Singular operators in multiwavelet bases

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We review some recent results on multiwavelet methods for solving integral and partial differential equations and present an efficient representation of operators using discontinuous multiwavelet bases, including the case for singular integral operators. Numerical calculus using these representations produces fast ***O(N)*** *methods for multiscale solution of integral equations when combined with low separation rank methods. Using this formulation, we compute the Hilbert transform and solve the Poisson and Schrödinger equations. For a fixed order of multiwavelets and for arbitrary but finite-precision computations, the computational complexity is* ***O(N)****. The computational structures are similar to fast multipole methods but are more generic in yielding fast* ***O(N)*** *algorithm development.*

Introduction

Using the multiwavelet representations of functions and operators, we present a multiscale solution method for integral and differential equations and integral transforms. The Hilbert transform, the Poisson equation, and the Schrödinger equation provide important examples with a wide range of applications in computational chemistry, physics, and electromagnetic and fluid dynamics. We also describe a representation with a low separation rank (LSR), which is exact up to arbitrary but finite precision.

Theoretically, it has been clear for some time [1] that a multiresolution representation of homogeneous operators should lead to useful numerical algorithms. However, the straightforward transition from algorithms in one spatial dimension to those in two, three, and beyond yields algorithms that are too costly for high-accuracy practical applications. Recently [2] it was observed that many physically interesting operators have a low separation rank. Using the low separation rank representation of these operators with multiwavelets, we have developed practical multiresolution algorithms in higher dimensions for important classes of problems [3].

In this paper we summarize an approach using multiwavelet bases which incorporates adaptive refinement, and fast $O(N)$ operations for a guaranteed solution of arbitrary but finite precision. The advantages of each of these concepts have been elucidated in the literature. We have integrated them to solve some real-world problems.

In the multiwavelet representation of functions, the integral equation $f(x) = \int K(x, y)g(y)dy$ is converted to a sparse matrix-vector multiplication, $f = Ag$, where f and g are vectors of coefficients representing the function $f(x)$ and $g(x)$, and A is the matrix of coefficients for the representation of the kernel $K(x, y)$.

In estimating the complexity of the algorithms discussed in this paper, we select a fixed but arbitrary accuracy and then estimate the number of operations or significant coefficients to achieve that accuracy (in the operator norm). We note that this count is somewhat different from that obtained by estimating the number of arithmetic operations necessary to obtain a solution with a given accuracy, where the discretization of the operator depends on accuracy as well.

Multiresolution analysis and low-separation-rank representation

It has been shown in [1] that singular operators have their most natural representation in multiresolution bases. Using bases of compactly supported Daubechies wavelets [4] (and their variations), and two-scale

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difference equations, one finds a regularization method for computing such representations by solving a linear system of equations [5]. By solving such a linear system, the issue of discretizing kernels near its singularity is avoided.

In many problems, the choice of basis should accommodate not only the integral operators but also differential operators and the boundary conditions. Multiwavelet bases developed in [6] satisfy many of these requirements. As is well known, multiwavelet bases retain some properties of wavelet bases, such as vanishing moments, orthogonality, and compact support. The basis functions do not overlap on a given scale and are organized in small groups of several functions (thus, multiwavelets) sharing the same support. On the other hand, some of the basis functions are discontinuous, similar to the Haar basis and in contrast to wavelets with regularity. Because of the vanishing moments of the basis functions, a wide class of integro-differential operators has effectively sparse representations in these bases. (By an effectively sparse matrix representation, we mean a representation that differs from a sparse matrix by a matrix with a small norm.) More recently, it was demonstrated in [7] that such bases are useful for adaptively solving partial differential equations (PDEs) with boundary conditions.

As a part of the program to develop multidimensional adaptive PDE solvers, we construct representations for homogeneous convolution operators in dimensions $d = 2$, 3, and higher. Another method using representations of low separation rank for functions and operators is described in [2], and we outline this approach as well. Let us start with the straightforward multiwavelet generalization of [1]. For the multiwavelet bases, the computational costs are $O(k^4N)$ in two dimensions and $O(k^6N)$ in three dimensions, where order-k multiwavelets are used and N is the number of boxes in which significant coefficients exist. In many applications, such as computational chemistry, it is too expensive to compute with such algorithms. The algorithms that we present here have computational complexity of $O(k^2N)$ and $O(k^3N)$, respectively.

In our solution method, the use of a localized, discontinuous, and adaptive basis of multiwavelets is combined with a representation of functions and operators that generalizes the separation of variables. This is all performed with controlled accuracy in finite-precision arithmetic. The notable features of multiwavelet representation of operators are the following:

- Multiwavelets form an orthonormal basis.
- The basis functions have disjoint local support.
- The basis functions (except on the coarsest scale) have vanishing moments.
- Two-scale relations are available for computing at adjacent scales.

We also have

- A choice of interpolating basis for the scaling functions.
- Adaptive representation and local refinement.
- A high-order approximation near the boundaries.

The computational advantages are the following:

- A sparse representation of a large class of operators.
- Fast algorithms with guaranteed precision for many common operations, such as inversion, multiplication, and addition within this class.

