The solution of multi-scale partial differential equations using wavelets

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1 Introduction

Wavelets are a powerful new mathematical tool which offers the possibility to treat in a natural way quantities characterized by several length scales. In this article we will show how wavelets can be used to solve partial differential equations which are characterized by widely varying length scales and which are therefore hardly accessible by other numerical methods. The standard way to solve partial differential equations is to express the solution as a linear combination of so-called basis functions. These basis functions can for instance be plane waves, Gaussians or finite elements. Having discretized the differential equation in this way makes it amenable to a numerical solution. Wavelets are just another basis set which however offers considerable advantages over alternative basis sets. Its main advantages are:

1. The basis set can be improved in a systematic way:
   If one wants the solution of the differential equation with higher accuracy one can just add more wavelets in the expansion of the solution. This will not lead to any numerical instabilities.

2. Different resolutions can be used in different regions of space:
   If the solution of the differential equation is varying particularly rapidly in a particular region of space one can increase the resolution in this region by adding more high resolution wavelets centered around this region.

3. There are few topological constraints for increased resolution regions:
   The regions of increased resolution can be chosen in arbitrarily, the only requirement
being that a region of higher resolution be contained in a region of the next lower resolution.

4. The matrix elements of the differential operators are very easy to calculate

5. The numerical effort scales linearly with respect to system size:

Three-dimensional problems of realistic size require usually a very large number of basis functions. It is therefore of utmost importance, that the numerical effort scales only linearly (and not quadratically or cubically) with respect to the number of basis functions. If one uses iterative matrix techniques, this requirement is equivalent to the two requirements, namely that the matrix vector multiplications which are necessary for all iterative methods can be done with linear scaling and that the number of matrix vector multiplications is independent of the problem size. The first requirement is fulfilled since the matrix representing the differential operator is sparse. The second requirement is related to the availability of a good preconditioning scheme which can be easily found by analyzing the Fourier properties of wavelets.

2 A first tour of some wavelet families

Many families of wavelets have been proposed in the mathematical literature. If one wants to use wavelets for the solution of differential equations, one therefore has to choose one specific family which is most advantageous for the intended application. Within one family there are also members of different degree. We believe that the so-called bi-orthogonal interpolating wavelets \[6\] are the most useful ones in the context of differential equations and we will therefore mainly concentrate on this class. Each wavelet family is characterized by two functions, the mother scaling function \(\phi\) and the mother wavelet \(\psi\). For the case of a fourth order interpolating wavelet they are shown in Figure 1.

![Figure 1: The interpolating scaling function and wavelet of degree 4](image)

Another family which will be introduced is the Haar wavelet family shown in Figure 2. It is too crude to be useful for any numerical work, but its simplicity will help us to illustrate some basic wavelet concepts.
To obtain a basis set at a certain resolution level $k$ one can use all the integer translations of the mother scaling function of some wavelet family.

$$\phi_i^k(x) = \phi(2^k x - i)$$

Note that with this convention higher resolution corresponds to larger values of $k$. Exactly the same scaling and shifting operations can of course also be applied to the wavelets.

$$\psi_i^k(x) = \psi(2^k x - i)$$

This set of wavelet basis functions can be added as a basis to the scaling functions as will be explained in the following for the case of the Haar wavelet family.

### 3 The Haar wavelet

In the case of the Haar family, any function which can exactly be represented at any level of resolution is necessarily piecewise constant. One such function is shown in Figure 3.

Evidently this function can be written as a linear combination of the scaling functions $\phi_i^4(x)$

$$f = \sum_{i=0}^{16} s_i^4 \phi_i^4(x)$$
where $s_4^i = f(i/16)$.

Another, more interesting, possibility consists of expanding a function with respect to wavelets of different resolution. This is possible because a scaling function (and wavelet) at resolution level $k$ is always a linear combination of a scaling function and a wavelet at the next coarser level $k - 1$ as shown in Figure 4.

![Figure 4: A skinny scaling function is a linear combination of a fat scaling function and a wavelet.](image)

Using this relation, we can write any linear combination of the two scaling functions $\phi_{2i}^k(x)$ and $\phi_{2i+1}^k(x)$ as a linear combination of $\phi_{i}^{k-1}(x)$ and $\psi_{i}^{k-1}(x)$.

Denoting the expansion coefficients with respect to $\psi_{i}^{k}(x)$ as $d_{i}^{k}$, we obviously obtain

$$s_{i}^{k-1} = \frac{1}{2} s_{2i}^{k} + \frac{1}{2} s_{2i+1}^{k} ; \quad d_{i}^{k} = \frac{1}{2} s_{2i}^{k} - \frac{1}{2} s_{2i+1}^{k} \quad (4)$$

So to calculate the expansion coefficients with respect to the scaling functions at the next coarser level, we have to take an average over expansion coefficients at the higher resolution level. Because we have to take some weighted sum these coefficients are denoted by $s$. To get the expansion coefficients with respect to the wavelet, we have to take some weighted difference and the coefficients are accordingly denoted by $d$. The wavelet part contains mainly high frequency components and by doing this transformation we therefore peel off the highly oscillatory parts of the function. The remaining part represented by the coefficients $s_{i}^{k-1}$ is therefore smoother. For the case of our example in Figure 3 the remaining scaling function part after one transformation step is shown in Figure 4.

