



Shannon–Gabor wavelet distributed approximating functional

D.K. Hoffman ^a, G.W. Wei ^b, D.S. Zhang ^b, D.J. Kouri ^b

^a *Iowa State University, Ames, IA 50011, USA*

^b *Department of Chemistry and Department of Physics, University of Houston, Houston, TX 77204-5641, USA*

Received 8 January 1998; in final form 27 January 1998

Abstract

The Shannon sampling theorem is critically reviewed from a physical point of view. An approximate sampling formula is proposed, combining Shannon sampling with a Gabor-distributed approximating functional (DAF) window function, which results in new Shannon–Gabor wavelet DAFs (SGWDs). They are extremely smooth, decay rapidly, have simultaneous time-frequency localization, and are also generalized delta sequences (reducing to the Dirac delta function under the limit of a zero window width). Shannon's sampling theorem is recovered exactly when the window is infinitely wide. Finally, SGWDs are well-behaved $L^2(R)$ kernels, and thus can be used for solving differential equations. © 1998 Elsevier Science B.V. All rights reserved.

In the last decade the development of wavelets and associated multiresolution techniques [1–3] has had tremendous impact not only in signal and image processing but also in science and engineering. From a mathematical point of view, wavelets are functions generated from a single function (the mother wavelet) by dilation and translation. They are most important when they form building blocks for some space, such as $L^2(R)$, whether as a frame [1–3] or as an orthonormal basis [1–3]. From a physical point of view, the wavelet transform is a mathematical technique that can be used to split a signal into different frequency components so that each component can be studied with a resolution matched to its scale, thus providing excellent frequency and spatial resolution. Being closely associated with the theory of approximations and of minimum support bases, wavelets have the potential to fill the gap between accurate global methods and convenient local methods for numerically solving ordinary differential equations (ODEs) and partial differential equations

(PDEs). Such an intermediate method is expected to have global method-accuracy and local method-flexibility for handling both linear and nonlinear problems. Thus, enormous effort has been expended on developing wavelet based ODE and PDE solvers [4–8], including the recently reported adaptive wavelet algorithms [9,10]. However, these efforts are hindered, to a certain degree, by the difficulty of implementing general boundary conditions in the multiresolution analysis and by the lack of sufficiently accurate and robust wavelets (in the sense of computational physics, where accuracy of one part in 10^6 or better is often required). Glowinski et al. [8] have recently demonstrated that their wavelet-Galerkin approach provides results comparable to those of finite element methods for the Neumann problem using fictitious domains. In a recent work, we have constructed various wavelet-DAFs and DAF-Wavelets [11,12] for solving ODEs and PDEs. In this Letter, we propose a new wavelet-DAF, called the Shannon-Gabor-wavelet distributed approx-

imating functional (SGWD), which has a number of convenient features for various numerical purposes. In particular, we demonstrate its use for numerical sampling and for solving the Schrödinger equation.

One of the most important motivations for wavelet development is provided by Shannon's sampling theorem [13]

$$f(x) = \sum_{n=-\infty}^{\infty} f(x_n) \frac{\sin \eta(x-x_n)}{\eta(x-x_n)}, \quad f \in \mathbf{B}_{\eta}^2, \\ x_n = \frac{n\pi}{\eta}, \quad (1)$$

where \mathbf{B}_{η}^2 is the Paley–Wiener space of band limited functions. The reproducing kernel

$$\frac{\sin \eta(x-y)}{\eta(x-y)} = \sum_{n=-\infty}^{\infty} \frac{\sin \eta(x-x_n)}{\eta(x-x_n)} \frac{\sin \eta(y-x_n)}{\eta(y-x_n)} \quad (2)$$

is related to the earlier Whittaker's cardinal series [14,15]

$$\frac{\sin \eta(x-x_n)}{\eta(x-x_n)} = \frac{(-1)^n \sin \eta x}{\eta x - n\pi} \quad (3)$$

and it can be used to generate an orthonormal basis for the reproducing kernel Hilbert space \mathbf{B}_{η}^2 . The most striking property of Shannon's sampling theorem is that one can recover a continuous (band-limited) function $f(x)$ on the real line $x \in R$ from an infinite, discrete set of known values $\{f(x_n)\}$. By setting $\eta = \pi$, one obtains the well-known Shannon's father wavelet [1–3]

$$\phi(x) = \frac{\sin \pi x}{\pi x}. \quad (4)$$

Its Fourier transform is given by

$$\hat{\phi}(x) = \chi_{[-1/2, 1/2)}, \quad (5)$$

where χ is the characteristic function of the interval $[-\frac{1}{2}, \frac{1}{2})$. It is easy to show that