The LSR representation of a d-dimensional function, $f : R^d \rightarrow R$, generalizes the notion of separation of variables. The separated representation of a function (or operator) in many dimensions [2], to an arbitrary but finite precision ε, is a sum of products of functions of lower dimension such that

$$\left| f(x_1, x_2, \cdots, x_d) - \sum_{i=1}^{m} s_i \phi_1^i(x_1) \phi_2^i(x_2) \cdots \phi_d^i(x_d) \right| < \varepsilon.$$

The number of terms m, in the above sum, is called the *separation rank* and is distinct from the operator rank. This type of representation is important in obtaining fast methods because in many situations the number of terms scales as $O(-\log \varepsilon)$ with respect to the threshold of accuracy and as $O(d)$ or even $O(\log d)$ with respect to the number of variables [2]. The modern fast multipole method (e.g., for the Poisson kernel $1/r$) is based on essentially this type of approximation, with the functions being plane waves with the region of validity in selected directions [8–10]. In [2] a computational algorithm was developed for LSR in which the set of functions $\{\phi_l^i(x_l)\}$ is not fixed, and one does not try to solve equations using them as a basis. The sum is used as an approximation technique for functions and operators, and an algorithm was developed for minimizing the number of terms at each step.

The benefits of LSR representations for many operators are the following:

- All operations are one-dimensional.
- Storage requirements are low.
- Constructive algorithms exist for the reduction of separation rank.
- For many physically significant operators it removes the curse of dimensionality.

Although it is not known whether all operators and functions in practical applications have a short LSR representation, many important operators, such as the multiparticle Schrödinger operator and the inverse Laplacian, can be efficiently represented in this form.

We apply our framework for numerical calculus of operators. These operations are important in applications in which functions of operators must be computed. For example, the Schultz iteration[1] for the computation of the inverse requires operator products and sums.

Let us start by providing a formal description of a multiresolution analysis (MRA) for a multiwavelet [11, 12]. Such an MRA is defined as an ascending chain of embedded closed subspaces of the Hilbert space $L_2([0, 1])$,

$$\cdots \subset V_0 \subset V_1 \subset V_2 \subset \cdots,$$

with the properties that

$$L_2([0, 1]) = \overline{\cup_j V_j}, \qquad \cap V_j = \{0\}.$$

Additional requirements are as follows:

1. The subspace V_0 is invariant under integer translations.
2. The subspaces V_j are all scaled version of one another. One or more scaling functions ϕ are in V_j if and only if $\phi(2^j x)$ is in V_0.
3. One or more scaling functions ϕ are in V_0 such that their rescaled and shifted versions, of the form $2^{j/2}\phi(2^j x - k)$, constitute an orthonormal basis[2] of V_j.

Well-known examples are the Haar basis, in which the scaling function is the characteristic function restricted to the interval [0, 1], the Battle–Lemarie wavelet with spline scaling function, and the Daubechies families of wavelets [4], as well as multiwavelets [6]. For computational purposes, we start from a coarse subspace V_0 and generate a finite ascending sequence of finer subspaces as needed.

Multiwavelets

In this section, we review fundamental properties of the Legendre multiwavelet bases [6, 7] for $L^2([0, 1])$.

For $k = 1, 2, \cdots$ and $n = 0, 1, 2, \cdots$, the vector space of scaling functions of level n and degrees 0 to $k - 1$ is

$$V_n^k = \left\{ \begin{matrix} f : f|_{[2^{-n}l, 2^{-n}(l+1)]} \text{ is a polynomial of degree} \\ \text{less than } k, \text{ for } l = 0, \cdots, 2^n - 1, \text{ and 0 elsewhere} \end{matrix} \right\}.$$

The space V_n^k has dimension $2^n k$ and

$$V_0^k \subset V_1^k \subset \cdots \subset V_n^k.$$

The multiwavelet subspace W_n^k, $n = 0, 1, 2, \cdots$, is defined as an orthogonal complement of V_n^k in V_{n+1}^k,

$$V_{n+1}^k = V_n^k \oplus W_n^k,$$

and the dimension of W_n^k is $2^n k$. Therefore,

$$V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus W_2^k \oplus \cdots \oplus W_{n-1}^k.$$

We define $V^k = \cup_{n=0}^{\infty} V_n^k$ and observe that V^k is dense in the space of square integrable functions $L^2([0, 1])$ with respect to the L^2 norm.

Given a basis $\phi_0, \cdots, \phi_{k-1}$ of V_0^k of scaling functions, the space V_n^k is spanned by $2^n k$ functions which are obtained from $\phi_0, \cdots, \phi_{k-1}$ by dilation and translation,

$$\phi_{jl}^n(x) = 2^{n/2}\phi_j(2^n x - l), j = 0, \cdots, k - 1, l = 0, \cdots, 2^n - 1.$$

We introduce the multiwavelet basis as a set of piecewise orthonormal polynomials $\psi_0, \cdots, \psi_{k-1}$ for W_0^k,

$$\int_0^1 \psi_i(x)\psi_j(x)dx = \delta_{ij}.$$

Since $V_0^k \perp W_0^k$, the first k moments of $\psi_0, \cdots, \psi_{k-1}$ vanish,

$$\int_0^1 \psi_j(x)x^i dx = 0, \qquad i, j = 0, 1, \cdots, k - 1.$$

The space W_n^k is spanned by $2^n k$ functions obtained from $\psi_0, \cdots, \psi_{k-1}$ by dilation and translation $\psi_{jl}^n(x) = 2^{n/2}\psi_j(2^n x - l)$, with $j = 0, \cdots, k - 1$ and $l = 0, \cdots, 2^n - 1$. The support of ψ_{jl}^n is the interval $[2^{-n}l, 2^{-n}(l + 1)]$. The condition of orthonormality of the wavelet basis functions yields

$$\int_0^1 \psi_{il}^n(x)\psi_{jm}^{n'}(x)dx = \delta_{ij}\delta_{lm}\delta_{nm'}.$$

We note that in constructing multiwavelets there are two natural choices in selecting the basis. One choice provides additional vanishing moments for some of the basis functions [6], whereas the other organizes the basis by the type of singularity at the boundary between the subintervals [7].

