the box b.

Γ_b will denote the p-term incoming singular function expansion for the box b due to all particles in $T(V_b)$.

Δ_b will denote the p-term incoming singular function expansion for the box b due to all charges in $T(X_b)$.

$\Psi_b(r)$ is the result of evaluation of the expansion Ψ_b at a particle $r \in T(b)$.

$\alpha_b(r)$ will denote the potential at $r \in T(b)$ due to all particles in $T(U_b)$.

$\beta_b(r)$ will denote the potential at $r \in T(b)$ due to all particles in $T(W_b)$.

$\gamma_b(r)$ will denote the potential at $r \in T(b)$ due to all particles in $T(Y_b)$.

$F(r)$ will denote the potential at r.

$A_{b,c}$ will denote the translation operator (a $p \times p$ matrix) in the Theorem 3.2 for the boxes b and c such that $b = Y^{(l-1,m_1,m_2)}$ and $c = Y^{(l,k_1,k_2)}$.

$B_{b,c}$ will denote the translation operator (a $p \times p$ matrix) in the Theorem 3.3 for the boxes b and c such that $b = Y^{(l,m_1,m_2)}$ and $c = Y^{(l,k_1,k_2)}$.

$C_{b,c}$ will denote the translation operator (a $p \times p$ matrix) in the Theorem 3.4 for the boxes b and c such that $b = Y^{(l+1,m_1,m_2)}$ and $c = Y^{(l,k_1,k_2)}$.

4.2 Informal Description of the Algorithm

1. Create the adaptive quad-tree. Compute the outgoing and incoming singular functions for each box in the computational tree, by the means of the Theorem 2.11.

2. For each childless box b, the interactions between particles in $T(b)$ and $T(U_b)$ are evaluated directly. For each particle $r \in T(b)$ the result is $\alpha_b(r)$.

3. For each childless box b, form an outgoing singular function expansion Φ_b by the means of Theorem 3.1. For each parent box b, use Theorem 3.2 to translate and merge the outgoing singular function expansions of its children into the outgoing singular function expansion Φ_b.

4. Use Theorem 3.3 to convert the outgoing singular expansion of each box in V_b into the incoming singular function expansion in the box b, adding the resulting expansions together to obtain Γ_b.

5. Convert the potential of all particles in $T(X_b)$ into a incoming singular function expansion in the box b, adding the resulting expansions to obtain Δ_b. Add Δ_b to Γ_b.

6. For each childless box b, evaluate the potential $\beta_b(r)$ due to all particles in $T(W_b)$ by evaluating the outgoing singular function expansions Φ_c for each box $c \in W_b$.

7. Translate the incoming singular function expansion Γ_B of b's parent B to the box b by the means of Theorem 3.4. Add the resulting local expansion to Γ_b.

8. For each childless box b, evaluate the local expansion Γ_b at every particle $r \in b$ and add the result to $\alpha_b(r)$ and $\beta_b(r)$, obtaining the potential $F(r)$ at r.

4.3 Detailed Description of the Algorithm

Step 1: Initialization

Comment [Set the order n of Legendre expansions, the number of terms p in all singular function expansions, and the maximum number s of the particles in a childless box. Create the computational tree.]

do $l = 0, 1, 2, \ldots$
  do $b \in B_l$
    if b contains more than s particles **then**
      subdivide b into four smaller boxes,
      ignore empty boxes, add nonempty boxes to B_{l+1}.
    endif
  enddo
enddo

Comment [For each box b in the computational tree, compute the outgoing and incoming singular value decompositions of the kernel K.]

do $l = 0, 1, 2, \ldots$
  do $b \in B_l$
    Set $b = Y^{(l,k_1,k_2)}$. Compute two singular value decompositions for $x \in X^{(l,k_1,k_2)}$, $y \in Y^{(l,k_1,k_2)}$.

$$K(x,y) = \sum_{k=1}^{\infty} u_{b;k}^{out}(x) \cdot s_{b;k}^{out} \cdot v_{b;k}^{out}(y),$$

$$K(y,x) = \sum_{k=1}^{\infty} u_{b;k}^{in}(y) \cdot s_{b;k}^{in} \cdot v_{b;k}^{in}(x).$$

enddo
enddo

Step 2: Local Interactions

Comment [For each childless box b, evaluate interactions with the particles in $T(U_b)$ directly, obtaining the potential due to nearby particles.]

do $l = 0, 1, 2, \ldots$
do $b \in B_l$, b is childless
do $x_i \in T(b), x_j \in T(U_b)$

$$\alpha_b(x_i) = \alpha_b(x_i) + \sum_j q_j \cdot K(x_i, x_j).$$

enddo
enddo
enddo

Cost [$9(N/s) \cdot s \cdot s + 8(N/s) \cdot s \cdot s$ operations.]