$$\phi_{n,m}(x) = 2^{-m/2} \phi(2^{-m}x - n) \quad (n, m \in Z), \quad (6)$$

is an orthonormal sequence for constructing an $L^2(R)$ multiresolution analysis [1,2]. One can also show that the Shannon mother wavelet is given by

$$\psi(x) = \frac{\sin(2\pi x) - \sin(\pi x)}{\pi x}. \quad (7)$$

Shannon's wavelets are not efficient from computational point of view because of their slow decay as x becomes large. This is implied from the ideal lowpass property of ϕ , Eq. (5). To obtain a better upper bound on the truncation error that decreases faster with N , Helms and Thomas [16] proposed the following self-truncating sampling expansion for $f(x)$ band-limited to $r\eta$:

$$f(x) = \sum_{n=-\infty}^{\infty} f(x_n) \frac{\sin \eta(x-x_n)}{\eta(x-x_n)} \\ \times \left[\frac{\sin \frac{\eta p}{m}(x-x_n)}{\frac{\eta p}{m}(x-x_n)} \right]^m, \quad (8)$$

where $p = 1 - r, 0 < r < 1$. In practical computations, they set $m = Np\pi/e$. Mathematical sampling theory is focused on the exactness of expressions (1) and (8). However, in the real world, since one cannot actually use infinitely many sampling points, the "exactness" of Eqs. (1) and (8) can never actually be realized. Moreover, there is an inherent paradox [17] in the notion of bandlimited signals. The usual definition implies that a bandlimited signal is an entire function, whose Fourier transform has compact support. However, an entire function cannot have compact support unless it is identically zero in the entire domain. Therefore, it cannot be *both* bandlimited and time-limited, unless it is identically zero. This contrasts with the fact that physically realizable states can be treated as well-behaved Schwartz space functions, which are *effectively* both bandlimited and time-limited [18]. The bandwidths in the frequency and time domains are related by the Heisenberg uncertainty principle. Thus, for all practical purposes, it is justified to give up exactness and construct the following *approximate sampling formula*:

$$f(x) \approx \sum_{n=-W}^W f(x_n) \frac{\sin \eta(x-x_n)}{\eta(x-x_n)} w_{\sigma}(x-x_n), \quad (9)$$

where $w_{\sigma}(x-x_n)$ can be regarded as a window function or a positive weight function with an appro-

privately behaved scaling factor σ . The points $\{x_n\}$ are centered around x with a bandwidth of $2W + 1$ (or $2W$). It is convenient to consider the following Gabor-DAF weight function [19]

$$w_\sigma(x - x_n) = e^{-(x-x_n)^2/2\sigma^2}, \quad \sigma \geq 0. \quad (10)$$

This leads us to define an interesting Shannon–Gabor wavelet DAF (SGWD) as

$$\Phi(x) = \frac{\sin \pi x}{\pi x} e^{-x^2/2\sigma^2}, \quad (11)$$

which we also use as a father wavelet. Note that the SGWD is different from either the Shannon father wavelet ϕ or the Gabor wavelet, $e^{-x^2/2\sigma^2} \cos(ax)$. It is interesting to examine two limiting cases of the SGWD:

$$\lim_{\sigma \rightarrow \infty} \Phi(x) = \frac{\sin \pi x}{\pi x} \quad (12)$$

and

$$\lim_{\sigma \rightarrow 0} \frac{1}{2\pi\sigma} \Phi(x) = \frac{\sin \pi x}{\pi x} \delta(x) = \delta(x). \quad (13)$$

Eq. (9) becomes exact in the first limit (providing $W \rightarrow \infty$). The second limit, Eq. (13), indicates that the SGWD is a delta sequence. Using this fact, we can construct an interpolating SGWD

$$\delta_{\text{DAF}}(x - x_n | \sigma) = \frac{\sin \eta(x - x_n)}{\eta(x - x_n)} e^{-(x-x_n)^2/2\sigma^2}. \quad (14)$$

The best σ values for numerical purposes are determined by the grid spacing π/η (the dilation factor). For a given η , there is a wide range of σ 's that deliver excellent numerical results. A family of wavelets can be generated by dilations and translations of the SGWD through the usual two-scale relation

$$\Phi_{m,n} = 2^{-m/2} \Phi(2^{-m}x - n). \quad (15)$$

Except for the limiting case, this family is not orthogonal, in general (as is consistent with the Balian-Low theorem [1]). A corresponding mother DAF-wavelet (SGDW) is given by

$$\Psi(x) = \frac{1}{\pi x} \left[\sin(2\pi x) e^{-2x^2/\sigma^2} - \sin(\pi x) e^{-x^2/2\sigma^2} \right]. \quad (16)$$

This result can also be obtained from a multiresolution analysis. Though the present SGWDs and SGWDs are not orthogonal, they have Gaussian envelope decay and are smooth in both the time and frequency domains (see Fig. 1). This implies that they have potential for important applications for image and signal processing and for numerically solving ODEs and PDEs.