Example: A multiwavelet basis can be constructed using the system of the Legendre polynomials, $P_j(x), j = 0, \cdots, k - 1$, rescaled to the unit interval (cf. **Figures 1** and **2**),

$$\phi_j(x) = \begin{cases} \sqrt{2j + 1}\, P_j(2x - 1) & x \in [0, 1], \\ 0 & x \notin [0, 1]. \end{cases}$$

If a function is projected to the level-n subspace V_n^k, it is approximated on subintervals constructed by dividing the interval [0, 1] into 2^n equal subintervals. In the scaling function basis, a function f projected onto V_n^k is represented as

$$f(x) = \sum_{l=0}^{2^n-1} \sum_{j=0}^{k-1} s_{jl}^n \phi_{jl}^n(x);$$

[1] The Schultz iteration $B_{k+1} = 2B_k - B_k A B_k$, $B_0 = \alpha A^*$ with $\alpha \le |A^*A|^{-1}$, is used for computing A^{-1}. The operator A^* is the adjoint of A. It is easy to show convergence to the inverse of A or its pseudo-inverse if A is singular.

[2] Since we are using only orthonormal bases, the usual Riesz condition is replaced by Condition 3.

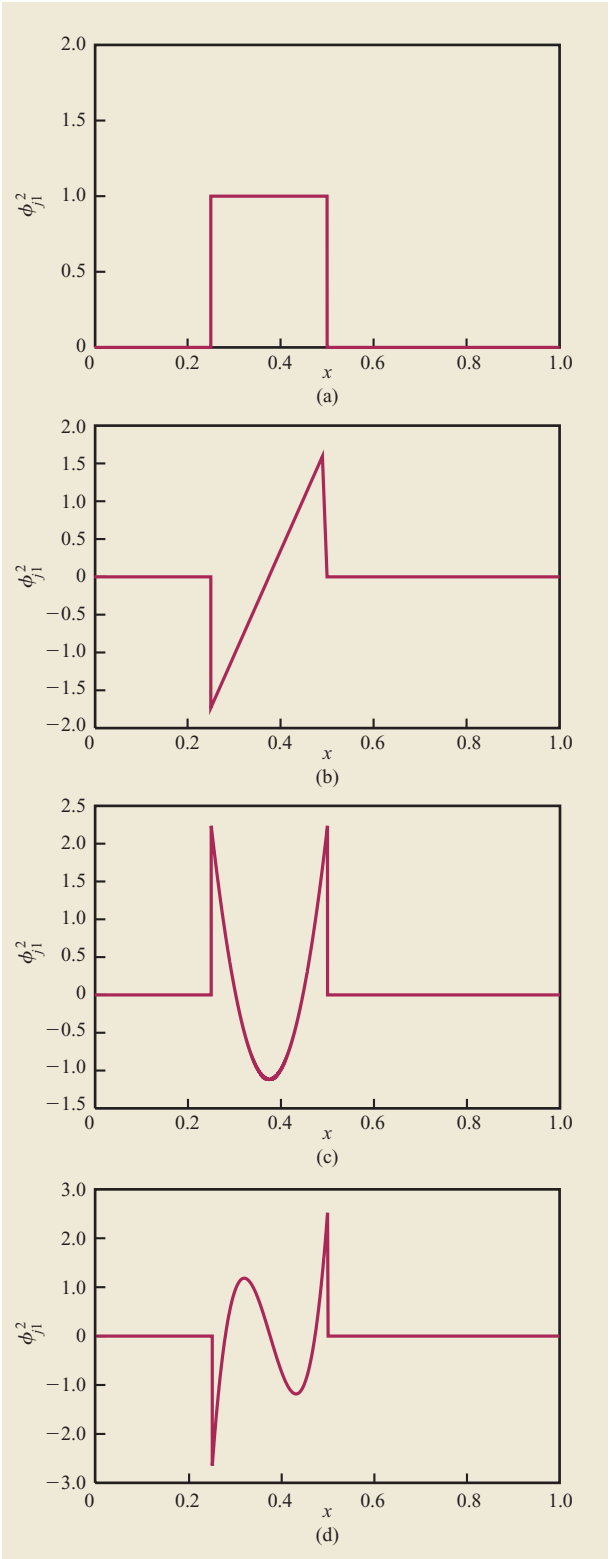

Figure 1

Four scaling functions ϕ_{j1}^2 at level $n = 2$: (a) $j = 0$; (b) $j = 1$; (c) $j = 2$; (d) $j = 3$.