For any data set whose size is a power of 2, we can now apply this transformation repeatedly. In each step the number of $s$ coefficients will be cut into half. So we have to
stop the procedure as soon as there is only one $s$ coefficient left. Such a series of transformation steps is called a forward Haar wavelet transform. The wavelet representation of the function in Equation 3 is then

$$f = s_0^0 \phi_1^0(x) + d_1^0 \psi_1^0(x) + \sum_{i=1}^{2} d_i^1 \psi_i^1(x) + \sum_{i=1}^{4} d_i^2 \psi_i^2(x) + \sum_{i=1}^{8} d_i^3 \psi_i^3(x).$$  

(5)

Note that in both cases we need exactly 16 coefficients to represent the function. Functional representations of this type will be the focus of this article.

By doing a backward wavelet transform, we can go back to the original expansion of Equation 3. Starting at the lowest resolution level, we have to split up each scaling function and wavelet on the coarse level into scaling functions at the finer level.

$$s_{2i}^{k+1} = s_i^k + d_i^k; \quad s_{2i+1}^{k+1} = s_i^k - d_i^k$$  

(6)

4 The concept of Multi-Resolution Analysis

In the previous sections a very intuitive introduction to wavelet theory was given. The formal theory behind wavelets is called Multi-Resolution Analysis (MRA). The reader interested in the formal theory can consult Daubechies’s book. We will list here only a few facts which are useful for numerical work.

A bi-orthogonal wavelet family of degree $m$ is characterized by 4 finite filters denoted by $h_j, \tilde{h}_j, g_j, \tilde{g}_j$. A filter is just a short vector which is used in convolutions. Those filters satisfy certain orthogonality and symmetry relations. Scaling functions and wavelets at a coarse level can be written as the linear combinations of scaling functions at a higher resolution level. These important relations are called refinement relations.

$$\phi(x) = \sum_{j=-m}^{m} h_j \phi(2x - j)$$  

(7)

$$\psi(x) = \sum_{j=-m}^{m} g_j \phi(2x - j)$$  

(8)

$$\tilde{\phi}(x) = 2 \sum_{j=-m}^{m} \tilde{h}_j \tilde{\phi}(2x - j)$$  

(9)
\[ \tilde{\psi}(x) = 2 \sum_{j=-m}^{m} \tilde{g}_j \tilde{\phi}(2x - j) \] (10)

The expansion coefficients at different resolution levels are related by the wavelet transform equations. The analysis (forward) transform is given by

\[ s_k^{k-1} = \sum_{j=-m}^{m} \tilde{h}_j s_{j+2i}^k \quad ; \quad d_k^{k-1} = \sum_{j=-m}^{m} \tilde{g}_j s_{j+2i}^k \] (11)

and a wavelet synthesis (backward) transform is given by

\[ s_{2i}^{k+1} = \sum_{j=-m/2}^{m/2} h_{2j} s_{i-j}^k + g_{2j} d_{i-j}^k \quad ; \quad s_{2i+1}^{k+1} = \sum_{j=-m/2}^{m/2} h_{2j+1} s_{i-j}^k + g_{2j+1} d_{i-j}^k \] (12)

These two equations are generalizations of Equations (4) and (6) which we derived in an intuitive way and with a different normalization convention.

The fundamental functions satisfy the following orthogonality relations

\[ \int \tilde{\phi}_i^k(x) \tilde{\phi}_j^q(x) dx = \delta_{i,j} \] (13)
\[ \int \tilde{\psi}_i^k(x) \tilde{\phi}_j^q(x) dx = 0 \ , \ k \geq q \] (14)
\[ \int \tilde{\phi}_i^k(x) \tilde{\psi}_j^q(x) dx = 0 \ , \ k \geq q \] (15)
\[ \int \psi_i^k(x) \psi_j^q(x) dx = \delta_{k,q} \delta_{i,j} \] (16)

The scaling function is usually normalized to 1

\[ \int \phi(x) dx = 1 \] (17)

5 The fast wavelet transform

Let us first look at the forward transform given by Equation (11). The peeling off of the high frequency components in the forward transform can be illustrated in the following way:

\[ s^4 \rightarrow s^3 \rightarrow s^2 \rightarrow s^1 \rightarrow s^0 \]
\[ \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \]
\[ d^3 \quad d^2 \quad d^1 \quad d^0 \]