Step 3: Outgoing Singular Function Expansions

Comment [For each childless box b, form the outgoing singular function expansion Φ_b.]

do $l = 0, 1, 2, \ldots$
do $b \in B_l$, b is childless
Evaluate the coefficients of the outgoing singular function expansion for the square b by the means of the Theorem 3.1.,

$$\Phi_{b;k} = \sum_{x_j \in b} q_j \cdot v_{b;k}^{out}(x_j),$$

for all $k = 1, \ldots, p$.
enddo
enddo

Cost [Np operations.]

Step 4: Upward Sweep

Comment [For each parent box b, form the outgoing singular function expansion Φ_b by translating the outgoing singular function expansions of b's children and adding the resulting expansions together.]

do $l = \ldots, 2, 1, 0$
  do $b \in B_l$, b is a parent box
    Use Theorem 3.2 to translate and merge the outgoing singular function expansions of $b's$ children b_1, b_2, b_3, b_4 into the outgoing singular function expansion Φ_b

$$\Phi_b = \Phi_b + A_{b,b_1} \cdot \Phi_{b_1} + A_{b,b_2} \cdot \Phi_{b_2} + A_{b,b_3} \cdot \Phi_{b_3} + A_{b,b_4} \cdot \Phi_{b_4}$$

  enddo
enddo

Cost [$(4/3)(N/s) \cdot p^2$ operations.]

Step 5: Adaptive Part

Comment [For each childless box b, form the incoming singular function expansion Δ_b due to particles located in List 4 of b.]

do $l = 0, 1, 2, \ldots$
  do $b \in B_l$, b is childless
    Use Theorem 3.1 to evaluate the coefficients of the incoming singular function expansion Δ_b for the square b

$$\Delta_{b;k} = \sum_{x_i \in X_b} q_i \cdot v^{in}_{b;k}(x_i),$$

    for all $k = 1 \ldots, p$.
  enddo
enddo

Cost [$8(N/s) \cdot p \cdot s$ operations.]

Comment [For each box b, evaluate the outgoing singular function expansion Φ_b at each particle located in boxes c in List 4 of b.]

do $l = 0, 1, 2, \ldots$
  do $b \in B_l$, b is childless
    do $x_i \in X_b$

$$\beta_b(x_i) = \beta_b(x_i) + \sum_{k=1}^{p} \Phi_{b;k} \cdot s_{b;k}^{out} \cdot u_{b;k}^{out}(x_i).$$

enddo
enddo
enddo

Cost [$8(N/s) \cdot p \cdot s$ operations.]

Step 6: Outgoing to Incoming

Comment [For each box b, convert the outgoing singular function expansion Φ_c for each box c in List 2 of b, into the incoming singular function expansion Γ_b, adding the resulting expansions together.]

do $l = 0, 1, 2, \ldots$
do $b \in B_l$

For all boxes $c \in V_b$, convert the outgoing singular function expansion into the incoming singular function expansion for the box b by the means of Theorem 3.3. Add the resulting singular function expansions to Γ_b

$$\Gamma_b = \Gamma_b + \sum_{c \in V_b} B_{b,c} \cdot \Phi_c.$$

Add Γ_b and Δ_b to obtain the incoming singular function expansion Ψ_b

$$\Psi_b = \Gamma_b + \Delta_b.$$

enddo
enddo

Cost [$27 \cdot (4/3)(N/s) \cdot p^2$ operations.]

Step 7: Downward Sweep

Comment [For every parent box b, translate the incoming singular function expansion Ψ_b to b's children incoming singular function expansions.]

do $l = 0, 1, 2, \ldots$
do $b \in B_l$, b is a parent box
do $c \in B_{l+1}$, c is a $b's$ child

Translate the incoming singular function expansion Ψ_b by the means of Theorem 3.4. Add the resulting local expansion to Ψ_c

$$\Psi_c = \Psi_c + C_{c,b} \cdot \Psi_b.$$

enddo
enddo
enddo

Cost [$(4/3)(N/s) \cdot p^2$ operations.]