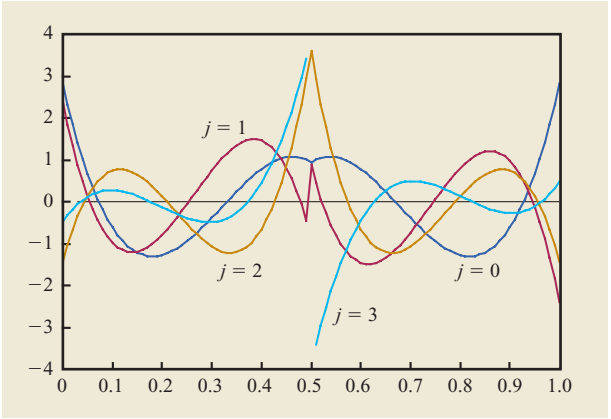

Figure 2

Four Legendre multiwavelet basis functions $\psi_{j0}^0(x)$ at level $n = 0$ with $j = 0, 1, 2, 3$.

in the multiwavelet basis, the function f is expressed as

$$f(x) = \sum_j s_j \phi_{j0}^0(x) + \sum_{n'=0}^{n-1} \sum_{l=0}^{2^{n'}-1} \sum_{j=0}^{k-1} d_{jl}^{n'} \psi_{jl}^{n'}(x).$$

The scalars $s_{jl}^n = \int f(x)\phi_{jl}^n(x)dx$ and $d_{jl}^{n'} = \int f(x)\psi_{jl}^{n'}(x)dx$ are respectively called the scaling and multiwavelet coefficients. These can be computed directly using Gauss–Legendre quadrature or by the following two-scale relations from a fine scale to a coarse scale.

The scaling and multiwavelet functions satisfy the two-scale relations

$$\phi_i(x) = \sqrt{2} \sum_{j=0}^{k-1} [h_{ij}^{(0)} \phi_j(2x) + h_{ij}^{(1)} \phi_j(2x-1)]$$

and

$$\psi_i(x) = \sqrt{2} \sum_{j=0}^{k-1} [g_{ij}^{(0)} \phi_j(2x) + g_{ij}^{(1)} \phi_j(2x-1)],$$

where $h_{ij}^{(0)}$, $h_{ij}^{(1)}$, $g_{ij}^{(0)}$, and $g_{ij}^{(1)}$ are coefficients which are easily computed given the scaling and multiwavelet basis. By using these relations, further two-scale relations can be derived for the scaling and multiwavelet coefficients from scale n and $n + 1$,

$$s_{il}^n = \sqrt{2} \sum_{j=0}^{k-1} (h_{ij}^{(0)} s_{j,2l}^{n+1} + h_{ij}^{(1)} s_{j,2l+1}^{n+1})$$

and

$$d_{il}^n = \sqrt{2} \sum_{j=0}^{k-1} (g_{ij}^{(0)} s_{j,2l}^{n+1} + g_{ij}^{(1)} s_{j,2l+1}^{n+1}).$$

Similarly, there is an algorithm for reconstructing scaling coefficients from multiwavelet representations. If the scaling coefficients at level m have been computed,

$$s_{il}^{m+1} = \sum_{j=0}^{k-1} \left(h_{ji}^{(0)} s_{jl}^{m} + g_{ji}^{(1)} d_{jl}^{m} \right)$$

and

$$s_{i,2l+1}^{m+1} = \sum_{j=0}^{k-1} \left(h_{ji}^{(1)} s_{jl}^{m} + g_{ji}^{(1)} d_{jl}^{m} \right).$$

These formulas are multiwavelet versions of the fast wavelet transform and are a key ingredient for fast algorithms.

In [7], interpolating multiwavelet bases are constructed as a linear combination of the Legendre multiwavelets. The advantage of interpolating bases is that the function values and coefficients of scaling functions differ by only a factor.

Scaling of homogeneous operators

Multiwavelet representation of linear homogeneous operators of degree α, $T(f)(\lambda x) = \lambda^{\alpha} T(f)(x)$, can be obtained by computing coefficients on only one scale.

Proposition

For a homogeneous convolution operator T of degree d, the scaling coefficients,

$$[r_{lm}^{n}]_{ij} = \int_{2^{-n}l}^{2^{-n}(l+1)} \phi_{il}^{n}(x) T \phi_{jm}^{n}(x) dx,$$

are equal to $2^{nd}[r_{0,l-m}^{0}]$.

Since the derivative operator d/dx is homogeneous of degree 1, the multiwavelet coefficients scale as $[r_{lm}^{n}]_{ij} = 2^{n}[r_{0,l-m}^{0}]_{ij}$. The second derivative operator d^2/dx^2 scales as $[r_{lm}^{n}]_{ij} = 2^{2n}[r_{0,l-m}^{0}]_{ij}$. Further descriptions of this type of relations can be found in [13].

Nonstandard form

Given a multiresolution analysis and projection operators $P_n^k : L^2([0, 1]), \rightarrow V_n^k$ onto the scaling function subspace, and $Q_n^k : L^2([0, 1]) \rightarrow W_n^k$ onto the multiwavelet subspace, an operator T can be represented as a telescopic series,

$$T = T_0 + \sum_{n=0}^{\infty} (A_n^k + B_n^k + C_n^k),$$

where $A_n^k = Q_n^k T Q_n^k$, $B_n^k = Q_n^k T P_n^k$, $C_n^k = P_n^k T Q_n^k$, and $T_n^k = P_n^k T P_n^k$.

The nonstandard form is defined in [1] as a collection of triples, $T = \{T_0^k, (A_n^k, B_n^k, C_n^k)_{n=0,1,\ldots}\}$, where each triple (A_n^k, B_n^k, C_n^k) corresponds to a particular scale. The advantage of the nonstandard form over the usual multiwavelet series expansion is the explicit separation of scales.

