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Gregory Beylkin

**7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**
Program in Applied Mathematics
University of Colorado, Boulder
Campus Box 526
Boulder, CO 80309-0526

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AASERT grant N00014-91-J-4037 supported the research of two graduate students, James M. Keiser and Robert Cramer. James Keiser has completed his research and defended his thesis April 17, 1995. The results of his research were described in the report submitted 5/31/95. At about the same time (May 1995) a one year no cost extension for this grant was approved in order to allow Robert Cramer to finish his research towards a Ph.D. At the time of this writing, Robert Cramer has achieved the goals of his thesis work and is in the process of finishing his thesis (which he will defend this summer).

The work of Robert Cramer is concerned with computing particle interactions in a manner consistent with projection methods. Using a wavelet-based approach, it appears possible to construct a high order generalization of local correction methods.



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SEATTLE REGIONAL OFFICE
1107 NE 45TH STREET. SUITE 350
SEATTLE WA 98105-4631

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ROBERT J. SILVERMAN

## Report for AASERT grant N00014-91-J-4037

AASERT grant N00014-91-J-4037 supported the research of two graduate students, James M. Keiser and Robert Cramer. James Keiser has completed his research and defended his thesis April 17, 1995. The results of his research were described in the report submitted 5/31/95. At about the same time (May, 1995) a one year no cost extension for this grant has been approved in order to allow Robert Cramer to finish his research towards Ph.D. At the time of this writing, Robert Cramer has achieved the goals of his thesis work and is in the process of finishing his thesis (which he will defend this summer).

The work of Robert Cramer is concerned with computing particle interactions in a manner consistent with projection methods. Using a wavelet-based approach, it appears possible to construct a high order generalization of local correction methods (local correction methods typically work well if low accuracy is required). A brief outline is presented below.

### Summary of Robert Cramer's thesis

The work of Robert Cramer concerns a fast wavelet based method for computing "particle interactions". By "particle interactions" we understand discrete sums representing interactions between points in space. We assume that the interaction between any two particles depends only on the distance between them.

We wish to compute the sums

$$g(x_m) = \sum_{\substack{n=1 \\ y_n \neq x_m}}^{N} K(x_m - y_n) f(y_n)\,, \qquad 1 \leq m \leq M$$

in a number of operations proportional to $(M+N)$ (rather than $M \cdot N$) with a fixed but arbitrary accuracy. In the context of a particle simulation, the function $f(y)$ represents the charge density sampled at the discrete set of points $\{y_1, \ldots, y_N\}$, and $g(x)$ represents a potential field sampled at the discrete set of points $\{x_1, \ldots, x_M\}$. The requirement $x_m \neq y_n$ excludes the self-interaction (which is generally infinite).

It is often possible to view the summation problem as a discretization of a bounded integral operator,

$$g(x) = Kf(x) = \int K(x-y)f(y)\,dy\,.$$

However, our algorithms do not depend on this and, moreover, we are especially interested in kernels for which this interpretation is not valid.

The applications of such algorithms are numerous, and in the physical sciences include the study of stellar and galactic clusters, gas dynamics, fluid dynamics (vortex methods), flow of electrons in semi-conductor devices, and the study of ionized liquids and phase changes in chemistry. In addition, such algorithms permit the design of fast Fourier transforms for unequally spaced data.

A fast algorithm to compute these sums is provided by the Fast Multipole Method (FMM). We are looking for an alternative to FMM which will be more generic and fit naturally into projection-type methods. It appears that the wavelet approach leads to an algorithm which may be thought of as a high order generalization of the method of local corrections. These local corrections methods have largely been of relatively low order in accuracy (roughly $10^{-2}$ to $10^{-4}$), and have been restricted to kernels arising from differential equations, mainly Laplace's or Poisson's. Our approach yields methods of much broader scope, including arbitrary order accuracy, and the ability to handle a wider range of kernels. Using a multiresolution approach it appears possible to analytically construct an efficient high order approximation of the correction operator. The approach is efficient and should be competetive with FMM.

The fact which provides a common foundation for fast summation algorithms is that kernels of the type mentioned above can be split into the sum of a smooth kernel which describes the long-range interactions, and a singular kernel which influences only the short-range interactions. Thus, the strategy is to construct a globally smooth kernel, $K^{(\mathrm{LR})}$, which approximates $K(x-y)$ well if the distance $|x-y|$ is large, and then define the short-range part $K^{(\mathrm{SR})}$ through the equation

$$K^{(\mathrm{SR})} = K - K^{(\mathrm{LR})}\,.$$

The long-range part, being globally smooth and a convolution, can be efficiently applied

using the Fourier transform.

The singular or "high-frequency" part of the kernel is applied directly, but due to the rapid decay of $K^{(\mathrm{SR})}$ in the physical space, these short-range interactions involve only a few particles. For this reason, this stage of the computation can also be accomplished at relatively low computational cost.