For simplicity, we have restricted our discussion to the one dimensional case. It is straightforward to generalize the SGWDs to multidimensions. For example, an n -dimensional SGWD can be immediately written as

$$\Phi(x_1, x_2, \dots, x_n) = \prod_{i=1}^n \frac{\sin \pi x_i}{\pi x_i} e^{-x_i^2/2\sigma_i^2}. \quad (17)$$

In the remainder of this Letter, we demonstrate the usefulness, and test the accuracy, of the SGWD for both sampling and for numerically solving ODEs.

The goal of sampling is to extract information contained in a finite set of input data. The quality of this process is determined by the sampling kernel which provides the responses to discrete (impulse) data. From a computational point of view, sampling provides a representation of a function everywhere in a domain using only a set of discrete input values. Therefore, the accuracy and efficiency of the sampling is the essential property of *any* digital computational method. To represent a well-behaved signal on a grid efficiently, we choose interpolating points of the SGWD by setting $\eta = \pi/\Delta$, with Δ being the grid spacing. This is, however, not necessary. To illustrate, we use the function

$$f(x) = e^{-kx} [\cos(\alpha x) + \sin(\beta x)], \quad (18)$$

where we take $k = 1/5$, $\alpha = 2$ and $\beta = 3$. We use both SGWDs and the Shannon father wavelet to predict the off grid values of the function inside the interval $[0, \pi]$. While the total number of grid points used inside the interval is N , as required by Eq. (9), W “grid points” (signal values) outside each end of the interval are also used for computations. A comparison of performance for our SGWD and the Shannon father wavelet is given in Fig. 2 for $N = 41$, $W = 32$ and 64 , as a function of σ/Δ . It is seen that our SGWD, with appropriate window sizes, approximates $f(x)$, Eq. (18), some 10^{11} times more accu-

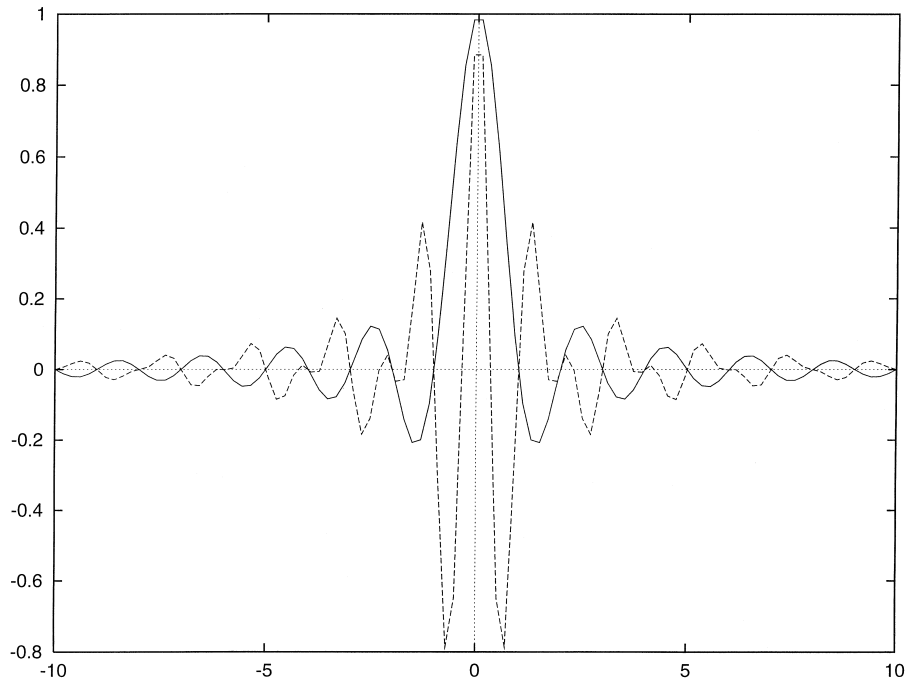


Fig. 1. The Shannon-Gabor father wavelet (solid line) and mother wavelet (dash line).