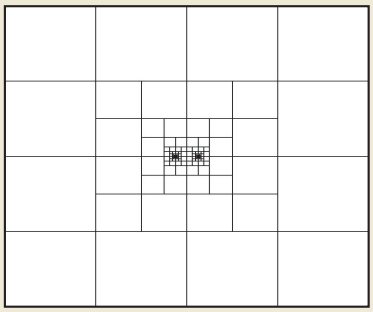

Figure 3

Adaptive refinement and thresholding are used to compute the energy levels of the hydrogen molecule, H_2. A two-dimensional slice of the three-dimensional adaptive refinement of cubes for the nuclear potential of the hydrogen molecule [3] shows where significant scaling and multiwavelet coefficients are required.

We use the nonstandard form of operators in multiwavelet bases. The nonstandard form does not explicitly contain matrix elements that are responsible for the interaction between different scales. This interaction is accounted for by the projection that must be performed after applying the nonstandard form. This projection requires $O(N)$ operations, resulting in algorithms that scale as $O(N)$, in contrast to the $O(N \log N)$ cost of applying operators to functions in the standard form, where scale-to-scale interactions are treated explicitly.

Most of the computation consists of a large number of independent small dense matrix multiplications involving small blocks of multiwavelet coefficients. Such operations are well suited to modern cache-based computer architectures.

Adaptivity

One of the attractive properties of multiwavelets is spatial refinement. This is especially important near regions with high gradients and discontinuities. By thresholding coefficients (i.e., setting all multiwavelet coefficients to zero when the absolute value of the coefficients is less than a threshold of accuracy), spatial adaptivity is naturally introduced. **Figure 3** shows an example of the refinement near the nuclear center of two hydrogen atoms in hydrogen gas, H_2, at level 8 with $k = 7$ and a precision of 10^{-5}.

Cross-correlation of multiwavelet functions

We use tensor products of multiwavelets in higher dimensions. For convolution operators, the integrals expressing the coefficients involve only the cross-correlations

of the basis functions. For example, in two dimensions, the coefficients for the kernel $K(x, y)$ in a box with a corner point $l = (l_1, l_2)$,

$$[r_l]_{ij} = \int K(x, y)\phi_i(x - l_1)\phi_j(y - l_2)dxdy,$$

must be calculated as a step in computing the nonstandard form.

Recurrence relation of cross-correlation functions

For computing representations of the convolution operators in the multiwavelet basis, we use the cross-correlation functions, $\Phi_{ij}(z) = \int \phi_i(z + y)\phi_j(y)dy$,

$$[r_l]_{ij} = \int\int K(x - y)\phi_i(x - l_1)\phi_j(y - l_2)dxdy$$

$$= \int K(z)\Phi_{ij}(z + l_2 - l_1)dz.$$

By substituting the recurrence relation for multiwavelets, we obtain the following recurrence relation for Φ_{ij}:

$$\Phi_{ij}(x) = \sum_{i',j'} [h_{ii'}^{(0)} h_{jj'}^{(1)} \Phi_{i'j'}(2x - 1) + (h_{ii'}^{(0)} h_{jj'}^{(0)} + h_{ii'}^{(1)} h_{jj'}^{(1)})\Phi_{i'j'}(2x) + h_{ii'}^{(1)} h_{jj'}^{(0)} \Phi_{i'j'}(2x + 1)].$$

Consequently, for a homogeneous kernel of degree α, the coefficients $[r_l]_{ij}$ satisfy a two-scale relationship, viz.,

$$[r_l]_{ij} = 2^{-\alpha-d} \sum_{i',j'} (h_{ii'}^{(0)} h_{jj'}^{(1)} [r_{2l-1}] + (h_{ii}^{0} h_{jj'}^{(0)} + h_{ii'}^{(1)} h_{jj'}^{(1)})[r_{2l}] + h_{ii'}^{(1)} h_{jj'}^{(0)} [r_{2l+1}]).$$

Among the cross-correlation functions we find some well-known functions used in numerical analysis. For example, the function $\Phi_{00}(x)$ is the so-called "hat function," and the function $\Phi_{i0}(x)$ is a shifted version of a Gegenbauer polynomial. The two-scale relations for the auto-correlation and the cross-correlation functions of multiwavelets are

$$\int \phi_i(x + y)\psi_j(y)dy = \sum_{i',j'} [h_{ii'}^{(0)} g_{jj'}^{(1)} \Phi_{i'j'}(2x - 1) + (h_{ii'}^{(0)} g_{jj'}^{(0)} + h_{ii'}^{(1)} g_{jj'}^{(1)} \Phi_{i'j'}(2x) + h_{ii'}^{(1)} g_{jj'}^{(0)} \Phi_{i'j'}(2x + 1)]$$

and

$$\int \psi_i(x + y)\psi_j(y)dy = \sum_{i',j'} [g_{ii'}^{(0)} g_{jj'}^{(1)} \Phi_{i'j'}(2x - 1) + (g_{ii'}^{(0)} g_{jj'}^{(0)} + g_{ii'}^{(1)} g_{jj'}^{(1)} \Phi_{i'j'}(2x) + g_{ii'}^{(1)} g_{jj'}^{(0)} \Phi_{i'j'}(2x + 1)].$$

These relations are used to produce the coefficients of the representation of the kernels.

Regularization

Beylkin and Cramer defined the notion of wavelet regularization [5]. A multiwavelet version is presented here. Simplistically, multiwavelet regularization is a procedure which replaces the computation of the multiwavelet coefficients using quadrature with a solution of linear equations describing the interactions between neighboring scales. The criteria for multiresolution regularization are outlined below.