Step 8

Comment [For every childless box b, evaluate incoming singular function expansions Ψ_b at each particle, obtaining the potential due to distant particles. Find the potential at $r \in b$ by adding $\alpha_b(r)$, $\beta_b(r)$, $\gamma_b(r)$ together.]

do $l = 0, 1, 2, \ldots$
do $b \in B_l$, b is childless
For each particle $x_j \in b$, evaluate

$$\gamma_b(x_j) = \sum_{k=1}^{p} \Psi_{b;k} \cdot s_{b;k}^{in} \cdot u_{b;k}^{in}(x_j).$$

Add $\alpha_b(x_j)$, $\beta_b(x_j)$, $\gamma_b(x_j)$ to obtain the potential $F(x_j)$ at $x_j \in b$

$$F(x_j) = \alpha_b(x_j) + \beta_b(x_j) + \gamma_b(x_j).$$

enddo
enddo

Cost [$N \cdot p$ operations.]

4.4 Complexity of the Algorithm

Since s is the average number of particles in a childless box at the finest level, there are approximately N/s childless boxes, and approximately

$$B = (1 + 1/4 + 1/4^2 + \ldots) \cdot (N/s) = \frac{4}{3} \cdot \frac{N}{s} \tag{106}$$

boxes in the tree hierarchy. Therefore, Step 3 requires Np work, Step 4 requires Bp^2 work, Step 6 requires $27Bp^2$ work, Step 7 requires Bp^2 work, Step 8 requires Np work, and Step 2 requires $9 \cdot N/s \cdot s \cdot s = 9Ns$ work. Thus, a reasonable estimate for the total operation count is

$$9Ns + 2Np + 29Bp^2 = 9Ns + 2Np + 29 \cdot \frac{4}{3} \cdot \frac{N}{s} \cdot p^2. \tag{107}$$

With $s = 2p$, the operation count becomes approximately

$$40\,Np. \tag{108}$$

The adaptive part of the algorithm in the Step 5 requires $O(8(N/s)ps + 8(N/s)ps) = O(16Np)$ work, and Step 3 requires additional $O(8(N/s)s^2) = O(8Ns)$ work. The total operation count is

$$17Ns + 18Np + 29Bp^2 = 17Ns + 18Np + 29(4/3)(N/s)p^2. \tag{109}$$

By setting $s = 1.5p$, the operation count becomes approximately

$$69\,Np. \tag{110}$$

5 Numerical Results

A FORTRAN program has been written implementing the algorithm described in the preceding section. All timings listed below correspond to calculations performed on an UltraSparc-I/167 computer with 128MB RAM, using double precision arithmetic. The order of Legendre expansions was $n = 4$, $n = 8$, and $n = 16$ and the number of singular functions varied from $p = 9$ to $p = 36$ to $p = 90$ in order to achieve roughly 3, 6 and 10 digits accuracy, respectively.

The results of these experiments are presented in the tables below. The first column contains the number of particles used in the simulation. The second column contains the time for construction of the computational tree and precomputation of values singular functions at locations of particles. This can be done once for any given configuration of particles. We do not include the time for precomputation of singular value decompositions in this column, since this can be done in advance for any given kernel. The third column contains the total run time of the algorithm. The fourth and the fifth columns contain the actual time required by the algorithm and the time required by the direct algorithm, respectively.

Finally, the last two columns contain the relative 2-norm E_2 and the relative maximum error E_∞ obtained at any one particle. They are defined by the formulae

$$E_2 = \left(\frac{\sum_{i=1}^N |f_i - \tilde{f}_i|^2}{\sum_{i=1}^N |f_i|^2} \right)^{1/2}, \quad E_\infty = \max_i \frac{|f_i - \tilde{f}_i|}{|f_i|}, \tag{111}$$

where f_i is the value of the potential at the i-th particle position obtained by the direct calculation, and $\tilde{f}_i$ is the result obtained by the algorithm.

For the first set of tests, the positions of particles were uniformly distributed in the unit square. For the second set of tests, two fifth of charged particles were distributed uniformly along two ellipses and the remaining of particles were distributed randomly in three circles with a gaussian density. The number of terms in the singular function expansions was set to 9, 36 and 90, and the number of particles in a childless box was set to 15, 61, and 153, respectively.

Several observations can be made from Tables 1–12 below, and from the more extensive numerical experiments performed by the authors.