We note that just two arrays of length n (where n is a power of 2) are necessary to do the transform as shown below:
original data
Array 1: \( s_0^4 \ s_1^4 \ s_2^4 \ s_3^4 \ s_4^4 \ s_5^4 \ s_6^4 \ s_7^4 \ s_8^4 \ s_9^4 \ s_{10}^4 \ s_{11}^4 \ s_{12}^4 \ s_{13}^4 \ s_{14}^4 \ s_{15}^4 \)

after first sweep
Array 2: \( s_0^3 \ s_1^3 \ s_2^3 \ s_3^3 \ s_4^3 \ s_5^3 \ s_6^3 \ d_0^3 \ d_1^3 \ d_2^3 \ d_3^3 \ d_4^3 \ d_5^3 \ d_6^3 \ d_7^3 \)

after second sweep
Array 1: \( s_0^2 \ s_1^2 \ s_2^2 \ s_3^2 \ s_4^2 \ d_0^2 \ d_1^2 \ d_2^2 \ d_3^2 \ d_4^2 \ d_5^2 \ d_6^2 \ d_7^2 \)

after third sweep
Array 2: \( s_0^1 \ s_1^1 \ d_0^1 \ d_1^1 \ d_2^1 \ d_3^1 \ d_4^1 \ d_5^1 \ d_6^1 \ d_7^1 \)

final data
Array 1: \( s_0^0 \ d_0^0 \ d_1^0 \ d_2^0 \ d_3^0 \ d_4^0 \ d_5^0 \ d_6^0 \ d_7^0 \)

Note that this transformation from the "original data" to the "final data" corresponds exactly to the transformation done in an intuitive way to get from Equation 3 to Equation 12. Just as in the case of a Fast Fourier transform we have \( \log_2(n) \) sweeps to do a full transform. However in the case of the wavelet transform the active data set (the \( s \) coefficients) is cut into half in each sweep. If our filters \( h \) and \( g \) have length \( 2m \) the operation count is then given by \( 2m(n + n/2 + n/4 + ...) \). Replacing the finite geometric series by its infinite value, the total operation count is thus given by \( 4mn \).

The backward transform (Equation 12) can pictorially be represented by the following diagram:

\[
\begin{array}{cccc}
S^4 & \leftarrow & S^3 & \leftarrow \ S^2 & \leftarrow \ S^1 & \leftarrow \ S^0 \\
\searrow & \swarrow & \searrow & \swarrow & \searrow & \swarrow \\
D^3 & & D^2 & & D^1 & & D^0 \\
\end{array}
\]

As can easily been seen the operation count is again \( 4mn \) and again it can be done with 2 arrays of length \( n \). Since each sweep in a wavelet transform is a linear operation it can be represented by a matrix. Denoting the matrix for one sweep in a forward transform by \( \tilde{F} \) and in a backward transform by \( B \) we have

\[
F^T = \tilde{F}^{-1} = B ; \quad \tilde{B}^T = B^{-1} = \tilde{F}
\]

where the tilde on the matrix means that the filter coefficients necessary to fill the matrix are replaced by their dual counterparts. Obviously all these matrices are sparse and banded.

Backward wavelet transforms can also be used to make plots of scaling functions and wavelets. To generate the scaling function we start with a data set where \( s_0^0 = 1 \) and \( d_k^i = 0 \) for all possible \( i \)'s and \( k \)'s up to a maximum resolution level \( k = K \). In the wavelet case the initial data set is \( s_0^0 = 0, d_0^0 = 1, \) and \( d_k^i = 0 \) for all other values of \( i \) and \( k \) up to the maximal resolution \( K \). By doing repeated backward transform sweeps, we express these two functions by skinner and skinner scaling functions and the \( s \) coefficients will finally be the functional values within the resolution of the eye.
6 Interpolating wavelets

In addition to being advantageous as basis sets, interpolating wavelets are also conceptually the simplest wavelets and we will therefore briefly describe their construction. The construction of interpolating wavelets is closely connected to the question of how to construct a continuous function \( f(x) \) if only its values \( f_i \) on a finite number of grid points \( i \) are known. One way to do this is by recursive interpolation. In a first step we interpolate the functional values on all the midpoints by using for instance the values of two grid points to the right and of two grid points to the left of the midpoint. These four functional values actually allow us to construct a third order polynomial and we can then evaluate it at the midpoint. In the next step, we take this new data set, which is now twice as large as the original one, as the input for a new midpoint interpolation procedure. This can be done recursively ad infinitum until we have a quasi continuous function.