The classical approach to regularization of hypersingular integrals interprets a divergent integral as a functional, or generalized function, operating on a class of test functions. The origin of the mathematical treatment of generalized functions (distributions) goes back to the theory introduced by L. Schwartz (e.g., [14]). Typically, one considers a regularization which is natural in the sense that the regularization of a sum of generalized functions corresponds to the sum of the regularizations, the derivative of a generalized function to the derivative of its regularization, and the product of a generalized function with an infinitely differentiable function to the regularization of the product [15].

In [5] a multiresolution definition of the regularization of singular and hypersingular homogeneous integrals was introduced using wavelets. The classical regularization was replaced by solving a system of linear equations consisting of two-scale relations for wavelet coefficients representing an integral operator in a multiresolution analysis. This system of equations is complemented by knowledge of the wavelet coefficients away from the singularity. Multiresolution regularization is consistent with the classical definition, since the classical regularization alters neither the degree of homogeneity of the kernel nor its asymptotic behavior at infinity. As it turns out, only these two properties uniquely determine the multiresolution definition of the regularized operator.

In this paper we generalize multiresolution regularization to multiwavelets. Currently our construction applies at most to singular operators. The accuracy of the multiresolution regularization is controlled by the accuracy of the solver for the linear system resulting from the relations depending on the number of multiwavelets and the number of levels.

It is sufficient to compute the scaling coefficients, since the multiwavelet coefficients can be derived from the two-scale relation. For practical purposes it is sufficient to assume that the scaling coefficients satisfy the asymptotic condition $[r_l]_{ij} = F_{ij}(l)$. Given an integral operator with a homogeneous kernel, the multiresolution regularization procedure is defined constructively and consists of the following three steps:

1. We assume that the scaling function coefficients $[r_l]_{ij}$ are known for a sufficiently large distance $|l|$ from the singularity.
2. The two-scale relations (e.g., for $[r_l]_{ij}$) are used to compute $[r_l]_{ij}$ for $1 < |l| < n$.
3. The two-scale relations produce a system of linear equations for coefficients in the range $|l| \leq 1$. Coefficients in this range appear on both sides of the two-scale difference equations.

In general, this criterion is written as

$$2^{n+\alpha} r = Ar + b,$$

where r represents the vector of coefficients. The matrix A consists of combinations of the coefficients of two-scale relations.

Let $x, y \in R^n$ and let T be a convolution operator with the kernel $K(x, y)$, homogeneous of degree α. Assuming that the solution to the linear system in condition 3 exists, we obtain a multiresolution kernel $T_0(x, y)$ with coefficients r_l from the construction above. We define the multiresolution regularized operators to be $T_j : V_j \to V_j, j \in Z$, with kernels $T_j(x, y) = 2^{-j-n} T_0(2^{-j}x, 2^{-j}y)$ on the chosen MRA as $j \to \infty$.

We illustrate this construction in one dimension. The two-scale relations for the coefficients representing the kernel with homogeneity degree α are

$$[r_l]_{ij} = 2^{-n-\alpha} \sum_{i',j'=0}^{k-1} h_{ii'}^{(0)} h_{jj'}^{(1)} [r_{2l-1}]_{i'j'} + (h_{ii'}^{(0)} h_{jj'}^{(0)} + h_{ii'}^{(1)} h_{jj'}^{(1)})[r_{2l}]_{i'j'} + h_{ii'}^{(1)} h_{jj'}^{(1)} [r_{2l+1}]_{i'j'},$$

where $[r_l]_{ij} = [r_{l0}^0]_{ij}$.

If the kernel has singularity at the origin and the multiwavelet coefficients are known for $|l| > 1$, the two-scale relations consist of three equations:

$$\begin{aligned}
[r_0]_{ij} - 2^{-(n+\alpha)} \sum \{ & h_{ii'}^{(0)} h_{jj'}^{(1)} [r_{-1}]_{i'j'} \\
& + (h_{ii'}^{(0)} h_{jj'}^{(0)} + h_{ii'}^{(1)} h_{jj'}^{(1)})[r_0]_{i'j'} + h_{ii'}^{(1)} h_{jj'}^{(1)} [r_1]_{i'j'} \} \\
= 2^{-(n+\alpha)} \sum \{ & h_{ii'}^{(0)} h_{jj'}^{(1)} [r_{-1}]_{i'j'} + (h_{ii'}^{(0)} h_{jj'}^{(0)} \\
& + h_{ii'}^{(1)} h_{jj'}^{(1)})[r_0]_{i'j'} + h_{ii'}^{(1)} h_{jj'}^{(1)} [r_1]_{i'j'} \};
\end{aligned}$$

$$\begin{aligned}
[r_1]_{ij} - 2^{-(n+\alpha)} \sum h_{ii'}^{(0)} h_{jj'}^{(1)} [r_1]_{i'j'} = 2^{-(n+\alpha)} \sum \{ & h_{ii'}^{(0)} h_{jj'}^{(1)} [r_1]_{i'j'} \\
& + (h_{ii'}^{(0)} h_{jj'}^{(0)} + h_{ii'}^{(1)} h_{jj'}^{(1)})[r_2]_{i'j'} \\
& + h_{ii'}^{(1)} h_{jj'}^{(1)} [r_3]_{i'j'} \};
\end{aligned}$$

and

$$\begin{aligned}
[r_{-1}]_{ij} - 2^{-(n+\alpha)} \sum h_{ii'}^{(1)} h_{jj'}^{(1)} [r_{-1}]_{i'j'} = 2^{-(n+\alpha)} \sum \{ & h_{ii'}^{(0)} h_{jj'}^{(1)} [r_{-3}]_{i'j'} \\
& + (h_{ii'}^{(0)} h_{jj'}^{(0)} + h_{ii'}^{(1)} h_{jj'}^{(1)})[r_{-2}]_{i'j'} \\
& + h_{ii'}^{(1)} h_{jj'}^{(1)} [r_{-1}]_{i'j'} \}.
\end{aligned}$$