1. The number of singular functions required to obtain 3-digit accuracy is 9; the corresponding order of the Legendre expansions is 4. The 6-digit scheme requires 36-term singular-function expansions, and Legendre expansions of order 8. In order to obtain 10

digits, we used 90-term singular function expansions, and obtained these (during the pre-computation stage) by starting with Legendre expansions of order 16.

2. For the 3-digit version of the scheme, the break-even point with the direct scheme is $n \sim 200$; for 6 digits, the break-even point is $n \sim 800$, and for 10-digits the scheme becomes faster than the direct one at $n \sim 3000$.

3. The efficiency of the algorithm does not suffer significantly when the charges in the simulation are clustered. On the other hand, unlike its counterpart for harmonic kernels, the algorithm of this paper does not seem to derive any advantage from the clustering of particles in the simulation.

4. The cost of the algorithm grows rapidly with the increase of accuracy requirements. The algorithm is considerably slower than modern versions of the FMM for harmonic fields, especially in high-accuracy environments (see, for example, [10]).

5.1 Generalizations and Conclusions

The algorithm of this paper has an obvious analogue in three dimensions: quad-trees are replaced with oct-trees, two-dimensional expansions are replaced with three-dimensional ones, and the programming becomes more involved. Such a scheme has been implemented (see [6]), and found to work satisfactorily, as long as the required precision is low. For accuracies better than three or four digits, the CPU time requirements of the three-dimensional scheme become excessive.

For many kernels, the algorithm of this paper can be accelerated via an approach similar to the one used by [4], [9], [10] to accelerate the FMM for harmonic fields in two and three dimensions. Specifically, most the operators (70), (90), (98) can be diagonalized; this requires that the kernel K be approximated by linear combinations of exponentials on appropriately chosen parts of the product $Y^{(l,k_1,k_2)} \times X^{(l,k_1,k_2)}$. Needless to say, this can not be done for a "general" kernel K; however, it appears to be possible for many kernels (and classes of kernels) of interest. Such a scheme would require several developments (both analytic and numerical); it would accelerate the two-dimensional version of the algorithm significantly. The real pay-off of such a project would be in three dimensions, where it would be likely to make large-scale high-precision simulations feasible.

6 Acknowledgments

We would like to thank Professor Leslie Greengard for many useful discussions and suggestions.

Figure 1: The computational box and three levels of refinement.

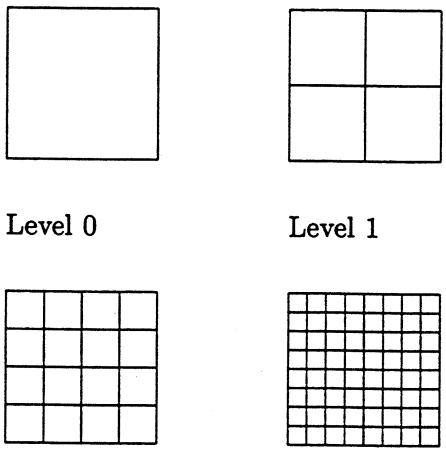


Figure 2: Non-uniform distribution of charges and its associated adaptive quad-tree.