Let us now show, how this interpolation prescription leads to a set of basis functions. Denoting by the Kronecker \( \delta_{i-j} \) a data set which has a nonzero entry only at the \( j \)-th position, we can write any initial data set also as a linear combination of such Kronecker data sets: \( f_i = \sum_j f_j \delta_{i-j} \). Now the whole interpolation procedure is clearly linear, i.e. the sum of two interpolated values of two functions is equal to the interpolated value of the sum of these two functions. This means that we can instead also take all the Kronecker data sets as the input for separate interpolation procedures, to obtain a set of functions \( \phi(x-j) \). The final interpolated function is then identical to

\[
f(x) = \sum_j f_j \phi(x-j)
\] (19)

If the initial grid values \( f_i \) were the functional values of a polynomial of degree less than four, we obviously will have exactly reconstructed the original function from its values on the grid points. Since any smooth function can locally be well approximated by a polynomial, these functions \( \phi(x) \) are good basis functions also in the case where \( f \) is not a polynomial and we will use them as scaling functions to construct a wavelet family.

The first construction steps of an interpolating scaling function are shown below for the case of linear interpolation. The initial Kronecker data set is denoted by the big dots. The additional data points obtained after the first interpolation step are denoted by medium size dots and the additional data points obtained after the second step by small dots.

Continuing this process ad infinitum will then result in the function shown in the left panel of Figure 6. If an higher order interpolation scheme is used the function shown in
the right panel of Figure 6 is obtained.

![Graph](image_url)

Figure 6: A Kronecker delta interpolated ad infinitum with linear interpolation (left panel) and 7-th order interpolation (right panel).

By construction it is clear, that $\phi(x)$ has compact support. If an $(m - 1)$-th order interpolation scheme is used, the filter length is $(m - 1)$ and the support interval of the scaling function is $[-(m - 1); (m - 1)]$.

It is also not difficult to see that the functions $\phi(x)$ satisfy the refinement relation. Let us again consider the interpolation ad infinitum of a Kronecker data set which has everywhere zero entries except at the origin. We can now split up this process into the first step, where we calculate the half-integer grid point values, and a remaining series of separate ad infinitum interpolations for all half-integer Kronecker data sets, which are necessary to represent the data set obtained by the first step. Doing the ad-infinitum interpolation for a half integer Kronecker data set with a unit entry at position $j$, we obviously obtain the same scaling function, just compressed by a factor of 2, $\phi(2x - j)$. If we are using a $(m - 1)$-th order interpolation scheme (i.e. $m$ input data for the interpolation process) we thus get the relation

$$\phi(x) = \sum_{j=-m+1}^{m-1} \phi(j/2) \phi(2x - j)$$

(20)

Comparing this equation with the refinement relation Equation 7 we can identify the first filter $h$ as

$$h_j = \phi(j/2) , \ j = -m + 1, m - 1$$

For the case of third order interpolation the numerical values of $h$ follow from the standard interpolation formula and are given by \{-1/16 , 0 , 9/16 , 1 , 9/16 , 0 , -1/16 \}.

Let us next determine the filter $\tilde{h}$. Let us consider a function $f(x)$ which is band-limited in the wavelet sense, i.e which can exactly be represented by a superposition of scaling functions at a certain resolution level $K$.

$$f(x) = \sum_{j} s_j^K \phi_j^K(x)$$
It then follows from the orthogonality relation Equation 13 that

\[ s_j^K = \int \tilde{\phi}_j^K(x) f(x) dx \]  

(21)

Now we have seen above that with respect to interpolating scaling functions, a band-limited function is just any polynomial of degree less than or equal to \( m - 1 \), and that in this case the expansion coefficients \( s_j^K \) are just the functional values at the grid points (Equation 19). We therefore have

\[ s_j^K = \int \tilde{\phi}_j^K(x) f(x) dx = f_j \]  

(22)

which shows that the dual scaling function \( \tilde{\phi} \) is the delta function.

\[ \tilde{\phi}(x) = \delta(x) \]  

(23)

Obviously the delta function satisfies a trivial refinement relation \( \delta(x) = 2\delta(2x) \) and from Equation 8 we conclude that \( \tilde{h}_j = \delta_j \). From the symmetry relations for the filters the two remaining filters \( \tilde{g}(i) \) and \( g(i) \) can be determined and we have thus completely specified our wavelet family.

Using these filters we can then determine the wavelet \( \psi \) and its dual counterpart \( \tilde{\psi} \) which turn out to be

\[ \psi(x) = \phi(2x - 1) \]  

\[ \tilde{\psi}(x) = -\frac{1}{16}\delta((x - \frac{1}{2}) - 3) + \frac{9}{16}\delta((x - \frac{1}{2}) - 1) - \delta((x - \frac{1}{2})) + \frac{9}{16}\delta((x - \frac{1}{2}) + 1) + \frac{1}{16}\delta((x - \frac{1}{2}) + 3) \]  

(25)

We see that the interpolating wavelet is a very special case in that its scaling function and wavelet have the same functional form and that the dual functions are related to the delta function. The non-dual functions are shown in Figure 1.

Lifting [5] is a very useful technique to modify an existing family of wavelets to meet specific needs. We can for instance lift the interpolating wavelets to obtain a new family whose wavelet has more vanishing moments \( M_l \).

\[ M_l = \int \psi_j^K(x) x^l dx \]

which will for instance improve the frequency properties of the wavelet.