Let us first describe the one-dimensional version of our algorithm and then indicate the modifications necessary to extend this approach to two or three dimensions. Let us consider a multiresolution analysis, i.e., a chain of closed subspaces of $L^2(\mathbf{R})$,

$$\cdots \subset V_2 \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \subset \cdots .$$

The approximation properties of a MRA follow from two essential ingredients. First, the basis functions $\phi_k^j$ are compactly supported, and this support becomes arbitrarily small as we go to finer and finer subspaces. Second, polynomials up to a given degree can be represented exactly in the MRA. Namely, with each MRA there is an associated parameter $M$, and for each $m = 0, \ldots, M$, there exist coefficients $s_k^j \in \mathbf{R}$, $k \in \mathbf{Z}$ such that

$$x^m = \sum_k s_k^j \phi_k^j(x).$$

Using the properties of compact support and the ability to accurately represent functions which behave like polynomials on compact intervals, it is possible to construct a kernel $T_j$ which operates on the subspace $V_j$, and which approximates $K$ as follows. Given any $\epsilon > 0$, there exists a constant $B = B(\epsilon)$, and an integer $j \leq 0$, such that

$$|K(x-y) - T_j(x,y)| < \epsilon \quad \text{whenever} \quad |x-y| > 2^j B\,.$$

Our multiresolution kernel has the explicit form

$$T_j(x,y) = \sum_k \sum_l t_{k-l}^j \phi_k^j(x) \phi_l^j(y)\,,$$

where the coefficients are given by

$$t_{k-l}^j = \int\int K(x-y) \phi_k^j(x) \phi_l^j(y)\, dy\, dx\,.$$

The short-range part is then defined by

$$K^{(\mathrm{SR})}(x,y) = \begin{cases} K(x-y) - T_j(x,y) & ,|x-y| \le 2^j B \\ 0 & ,|x-y| > 2^j B\,. \end{cases}$$

Computing the long-range contribution to the potential is reduced to the problem of applying a Toeplitz matrix to a vector which is accomplished using the FFT. To evaluate the short-range contribution, it is necessary to evaluate the kernel $T_j(x,y)$ at a given point $(x,y)$. For this we provide a Fourier series expansion of the kernel,

$$T_j(x,y) = \sum_{n=0}^{\infty} \cos\left[2n\pi\left(\frac{x+y}{2}\right)\right] \Phi_{n,j}(x-y)\,.$$

This series converges very quickly, and we typically retain only the first four terms. The functions $\Phi_{n,j}(\cdot)$ are expressed in terms of the basis function $\phi(\cdot)$, and are tabulated for rapid evaluation. Application of the short-range part of the kernel is thus an $O(M)$ procedure, as for a given point $x_m$, $1 \le m \le M$, only a few of the $N$ particles will be involved.

In two (and higher) spatial dimensions, we approximate the kernel $K(x-x', y-y')$ by constructing an MRA kernel

$$T_j(x,y,x',y') = \sum_{k,l} \phi_k^j(x)\phi_l^j(y) \sum_{k',l'} t_{k-k',l-l'}^j \phi_{k'}^j(x')\phi_{l'}^j(y')$$

to satisfy

$$|K(x-x', y-y') - T_j(x,y,x',y')| < \epsilon$$

whenever

$$\max\{|x-x'|, |y-y'|\} > 2^j B$$

for appropriately chosen $B = B(\epsilon)$ and $j \le 0$.

The long-range contribution is computed using the FFT, entirely analogous to the one-dimensional case. An additional step required in higher dimensions in order to rapidly evaluate $T_j(x,y,x',y')$ at a point $(x,y,x',y')$, is the step of computing the singular-value decomposition of the coefficient matrix $\{t_{k,l}^j\}$, to obtain the representation

$$t_{k,l}^j \approx \sum_{r=1}^{R} \sigma_r u_k^{(r)} v_l^{(r)}\,,$$

where $\{\sigma_r\}$ are the singular values and $R$ is the numerical rank. Due to the fact that the coefficient matrix $\{t^j_{k,l}\}$ is of low rank, the parameter $R$ is relatively small (for example, $R = 8$ for single precision). We obtain the two-dimensional equation for evaluating the short-range interactions,

$$\begin{aligned} T_j(x,y,x',y') &= \sum_{r=1}^{R} \sigma_r \\ &\times \left( \sum_{m=0}^{\infty} \cos\left[ 2m\pi \left( \frac{x+x'}{2} \right) \right] U^{(r)}_{j,m}(x-x') \right) \\ &\times \left( \sum_{n=0}^{\infty} \cos\left[ 2n\pi \left( \frac{y+y'}{2} \right) \right] V^{(r)}_{j,n}(y-y') \right) \end{aligned}$$

The functions $U^{(r)}_{j,m}$ and $V^{(r)}_{j,n}$ are again tabulated for rapid evaluation. The number of terms necessary to retain in the sums above is very small (typically four) since the series converges rapidly.

Further details may be obtained upon request from Robert Cramer,
bcramer@boulder.colorado.edu.