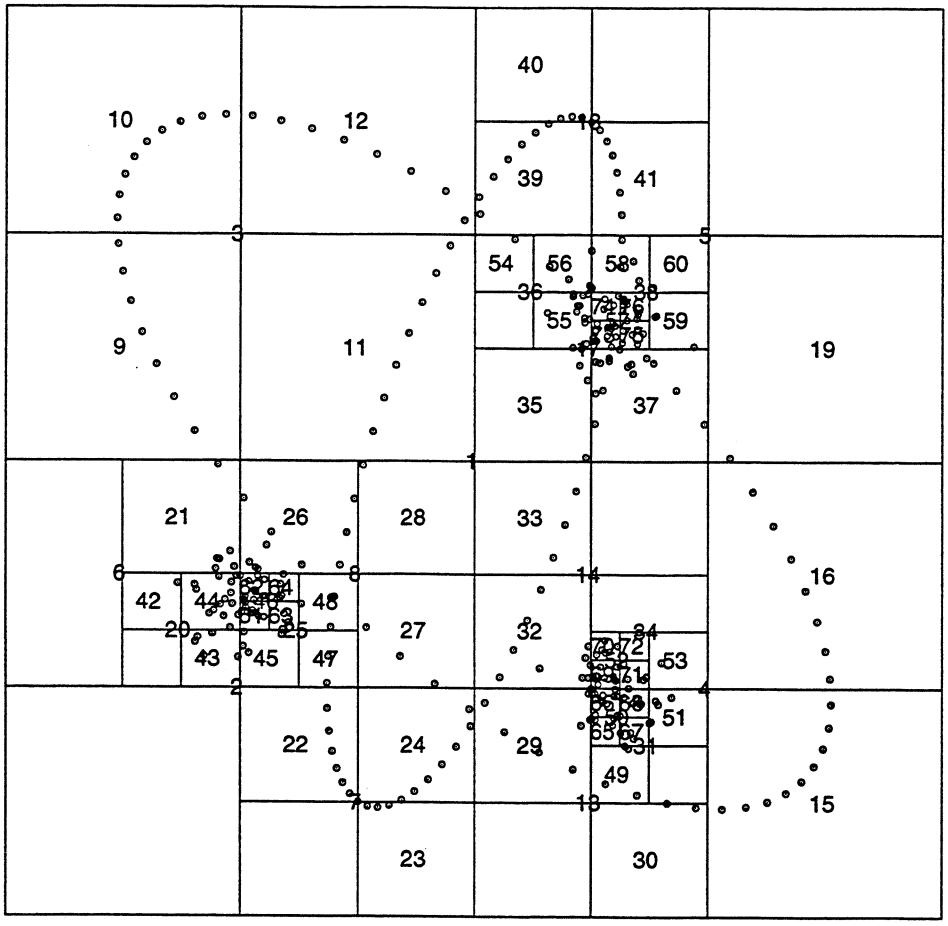
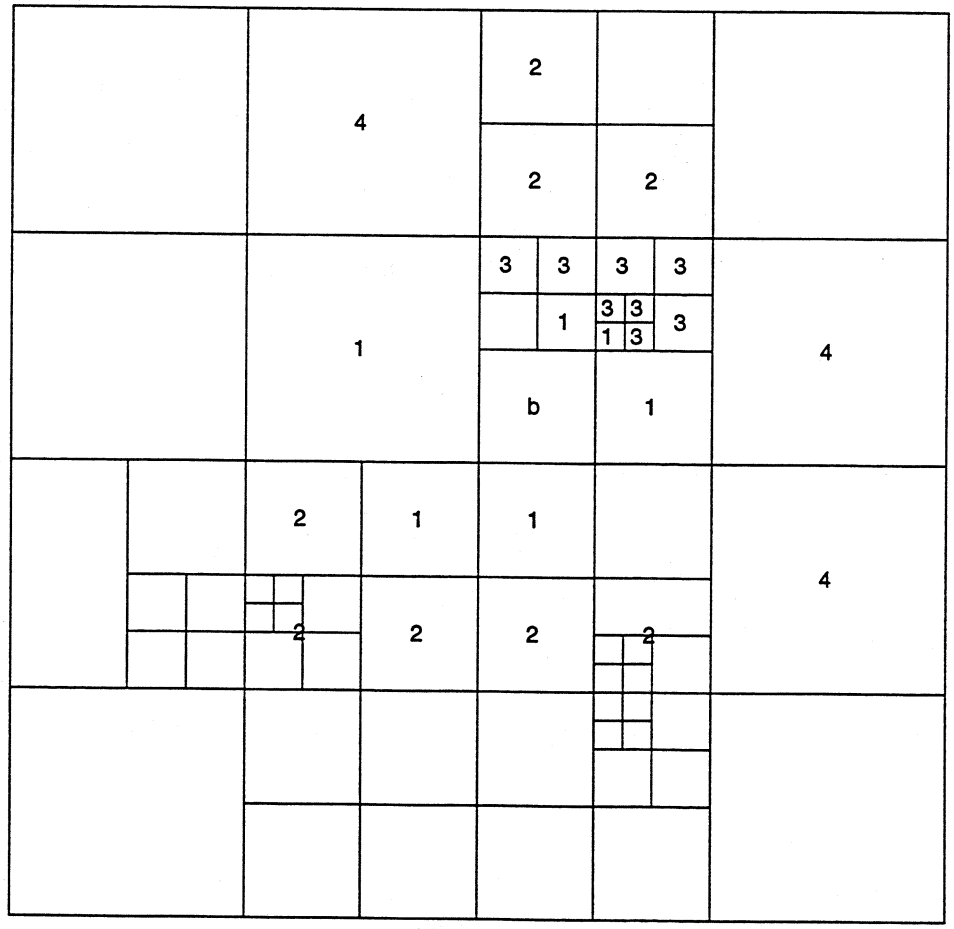


Figure 3: Box b and its associated Lists 1 to 4 for the charge distribution in Figure 2.