7 Expanding functions in a wavelet basis

As was demonstrated in the case of the Haar wavelet, there are two possible representations of a function within the framework of wavelet theory. The first one is called scaling function representation and involves only scaling functions. The second is called wavelet representation and involves wavelets as well as scaling functions. Both representations are completely equivalent and exactly the same number of coefficients are needed in the case where one has uniform resolution.
The scaling function representation is given by

\[ f(x) = \sum_j s_j^{K_{\text{max}}} \phi_j^{K_{\text{max}}}(x) \]  

(26)

The coefficients \( s_j^{K_{\text{max}}} \) can be calculated by integration through Equation 22. Once we have a set of coefficients \( s_j^{K_{\text{max}}} \) we can use a full forward wavelet transform to obtain the coefficients of the wavelet representation

\[ f(x) = \sum_j s_j^{K_{\text{min}}} \phi_j^{K_{\text{min}}}(x) + \sum_{K=K_{\text{min}}}^{K_{\text{max}}} \sum_j d_j^K \psi_j^K(x) \]

(27)

Alternatively, one could also directly calculate the \( d \) coefficients by integration

\[ d_j^K = \int \tilde{\psi}_j^K(x) f(x) dx \]  

(28)

Equation 28 follows from the orthogonality relations 14 to 16.

So we see that if we want to expand a function either in scaling functions or wavelets, we have to perform integrations at some point to calculate the coefficients. For general wavelet families this integration can be fairly cumbersome and require especially in 2 and 3 dimensions a substantial number of integration points. Furthermore it is not obvious how to do the integration if the function is only given in tabulated form. The interpolating wavelets discussed above are the glorious exception. Since the dual scaling function is a delta function (23) and since the dual wavelet is a sum of delta functions (25), one or a few data points are sufficient to do the integration exactly. One will therefore get exactly the same number of coefficients as one has data points and one has an invertible one-to-one mapping between the functional values on the grid and the expansion coefficients. This is even true in the case of nonuniform data sets, where we necessarily have to calculate the \( s \) and \( d \) coefficients directly by integration using 28. As follows from Equation 23 and 25, one just needs the functional values at the data point at which the wavelet will be centered and a few data points at one lower resolution level around this center. If one wants to calculate the interpolating wavelet center at the high resolution grid point indicated by the fat arrow in the figure below, one needs in the case of the 4-th order interpolating wavelets the 4 additional points indicated by thin arrows which belong to a more coarse grid and are therefore always available even if the fine grid does not extend into this region.

\[ \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet \]

In the case where one wants to represent functions with several length scales which need inhomogeneous real space grid structure the wavelet representation allows a much more compact representation than the scaling function representation, since one can neglect
all the tiny $d$ coefficients in the regions where one has little variation. To illustrate this let us look at the function $f$

$$f(x) = \sum_{l=1}^{8} \exp(-xl^2)$$

Evidently this function exhibits 8 different length scales. If one expands one simple Gaussian $\exp(-x^2)$ with respect to 4-th order interpolating scaling functions with a resolution of $1/16$, one gets a reasonably small error of $10^{-6}$. For the multi-scale function $f$, this error increases to more than $10^{-2}$ with the same resolution. If one however uses a scheme where one uses 32 wavelets on additional 5 resolution levels to improve the resolution as one approaches the origin one can again represent the function with an error of roughly $10^{-6}$ (it turns out that the expected 8 additional levels are not all needed). The total number of coefficients needed to represent the function in the interval $[-2, 2]$ is then $4 \times 16$ coefficients for the equal resolution ($1/16$) scaling function part plus $5 \times 32$ coefficients for the resolution enhancement with the wavelets, which makes all together 224 coefficients. This has to be compared with the 1024 scaling function coefficients which would be needed to represent the function over the whole interval with the maximum resolution of $(1/256)$, which we have obtained around the origin with this data compression scheme.

## 8 Wavelets in 2 and 3 dimensions

The easiest way to construct a wavelet basis in higher dimensional spaces is by forming product functions [2]. For simplicity of notation we will only consider here the 2-dimensional case, the generalization to higher dimensional spaces being obvious.

The space of all scaling functions of resolution level $k$ is given by

$$\phi_{i1,i2}^{k}(x,y) = \phi_{i1}^{k}(x)\phi_{i2}^{k}(y)$$

The wavelets consist of three types of products

$$\psi[sd]_{i1,i2}^{k}(x,y) = \phi_{i1}^{k}(x)\psi_{i2}^{k}(y)$$

$$\psi[ds]_{i1,i2}^{k}(x,y) = \psi_{i1}^{k}(x)\phi_{i2}^{k}(y)$$

$$\psi[dd]_{i1,i2}^{k}(x,y) = \psi_{i1}^{k}(x)\psi_{i2}^{k}(y)$$

A wavelet transform step in the 2-dimensional setting is done by first transforming along the $x$ and then along the $y$ direction (or vice versa).