We assume that the matrix coefficients $[r_l]_{ij}$ with $|l| \geq 2$ are known. The remaining coefficients become unknowns in the linear system. The important feature is that the relationships of coefficients at order k are recursive and depend only on coefficients from order 0 to $k - 1$. We use a preconditioned Generalized Minimal Residual (GMRES) solver with restart for solving the resulting linear system for each k.

The Hilbert transform

For singular integral operators, the multiwavelet coefficients can easily be computed away from the singularities of the kernel (e.g., by a quadrature). For the singular regions, we can use the two-scale relations to accurately compute the coefficients without using quadrature, as described above. The vanishing moment property of multiwavelets and the finite precision of the computation results in a sparse representation.

We illustrate this by using the Hilbert transform as an example:

$$Hf(y) = \frac{1}{\pi} \text{p.v.} \int \frac{f(x)}{x - y} dx.$$

The Hilbert transform appears in many important applications to wave propagtion and signal processing. The plot of the regularized Hilbert transform kernel using the multiresolution regularization procedure is shown in **Figure 4**.

The Poisson equation

The Poisson equation $\Delta\phi = \rho$ with the free-space boundary conditions occurs commonly in physics. In the differential form, wavelet and multiwavelet methods have been applied to solve the Poisson equation [16, 17]. In the integral formulation, for $x, y \in R^3$, the solution is

$$\phi(x) = \frac{1}{4\pi} \int \frac{\rho(y)}{|y - x|} dy.$$

In this formulation, the integral can be computed using the fast multipole method as well as our multiwavelet approach with the same complexity. The regularized Poisson kernel is shown in **Figure 5**.

We illustrate the accuracy of such a computation by the following example. Let

$$\rho(x, y, z) = \frac{65^3}{8\pi} \exp(-65r),$$

where

$$r = \sqrt{(x - 1/2)^2 + (y - 1/2)^2 + (z - 1/2)^2}.$$

The relative error of multiwavelet solutions for various k is shown in **Figure 6**.

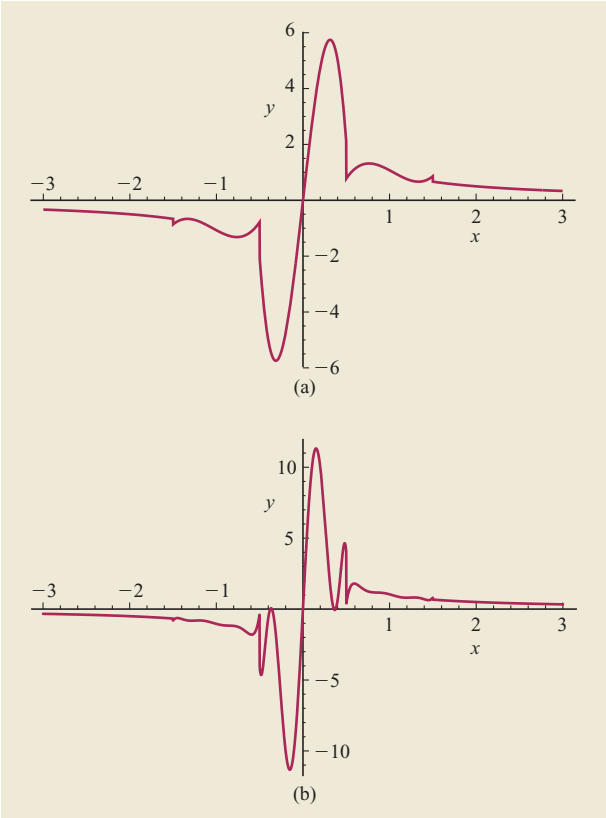

Figure 4

Plot of the regularized Hilbert kernel using multiwavelets of order (a) $k = 3$ and (b) $k = 7$.

Schrödinger's equation

In [3] a multiwavelet method is applied to solve the Schrödinger equation:

$$\left(-\frac{1}{2}\Delta + V\right)\Psi = E\Psi.$$

The integral form of this equation in three dimensions is

$$\Psi(r) = \frac{1}{4\pi}\int \frac{e^{-k|r-s|}}{|r-s|}V(s)\Psi(s)ds,$$

where V is the potential, Ψ is the wave function with the free-space boundary condition, and $k^2 = -2E$ is the energy [3, 18]. By using a fixed-point iteration scheme with a Davidson-like acceleration, a large number of chemical properties and reaction energies have been computed, so far for small molecules, using either the Hartree–Fock or density functional theory formulations. The total energy of the benzene molecule and the computational geometric features of our framework are shown in **Table 1** and **Figure 7**.