N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
200	0.007	0.009	0.015	0.019	0.11770E-03	0.85266E-03
400	0.015	0.018	0.034	0.076	0.27390E-03	0.19749E-02
800	0.024	0.047	0.071	0.310	0.29473E-03	0.20307E-02
1600	0.062	0.089	0.151	1.344	0.39506E-03	0.36146E-02
3200	0.105	0.213	0.318	5.371	0.42503E-03	0.38485E-02
6400	0.266	0.399	0.666	21.783	0.49194E-03	0.43736E-02

Table 1: Uniformly distributed particles. $K(x,y) = 1/|x-y|$, $s = 15$, $p = 9$, and $n = 4$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
400	0.066	0.042	0.107	0.075	0.37968E-07	0.36455E-06
800	0.124	0.130	0.254	0.309	0.30664E-07	0.23301E-06
1600	0.255	0.251	0.505	1.347	0.59016E-07	0.63131E-06
3200	0.492	0.684	1.176	5.375	0.67426E-07	0.67145E-06
6400	0.997	1.230	2.227	21.756	0.16065E-06	0.16568E-05

Table 2: Uniformly distributed particles. $K(x,y) = 1/|x-y|$, $s = 61$, $p = 36$, and $n = 8$.

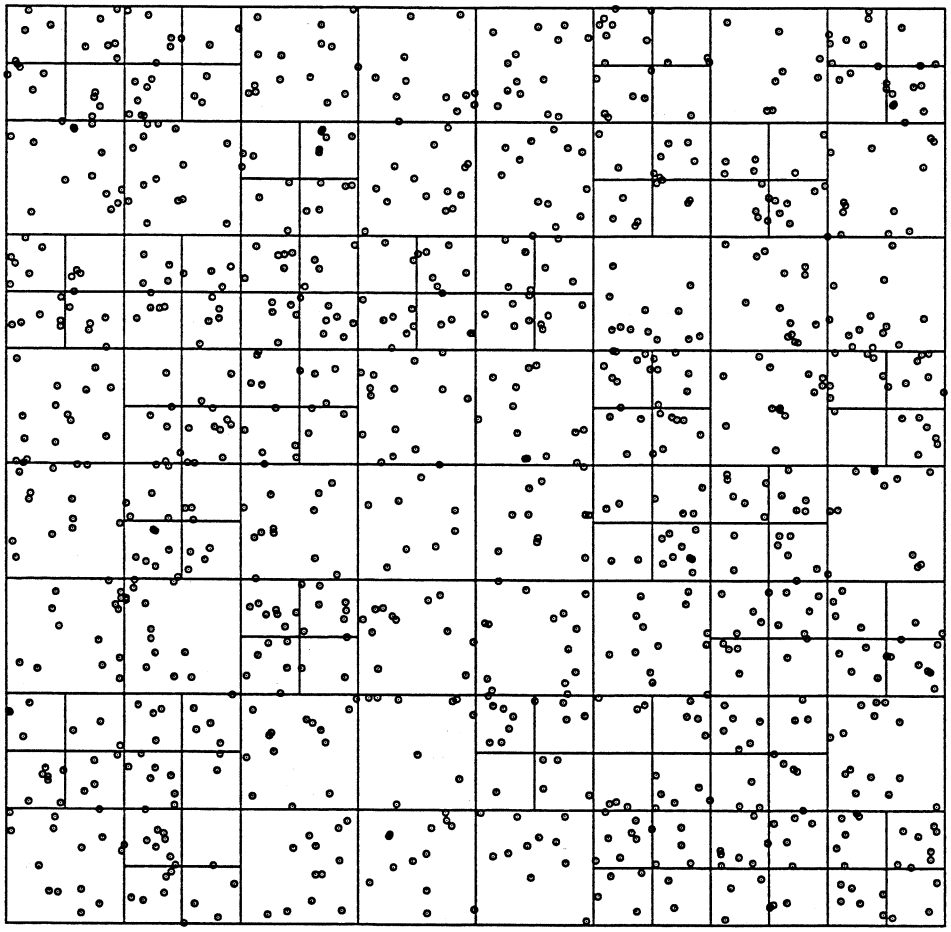
N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
800	0.832	0.213	1.045	0.316	0.35519E-11	0.27597E-10
1600	1.625	0.580	2.205	1.342	0.27911E-11	0.23206E-10
3200	3.210	1.374	4.515	5.371	0.47909E-11	0.35374E-10
6400	6.301	3.138	9.438	21.798	0.40687E-11	0.47116E-10