## 9 The standard operator form

In a bi-orthogonal wavelet basis it is natural to solve a differential equation in the collocation sense. Let us recall that in the collocation method one has two functional spaces, the space of the basis function which are used to represent the solution and the space of the test functions which are used to multiply the differential equation from the left to obtain
a linear system of equations. In our case the expansion set are the scaling functions and wavelets while the test set are their dual counterparts. Let’s consider the case of Poisson’s equation

$$\nabla^2 V = -4\pi \rho. \quad (33)$$

Given the expansion of the charge density \( \rho \) in a wavelet basis

$$\rho(x) = \sum_j s_j^{K_{min}} \phi_j^{K_{min}}(x) + \sum_{K=K_{min}}^{K_{max}} \sum_j d^K_j \psi^K_j(x) \quad (34)$$

we are looking for the wavelet expansion coefficients of the potential \( V \).

$$V(x) = \sum_j S_j^{K_{min}} \phi_j^{K_{min}}(x) + \sum_{K=K_{min}}^{K_{max}} \sum_j D^K_j \psi^K_j(x) \quad (35)$$

Plugging in the expansion for \( \rho \) and \( V \) (34) and (35) in Poisson’s equation (33) and multiplying from the left with the dual wavelet collocation test space we obtain a system of equations

$$A_s \vec{v} = \vec{\rho} \quad (36)$$

where \( \vec{v} \) is the vector containing both the \( s \) and \( d \) coefficients of the potential and \( \vec{\rho} \) is the same vector for the charge density \( \rho \). The matrix \( A_s \) represents the Laplacian in this wavelet basis and one says that it has standard form. This standard form is graphically shown in Figure 7.

![Figure 7: The structure of a matrix in the standard form.](image)

The problem with the standard form is that it is first of all rather complicated. There is coupling between all resolution levels and one has to calculate many different types of
matrix elements corresponding to all possible products of wavelets and scaling functions at different resolution levels and positions. The second point is that there are many blocks in that matrix which have no or only few zeroes. Let us look at the blocks representing the coupling between the scaling functions at the highest resolution level and the wavelets at the different resolution. In general each scaling function will extend over the whole computational volume and will therefore overlap with all the wavelets at any position. All these blocks will consequently have nonzero entries only. So this standard matrix form has more nonzero entries than we would like to have for optimal efficiency in the matrix vector multiplications which are required for all iterative linear equation solvers.

10 The non-standard operator form

The so-called nonstandard \[8\] form gives a much easier and efficient representation of our matrix. To derive it let us first assume, that our potential \( V \) and charge \( \rho \) are given in a scaling function basis. The Laplacian is then represented by a matrix \( A \) whose elements \( A_{i,j} \) are given by \[ \int \tilde{\phi}_i^k(x) \nabla^2 \phi_j^k(x) dx \]

The matrix equation

\[ A\vec{v} = \vec{\rho} \]

can graphically be represented in the following way:

\[ \begin{array}{c|c} <S|\{S\} & S \end{array} = \begin{array}{c} S \end{array} \]

Now we can of course perform one step of a forward wavelet transform on all our data, i.e. both on the vector to be multiplied with the matrix and on the vector which is the result of this matrix times vector multiplication. Correspondingly we have then to transform the matrix \( A \) using the matrices whose properties are given in Equation 18.

\[ \tilde{F}\vec{\rho} = (\tilde{F}AF^T)(\tilde{F}\vec{v}) \]

Graphically this gives:

\[ \begin{array}{c|c} <S|\{S\} & <S|\{\rho\} \end{array} = \begin{array}{c} S \end{array} \]

\[ \begin{array}{c|c} <D|\{S\} & <D|\{\rho\} \end{array} = \begin{array}{c} D \end{array} \]

If we recursively applied wavelet transform to the upper \( S \) part we would obviously obtain the standard operator form. To get the nonstandard form, we have to add another step where we artificially enlarge our matrix \( A \) by putting in 5 blocks of zeroes as shown below:
We see that our input and output vectors $\vec{v}$ and $\vec{\rho}$ also have to be adapted to this matrix structure leading to a redundant copy of the $S$ data set.

We can now recursively apply this 2-step procedure on the $<S|S>$ block of the resulting matrices. Doing this we obtain the so called non-standard form, which is graphically visualized in Figure 8.

As we see, we have now completely decoupled different resolution levels, since there are no blocks in this matrix between different levels. The coupling between different levels just enters through the wavelet transforms which have to be interleaved with the application of this nonstandard operator form. We also see that all the nonzero blocks of this nonstandard matrix representation are strictly banded and the application of this matrix to a vector scales therefore linearly.

