Journal of Computational Physics 305 (2016) 244–262

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Higher-order wavelet reconstruction/differentiation filters and Gibbs phenomena

Richard Lombardini [1], Ramiro Acevedo [2], Alexander Kuczala [3], Kerry P. Keys [4], Carl P. Goodrich [5], Bruce R. Johnson *

Department of Chemistry, Smalley-Curl Institute and Laboratory for NanoPhotonics, Rice University, Houston, TX 77005, USA

ARTICLE INFO

Article history:
Received 5 December 2014
Received in revised form 18 October 2015
Accepted 23 October 2015
Available online 30 October 2015

Keywords:
Wavelets
Projection
Reconstruction
Gibbs
Multidimensional
Boundary

ABSTRACT

An orthogonal wavelet basis is characterized by its approximation order, which relates to the ability of the basis to represent general smooth functions on a given scale. It is known, though perhaps not widely known, that there are ways of exceeding the approximation order, i.e., achieving higher-order error in the discretized wavelet transform and its inverse. The focus here is on the development of a practical formulation to accomplish this first for 1D smooth functions, then for 1D functions with discontinuities and then for multidimensional (here 2D) functions with discontinuities. It is shown how to transcend both the wavelet approximation order and the 2D Gibbs phenomenon in representing electromagnetic fields at discontinuous dielectric interfaces that do not simply follow the wavelet-basis grid.

1. Introduction

Wavelets are of general interest in developing systematically-improvable multiscale methods for solving differential equations in quantum mechanics, electromagnetism and many other applications. Orthogonal wavelet families such as those due to Daubechies [1] allow multiresolution description and compression of the solutions as well as fast forward and inverse wavelet transforms. These are efficient transformations between discretized real space functions and wavelet basis space coefficients. The forward (projection) transform is well controlled and may be carried out to a desired accuracy by using high-order numerical quadrature and, if needed, scale refinement procedures [2–4]. In contrast, the inverse (reconstruction) transform is usually described as being intrinsically limited by the *approximation order* of the wavelet family, which is a measure of its ability to approximate general smooth functions. Despite that common sentiment, Keinert and Kwon [5] and Neelov and Goedecker [6] demonstrated that one can beat this limit in reconstruction. Our group has recently generalized the latter results so that the reconstruction error can be tuned just as freely as the projection error [7]. There are particular consequences of this, as will be shown. For example, the increased tunability gives us the ability to use shorter-length wavelets while maintaining higher-order accuracy. More difficult generalizations are then pursued, e.g., maintaining high-

* Corresponding author.
E-mail address: johnson@rice.edu (B.R. Johnson).
1 Present address: Department of Physics and Earth Sciences, St. Mary's University, San Antonio, TX 78228, USA.
2 Present address: Physics Department, Wharton County Junior College, Sugar Land, TX 77479, USA.
3 Present address: Department of Physics, University of California San Diego, San Diego, CA 92093, USA.
4 Present address: Kenan-Flagler Business School, University of North Carolina, Chapel Hill, NC 27599, USA.
5 Present address: School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA.

http://dx.doi.org/10.1016/j.jcp.2015.10.035
0021-9991/

order accuracy at function discontinuities, which requires overcoming the wavelet Gibbs phenomenon. This is then carried over to the 2D Gibbs phenomenon with an electromagnetic example possessing a dielectric interface that is curved rather than aligned with the wavelet basis grid. The strategy adopted is developed with an eye toward wavelet solution of differential equations in multiple dimensions with arbitrarily-shaped interfaces without being intrinsically restricted to low-order accuracy. The present work bears on how well such solutions can be represented in wavelet bases in the first place.

The first focus is on 1D function expansions in father wavelets or scaling functions, $\phi(x-k)$, k an integer, and on inversion of a matrix $\mathbf{X}$ formed from projections of monomial powers $(x-\tau)^p$ onto this distributed basis. The parameter τ is a shift that may be varied so as to allow wavelet interpolation/extrapolation in reconstruction. The columns of $\mathbf{X}^{-1}$ can be applied to a series of neighboring coefficients to provide high-order real-space samples of the underlying function and its derivatives. The lengths of these local convolution filters and their error orders can be varied by varying the size of the original matrix. By translation invariance, the same filters can be applied to different groups of expansion coefficients of the same length. Furthermore, explicit formulae can be derived for the filters in terms of Lagrange interpolating polynomials and moments of $\phi(x)$.