Table 3: Uniformly distributed particles. $K(x,y) = 1/|x-y|$, $s = 153$, $p = 90$, and $n = 16$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
200	0.007	0.007	0.014	0.014	0.33680E-06	0.11237E-02
400	0.015	0.016	0.031	0.055	0.24487E-05	0.46567E-02
800	0.024	0.037	0.061	0.227	0.75789E-05	0.67792E-02
1600	0.063	0.077	0.140	1.016	0.36380E-04	0.82441E-02
3200	0.105	0.173	0.278	4.064	0.10114E-03	0.11347E-01
6400	0.267	0.353	0.619	16.397	0.42311E-04	0.12510E-01

Table 4: Uniformly distributed particles. $K(x,y) = 1/|x-y|^2$, $s = 15$, $p = 9$, and $n = 4$.

Figure 4: Uniformly distributed particles and the associated partition of the computational box.



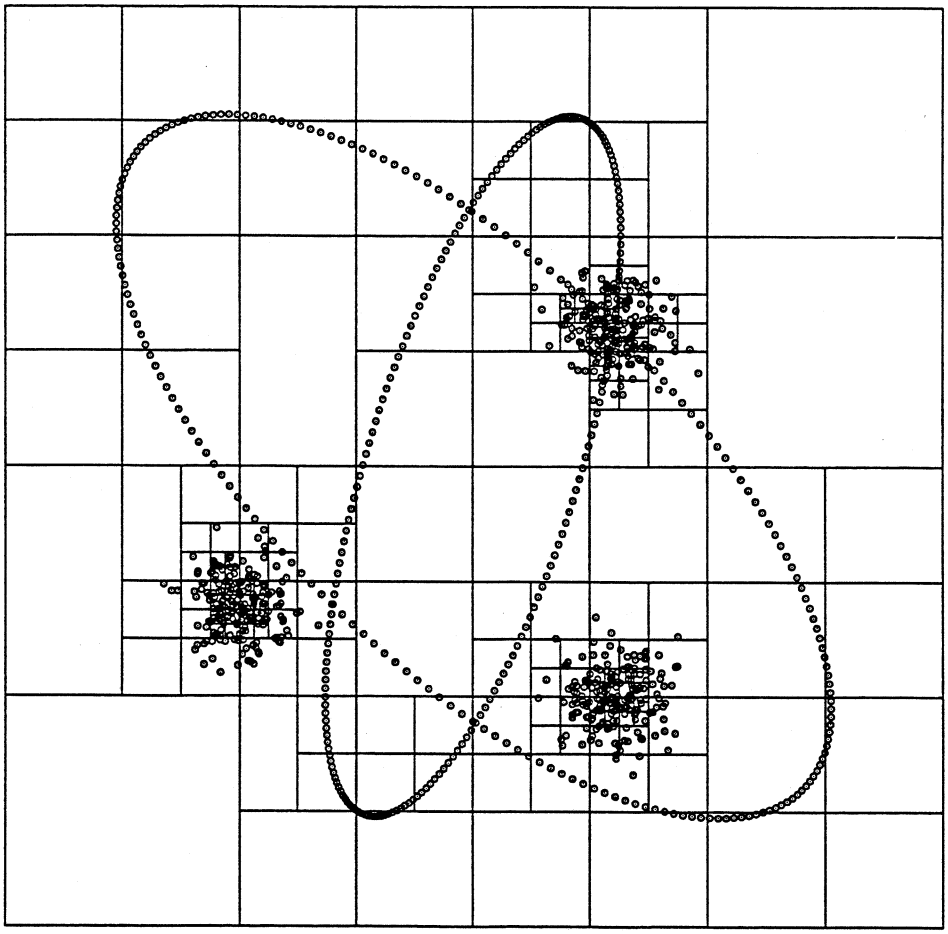
N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
400	0.065	0.033	0.099	0.055	0.33610E-09	0.96336E-06
800	0.126	0.098	0.223	0.225	0.74619E-09	0.55977E-06
1600	0.254	0.210	0.465	1.016	0.59034E-08	0.21584E-05
3200	0.493	0.529	1.022	4.090	0.18124E-07	0.17612E-05
6400	0.996	1.036	2.031	16.365	0.14692E-07	0.47616E-05

