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.

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]. F6sw3inni6.0801 39scend], asc 7encew3in in the multiwavelet basis, the function f is expressed as

$$f\ x) \square \sum_{j} s_j \square^{0}_{j0}\ x) \square \sum_{n'=0}^{n-1} \sum_{l=0}^{2^n-1} \sum_{j=0}^{k-1} d^{n'}_{jl} \square^{n'}_{jl}\ x).$$

The scalars $s^{n}_{jl} = \int f(x)\square^{n}_{jl}(x)dx$ and $d^{n'}_{jl} = \int f(x)\square^{n'}_{jl}(x)dx$ 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

$$\square_i\ x) \square\ \sqrt{2} \sum_{j=0}^{k-1} [h_{ij}^{\ 0)}\square_j\ 2x) \square h_{ij}^{\ 1)}\square_j\ 2x \square 1)]$$

and

$$\square_i\ x) \square\ \sqrt{2} \sum_{j=0}^{k-1} [g_{ij}^{\ 0)}\square_j\ 2x) \square g_{ij}^{\ 1)}\square_j\ 2x \square 1)],$$

where $h^{(0)}_{ij}$, $h^{(1)}_{ij}$, $g^{(0)}_{ij}$, and $g^{(1)}_{ij}$ 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 $n + 1$,

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

and

$$d^{n}_{il} \square\ \sqrt{2} \sum_{j=0}^{k-1}$$

of the basis functions. For example, in two dimensions, the coeffi

[redacted]. 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 $|l| \square 1$. Coefficients in this range appear on both sides of the two-scale difference equations.

In general, this criterion is written as

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

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 $\square$. 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 $j \to$.

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

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

$$+ h_{ii'}^{0)} h_{jj'}^{0)} \square h_{ii'}^{1)} h_{jj'}^{1)})[r_{2l}]_{i'j'} \square h_{ii'}^{1)} h_{jj'}^{1)} [r_{2l+1}]_{i'j'},$$

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

[redacted] multiwavelet coefficients are known for $|l| > 1$, the two-scale relations consist of three equations:

[redacted]

$$\square\ 2^{--]}$$

Schrödinger's equation

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

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

The integral form of this equation in three dimensions is

$$\Psi\ r) \square \frac{1}{4}$$

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 SchroN

and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN, 2003.
4. I. Daubechies, *Ten Lectures on Wavelets*, CBMS–NSF Regional Conference Series in Applied Mathematics, Vol. 61, SIAM, Philadelphia, PA, 1992.
5. G. Beylkin and R. Cramer, "A Multiresolution Approach to Regularization of Singular Operators and Fast Summation," *SIAM J. Sci. Comp.* **24**, No. 1, 81–117 (2002).
6. B. Alpert, "A Class of Bases in L^2 for the Sparse Representation of Integral Operators," *SIAM J. Math. Anal.* **24**, No. 1, 246–262 (1993).
7. B. Alpert, G. Beylkin, D. Gines, and L. Vozovoi, "Adaptive Solution of Partial Differential Equations in Multiwavelet Bases," *J. Comp. Phys.* **182**, 149–190 (2002).
8. L. Greengard and J. Lee, "A Direct Adaptive Solver of Arbitrary Order Accuracy," *J. Comp. Phys.* **125**, 415–424 (1996).
9. L. Greengard and V. Rokhlin, "A New Version of the Fast Multipole Method for the Laplace Equation in Three Dimensions," *Acta Numer.* **6**, 229 (1997).
10. V. Rokhlin, "Rapid Solution of Integral Equations of Classical Potential Theory," *J. Comp. Phys.* **60**, 187–207 (1985).
11. S. Mallat, "Multiresolution Approximation and Wavelet Orthonormal Bases of L_2," *Trans. Amer. Math. Soc.* **315**, 69–87 (1989).
12. Y. Meyer, *Wavelets and Operators*, Cambridge Studies in Advanced Mathematics, Vol. 37, Cambridge University Press, Cambridge, England, 1995.
13. G. Beylkin, "On the Representation of Operators in Bases of Compactly Supported Wavelets," *SIAM J. Numer. Anal.* **6**, 1716–1740 (1992).
14. L. Schwartz, *Theorie des Distributions*, Hermann, Paris, 1966.
15. I. M. Gel'fand and G. E. Shilov, *Generalized Functions*, Vol. 1, Academic Press, Inc., New York, 1964.
16. A. Averbuch, G. Beylkin, R. Coifman, and M. Israeli, *Multiresolution Solution of Elliptic and Parabolic PDEs*, the Samuel Neaman Workshop on Signal and Image Representation in Combined Space, Technion, Haifa, Israel, May 8-11, 1994, Y. Zeevi and R. Coifman, Eds., Academic Press, Inc., New York, 1998.
17. W. Dahmen, "Wavelet and Multiscale Methods for Operator Equations," *Acta Numer.* **6**, 55–228 (1997).
18. M. H. Kalos, "Monte Carlo Calculations of the Ground State of Three- and Four-Body Nuclei," *Phys. Rev.* **128**, No. 4, 1791–1795 (1962).

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