Conclusion

In this paper, we have reviewed multiwavelet methods for solving integro-differential equations and have described

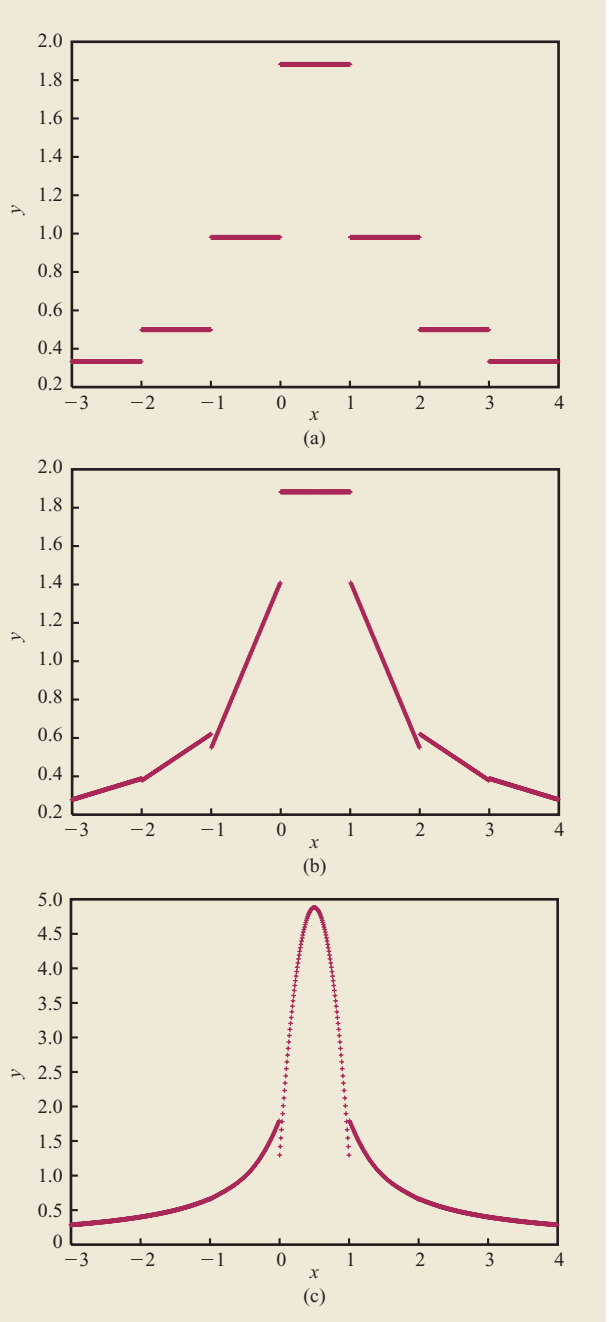

Figure 5

Two-dimensional slice of the multiwavelet-based regularized and "compressed" three-dimensional Poisson kernel using Legendre multiwavelets of order (a) $k = 0$, (b) $k = 1$, and (c) $k = 3$. The compressed kernel produces fast $O(N)$ direct Poisson solvers.

Table 1 The total energy of benzene computed using 7, 9, and 11 multiwavelets.

No. of multiwavelets	*Precision*	*Total energy* (eV)
7	10^{-3}	−230.194
9	10^{-5}	−230.19838
11	10^{-7}	−230.198345

new $O(N)$ multiscale simulation capabilities. The sparse representations of these operators were used to produce multiresolution methods for applying the Hilbert transform and solving the Poisson and Schrödinger equations.

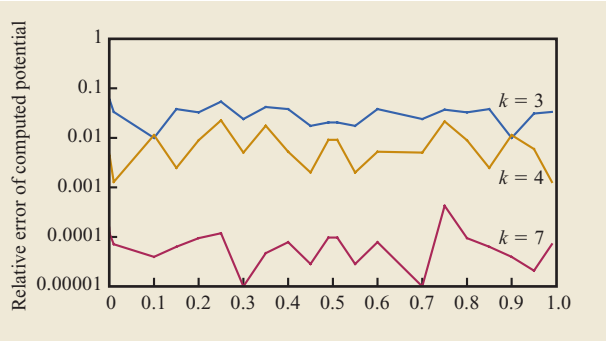

Figure 6

Relative error of the approximate solution for the example problem using the regularized kernel with $k = 3$, 4, and 7 multiwavelets.

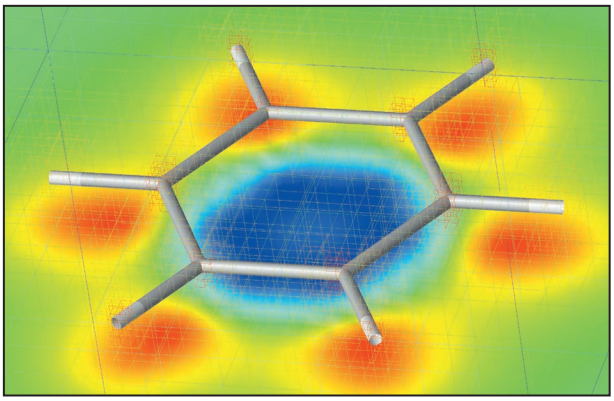

Figure 7

Graphic representation of a slice of the benzene molecule, showing the orbitals of the molecule. The orbitals were computed by means of a multiresolution method [3]. A ball-and-stick representation of the molecule is overlaid on an isocontour of a slice of one of the wave functions. The slice is colored according to the IBM OpenDX default colormap, and is a visual guide to the nodal structure of the orbitals and the structure within the isocontour. The grids represent support of the basis functions at different levels of refinement.

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