Table 5: Uniformly distributed particles. $K(x,y) = 1/|x-y|^2$, $s = 61$, $p = 36$, and $n = 8$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
800	0.826	0.180	1.006	0.231	0.14987E-12	0.17505E-09
1600	1.597	0.450	2.047	1.009	0.32363E-12	0.74589E-10
3200	3.205	1.217	4.422	4.104	0.20036E-11	0.25330E-09
6400	6.315	2.507	8.823	16.404	0.46900E-12	0.16662E-09

Table 6: Uniformly distributed particles. $K(x,y) = 1/|x-y|^2$, $s = 153$, $p = 90$, and $n = 16$.

Figure 5: Highly non-uniformly distributed particles and the associated partition of the computational box.



N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
200	0.008	0.010	0.019	0.019	0.13524E-03	0.87697E-03
400	0.016	0.029	0.045	0.076	0.20754E-03	0.11468E-02
800	0.029	0.058	0.087	0.309	0.26133E-03	0.12042E-02
1600	0.057	0.126	0.183	1.344	0.32551E-03	0.26410E-02
3200	0.114	0.245	0.358	5.368	0.37247E-03	0.34192E-02
6400	0.224	0.475	0.699	21.788	0.42360E-03	0.35911E-02

Table 7: Highly non-uniformly distributed particles. $K(x,y) = 1/|x-y|$, $s = 15$, $p = 9$, and $n = 4$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
400	0.065	0.060	0.125	0.076	0.59124E-07	0.61426E-06
800	0.140	0.139	0.279	0.315	0.77114E-07	0.11068E-05
1600	0.264	0.413	0.677	1.336	0.10049E-06	0.97051E-06
3200	0.528	0.834	1.363	5.439	0.12151E-06	0.12184E-05
6400	1.052	1.867	2.919	21.761	0.15353E-06	0.15668E-05

Table 8: Highly non-uniformly distributed particles. $K(x,y) = 1/|x-y|$, $s = 61$, $p = 36$, and $n = 8$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
800	0.805	0.250	1.055	0.314	0.40445E-11	0.87339E-10
1600	1.716	0.603	2.319	1.338	0.61795E-11	0.75092E-10
3200	3.334	1.769	5.103	5.442	0.88132E-11	0.85507E-10
6400	6.540	5.366	11.906	21.810	0.11716E-10	0.12124E-09

Table 9: Highly non-uniformly distributed particles. $K(x,y) = 1/|x-y|$, $s = 153$, $p = 90$, and $n = 16$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
400	0.016	0.023	0.039	0.055	0.44531E-04	0.19765E-02
800	0.029	0.045	0.075	0.226	0.72969E-04	0.37896E-02
1600	0.058	0.100	0.158	1.016	0.98016E-04	0.70910E-02
3200	0.115	0.197	0.312	4.064	0.24054E-03	0.57700E-02
6400	0.225	0.382	0.608	16.405	0.23213E-03	0.82506E-02

Table 10: Highly non-uniformly distributed particles. $K(x,y) = 1/|x-y|^2$, $s = 15$, $p = 9$, and $n = 4$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
400	0.065	0.045	0.110	0.054	0.61825E-08	0.15019E-05
800	0.140	0.108	0.247	0.234	0.10608E-07	0.20936E-05
1600	0.265	0.312	0.577	1.016	0.13661E-07	0.18906E-05
3200	0.521	0.639	1.160	4.059	0.38933E-07	0.21694E-05
6400	1.043	1.439	2.481	16.408	0.38956E-07	0.61407E-05

Table 11: Highly non-uniformly distributed particles. $K(x,y) = 1/|x-y|^2$, $s = 61$, $p = 36$, and $n = 8$.

N	$T_{init}(s)$	$T_{alg}(s)$	$T_{run}(s)$	$T_{dir}(s)$	E_2	E_∞
800	0.805	0.192	0.996	0.230	0.10539E-11	0.41111E-09
1600	1.717	0.477	2.194	1.010	0.68055E-12	0.18332E-09
3200	3.338	1.352	4.691	4.144	0.28719E-11	0.39139E-09
6400	6.540	4.045	10.586	16.411	0.29936E-11	0.21587E-09

Table 12: Highly non-uniformly distributed particles. $K(x,y) = 1/|x-y|^2$, $s = 153$, $p = 90$, and $n = 16$.

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