The structure of the matrix in Figure 8 is primarily valid for the case of uniform resolution where all the possible $d$ coefficients at the highest resolution level are nonzero.
It can however easily be seen that this nonstandard form retains its advantage in a case of varying resolution where only some of the \( d \) coefficients are nonzero. If the nonredundant input data set is sparse, the redundant input data set will be sparse as well. Since all the blocks are banded, the redundant output set will be sparse as well. Finally the nonredundant output set will then be sparse as well.

11 Calculation of differential operators in a wavelet basis

As we have seen in the preceding chapter we need the matrix elements

\[
\int \tilde{\phi}_i^k(x) \frac{\partial^l}{\partial x^l} \phi_j^k(x) \, dx
\]

(37)

\[
\int \bar{\psi}_i^k(x) \frac{\partial^l}{\partial x^l} \phi_j^k(x) \, dx
\]

(38)

\[
\int \tilde{\phi}_i^k(x) \frac{\partial^l}{\partial x^l} \psi_j^k(x) \, dx
\]

(39)

\[
\int \bar{\psi}_i^k(x) \frac{\partial^l}{\partial x^l} \psi_j^k(x) \, dx
\]

(40)

for the application of an operator in the nonstandard form. Matrix elements on different resolution levels are related by simple scaling relations. So we just have to calculate these 4 matrix elements for one resolution level. On a certain resolution level, we can use the refinement relations to express the matrix elements involving wavelets in terms of matrix elements involving scaling functions (at a better resolution level) only. So we just have to calculate the basic integral \( a_i \)

\[
a_i = \int \tilde{\phi}(x) \frac{\partial^l}{\partial x^l} \phi(x - i) \, dx
\]

(41)

Using the refinement relations Equations 7 and 9 for \( \phi \) and \( \tilde{\phi} \) we obtain

\[
a_i = \int \tilde{\phi}(x) \frac{\partial^l}{\partial x^l} \phi(x - i) \, dx
\]

(42)

\[
a_i = \sum_{\nu,\mu} 2 \tilde{h}_\nu h_\mu \int \tilde{\phi}(2x - \nu) \frac{\partial^l}{\partial x^l} \phi(2x - 2i - \mu) \, dx
\]

\[
= \sum_{\nu,\mu} 2 \tilde{h}_\nu h_\mu 2^l \int \tilde{\phi}(y - \nu) \frac{\partial^l}{\partial y^l} \phi(y - 2i - \mu) \, dy
\]

\[
= \sum_{\nu,\mu} \tilde{h}_\nu h_\mu 2^l \int \tilde{\phi}(y) \frac{\partial^l}{\partial y^l} \phi(y - 2i - \mu + \nu) \, dy
\]

\[
= \sum_{\nu,\mu} \tilde{h}_\nu h_\mu 2^l a_{2i - \nu + \mu}
\]

(43)
We thus have to find the eigenvector $\vec{a}$ associated with the eigenvalue of $2^{-l}$.

$$\sum_j A_{i,j} a_j = \left(\frac{1}{2}\right)^l a_i$$  \hspace{1cm} (44)

where the matrix $A_{i,j}$ is given by

$$A_{i,j} = \sum_{\nu,\mu} \tilde{h}_\nu h_\mu \delta_{j,2i-\nu+\mu}$$  \hspace{1cm} (45)

As it stands this eigensystem has a solution only if the rang of the matrix $A - 2^{-l}I$ is less than its dimension. For a well defined differential operator, i.e if $l$ is less than the degree of smoothness of the scaling function this will be the case.

The system of equations (44) determines the $a_j$’s only up to a normalization factor. For the case of interpolating wavelets the normalization condition is easily found from the requirement that one obtains the correct result for the function $x^l$. From the normalization of the scaling function (17) and from elementary calculus, it follows that

$$\int \phi(x) \frac{\partial^l}{\partial x^l} x^l \, dx = \int \phi(x) l! \, dx = l!$$  \hspace{1cm} (46)

On the other hand we know, that we can expand any polynomial of low enough degree exactly with the interpolating polynomials. The expansion coefficients are just $i^l$ by Equation (22). So we obtain

$$\int \phi(x) \frac{\partial^l}{\partial x^l} \sum_i i^l \phi(x - i) = \sum_i i^l a_i$$  \hspace{1cm} (47)

By comparing Equation (46) and (47) we thus obtain the normalization condition

$$\sum_i i^l a_i = l!$$  \hspace{1cm} (48)

The interpolating wavelet family offers also an important advantage for the calculation of differential operators. Whereas in general derivative filters extend over the interval $[-2m;2m]$ their effective filter length is only $[-m + 2; m - 2]$. Since higher-dimensional wavelets are products of one-dimensional ones differential operators in the higher-dimensional case can easily be derived from the one-dimensional results.