A fundamentally different situation occurs when there are boundary conditions, e.g., potential energy discontinuities in quantum mechanics, dielectric function discontinuities in Maxwell's equations and so on. Wavelet basis functions generally have overlapping supports and are not particularly graceful in satisfying pointwise boundary conditions. For functions with discontinuities, one encounters the wavelet Gibbs phenomenon, where reconstructions using the regular basis functions show significant errors in the neighborhood of the discontinuity [8,9]. One potential remedy is to try to work only with basis functions, or parts of them, that fall on one side of the boundary at a time. Those few $\phi(x-k)$ with support straddling the boundary become truncated and lose their mutual orthogonality. It is known that linear combinations of them may be orthogonalized to produce special edge functions terminating at the boundary [10–12], but these "intervalized" bases are not fully compatible with high order reconstruction as pursued here.

Instead, the nonorthogonal tail functions are used directly. Their truncated moments may be calculated and used in a generalized version of the distributed-moment matrix $\mathbf{X}$, followed by its inversion to produce edge-adapted reconstruction filters. There are some caveats: (i) a number of different filters are required near the boundary, (ii) the inversion of the matrix is only done numerically and, consequently, (iii) greater care must be taken to avoid effects due to finite precision. Nevertheless, this straightforward extension successfully allows reconstruction and differentiation filters near the edge that exhibit the desired higher-order errors and avoid the undesired Gibbs phenomenon.

New challenges arise for complex boundaries in multiple dimensions, and a different strategy is needed. In the finite-difference time-domain (FDTD) method in computational electromagnetics [13,14], one approach is to employ staircasing, i.e., replacing the actual boundary with a nearby boundary following grid faces (for discussion see, e.g., Zhao and Wei [15]), though this is not ideal. In a 2D problem with a curved boundary, we define similar staircased contours on either side that approach but do not cross the actual boundary. These mark the edges of the support to either side and allow exact moments to be calculated for use in projection and reconstruction. The reconstruction takes place at the boundary by appropriate shifts in the 2D moments, equivalent to mild polynomial extrapolation. (A related but different polynomial extrapolation of wavelet series has been used to handle edge effects in finite wavelet bases before [16].) As the scale is reduced, the average distances between the actual and staircased contours decreases and high-order reduction in error is achieved. There is some non-uniformity in the convergence of pointwise errors, but this is not fatal. In this way, 2D Gibbs oscillations are avoided, and confidence is gained that extension to arbitrary boundaries and higher dimensions will be effective.

The paper is organized as follows. In Section 2 the basics are discussed for wavelet projection and reconstruction via convolutional filters depending on moments. In Section 3 the generalization to include boundaries in 1D is made, and the further generalizations to include boundaries in 2D are made in Section 4. A brief summary of conclusions is given in Section 5, followed by appendices.

2. Wavelet projection and reconstruction filters

2.1. Wavelet transforms

Orthogonal compact-support Daubechies-type wavelet families [1,17] are characterized by $\phi(x)$ and the mother wavelet (or wavelet function) $\psi(x)$. These are limited in support to the interval $0 \le x \le L-1$, where L is an even integer. Each may be expressed as a finite sum of squeezed and translated copies of the scaling function,

$$\phi(x) = \sum_{k=0}^{L-1} c_k \phi(2x-k), \qquad \psi(x) = \sum_{k=0}^{L-1} d_k \phi(2x-k), \tag{1}$$

where c_k and d_k are known two-scale coefficients that are different for each wavelet family. More generally, it is useful to define orthonormal functions formed via scaling by λ and translating in units of λ,

$$\phi_k^\lambda(x) = \lambda^{-1/2}\phi(x/\lambda - k), \qquad \psi_k^\lambda(x) = \lambda^{-1/2}\psi(x/\lambda - k). \tag{2}$$

A general function may then be expanded as