The standard operator form can not only be used for the application of differential operators, but also for other operations. If one want to transform for instance from one wavelet family $\phi$ to another wavelet family $\Phi$ the basic integral becomes

$$a_i = \int \Phi(x) \phi(x - i) \, dx = \sum_{\nu,\mu} \tilde{H}_\nu h_\mu a_{2i-\nu+\mu}$$  \hspace{1cm} (49)

Another use is for scalar products where the fundamental integral is

$$a_i = \int \phi(x) \phi(x - i) \, dx = \frac{1}{2} \sum_{\nu,\mu} h_\nu h_\mu a_{2i-\nu+\mu}$$  \hspace{1cm} (50)
12 Solving Poisson’s equation for the $U_2$ dimer

Poisson’s equation is a prototype differential equation and we want to solve it therefore as an illustration of wavelet theory. To demonstrate the power of the wavelet method we applied it to the most difficult system we could think of in the area of electronic structure calculations, namely the calculation of the electrostatic potential of a three dimensional $U_2$ dimer [10]. In this example, we clearly find widely varying length scales. The valence electrons have an extension of 5 atomic units, the 1s core electrons of 2/100 atomic units and the nucleus itself was represented by a charge distribution with an extension of 1/2000 atomic units. So all together the length scales varied by 4 orders of magnitude and two regions of increasing resolution (around each nucleus) were needed. In order to have quasi perfect natural boundary conditions we embedded the molecule in a computational volume of side length $10^4$ atomic units. All together this necessitated 22 levels of resolution. Even though the potential itself varies by many orders of magnitude, we were able to calculate the solution with typically 7 digits of accuracy. We believe that it would not be possible with any other method to solve this kind of benchmark problem.

The solution of Poisson’s equation consists of several steps. Initially we have to find the wavelet expansion for a data set on a nonuniform real space grid structure shown in Figure 9 which represents the charge density. The resolution needed can in this example be estimated from the known extension and variation of the different atomic shells. Analogously to the one-dimensional case, this expansion can also easily be obtained for higher dimensional interpolating wavelets since all the dual function are related to delta functions. Let us point out, that also in this case the mapping from real space representation to the wavelet representation is invertible, and we could thus get back exactly the same real space values if we evaluate the wavelet expansion on the grid points.

![Figure 9: A grid with two centers of increased resolution around the two nuclei. Only 3 of the 22 levels used in the calculation are shown in this projection on a plane.](image)

Next we start a iteration loop for the potential. First we have to apply the Laplace operator to an approximate potential using the non-standard operator form. Subtracting from this result the charge density gives the residue vector which is the basis for all iterative methods [4], such as steepest descent and conjugate gradient methods. Unfortunately the condition number of the Laplace matrix worsens when more high resolution levels are added and the number of iterations needed to obtain convergence would dramatically increase if we used straightforward iterative methods. It this therefore absolutely
necessary to use a preconditioned iterative method which will give a condition number which is independent of the maximal resolution. In a preconditioning scheme one has to find an approximate inverse matrix of the Laplace matrix. If the Laplace matrix is strongly diagonally dominant, then just the inverse of the diagonal part (which is again diagonal) will be a good approximate inverse. Whether the Laplace matrix is strongly diagonally dominant depends on the kind of wavelet family which is used. In a plane wave representation the Laplace matrix is strictly diagonal. If therefore our wavelet family has good frequency localization properties the resulting matrix will be strongly diagonally dominant. Unfortunately our favorite interpolating wavelets have a very poor frequency localization making an iterative solution practically impossible. It is therefore necessary to do the preconditioning step within another family such as the lifted interpolating wavelets which have much better frequency localization properties as shown in Figure 10. Their improved frequency localization properties is related to the fact that several moments of the wavelet vanish.

![Figure 10: The Fourier spectrum of a 4-th order unlifted Lazy wavelet (left panel) and lifted wavelet (right panel). The spectrum is shown for 3 wavelets on neighboring resolution levels. One has reasonable frequency separation in the lifted but not in the unlifted case.](image)

As discussed above the transformation into another wavelet family can also be done with the help of the non-standard operator form. The preconditioned residue vector is then used to update the potential and we go back to the beginning of the iteration. Using lifted interpolating wavelets with 2 vanishing moments we were able to reduce the norm of the residue vector by one order of magnitude with 3 iterations independent of the maximal resolution. Despite their poor frequency localization properties, unlifted interpolating wavelets have recently also been proposed for the solution of Poisson’s equation [9].

13 Outlook and conclusions

Since we used mainly interpolating wavelets, all we did was essentially interpolating, which is one of the oldest technique in numerical analysis. However the framework pro-
vided by wavelet theory puts this whole interpolation procedure on the new and powerful
basis of multi-resolution analysis, expanding thus considerably the scope of interpolation
based techniques. In particular it assigns basis functions to certain interpolation schemes.
Wavelet based techniques allow us thus to solve differential equations which have several
length scales and to do this with linear scaling. It is thus to be expected, that wavelet
based techniques will catalyze progress in many fields of science and engineering, where
such problems exist. An detailed tutorial style book describing how to use wavelets for
the solution of partial differential equations will soon be published by the authors.

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