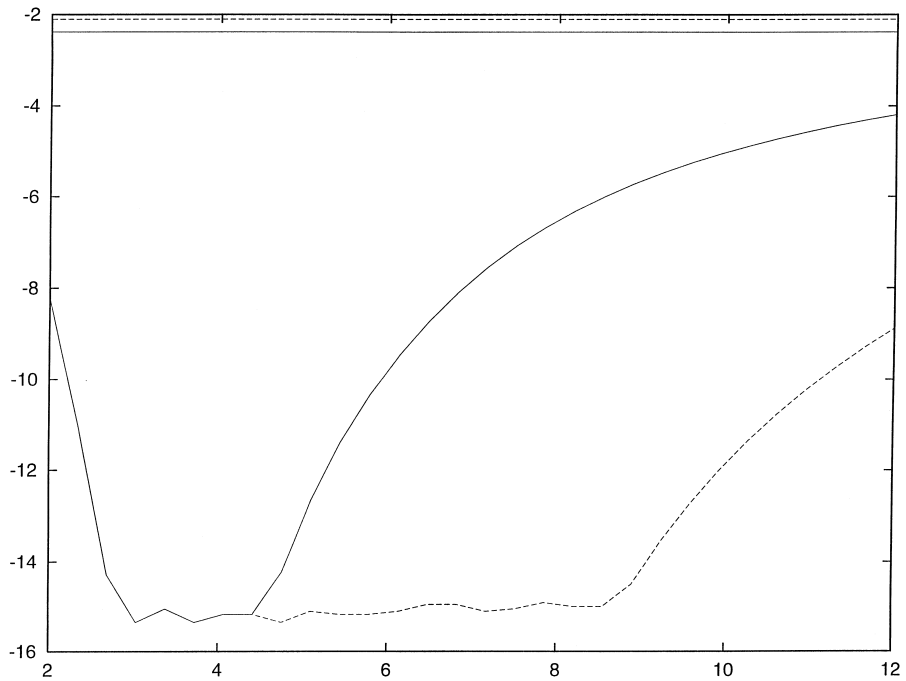


Fig. 2. L_∞ sampling errors for expression (18) using $N = 41$ input data. Solid lines are for $W = 32$. Dashed lines are for $W = 64$. The two straight lines (one dashed one solid) are from Shannon father wavelet calculations, while the other two lines are from the SGWD calculations.

rately than the Shannon father wavelet, using the same input. In particular, the Shannon sampling actually becomes *worse* as W increases. This is due to the exponential divergence of $F(x)$ at $x \rightarrow -\infty$. This indicates that our SGWDs will be very efficient for signal and image processing. To demonstrate further the computational utility of our SGWD, we next use it to solve the Schrödinger equation numerically.

To use the SGWD for numerical solutions of ODEs, a SGWD representation of derivative operators is first required. The simplest way [20] to achieve this is to note that Eq. (9) implies [21–23]

$$\begin{aligned} f^{(q)}(x) &\approx \sum_{n=-W}^W f(x_n) \frac{\partial^q}{\partial x^q} \\ &\times \left[\frac{\sin \eta(x-x_n)}{\eta(x-x_n)} w_\sigma(x-x_n) \right] \\ &= \sum_{n=-W}^W f(x_n) \delta_{\text{DAF}}^{(q)}(x-x_n|\sigma), \end{aligned} \quad (19)$$

where $f^{(q)}(x)$ is the q th derivative of $f(x)$. This provides a simple scheme for numerical discretization of linear and nonlinear ODEs and PDEs. Obviously, other schemes can also be used. In the present computations, the SGWD parameters are taken as $W = 40$ and $\sigma/\Delta = 4.0$ for all examples.

We choose a standard problem, a two-dimensional harmonic oscillator, a) to demonstrate the usefulness, b) test the accuracy and c) explore the limitations of the SGWD method by calculating the eigenfunctions and eigenvalues of the Schrödinger equation

$$\begin{aligned} &\left[-\frac{\hbar^2}{2m} \sum_{i=1}^2 \frac{\partial^2}{\partial x_i^2} + \frac{1}{2}(x_1^2 + x_2^2) \right] \Phi_k(x_1, x_2) \\ &= E_k \Phi_k(x_1, x_2). \end{aligned} \quad (20)$$

Here Φ_k and E_k are the k th eigenfunction and eigenvalue respectively. The eigenvalues are given by

$$E_{k_1, k_2} = 1 + k_1 + k_2, \quad 0 \leq k < \infty, \quad 0 \leq k_1 \leq k_2, \quad (21)$$

with a degree of degeneracy ($k_d = k + 1$) in each energy level $E_k = 1 + k$.

We first construct the two-dimensional version of the SGWD representation of the Hamiltonian opera-

tor, Eq. (20). The eigenvalues and eigenfunctions are obtained by subsequent numerical diagonalization of the discrete SGWD-Hamiltonian. We have used 40 grid points in each dimension to obtain the first 16 eigenvalues and eigenfunctions. As listed in Table 1, all results are accurate to at least 10 significant figures for the first 16 eigenstates. This calculation demonstrates the SGWD method is extremely accurate for handling degenerate eigenvalue problems.

In conclusion, we have constructed SGWDs by combining the Shannon father wavelet with a Gabor-DAF window function in a DAF-manner [21]. As a result, the SGWDs have excellent smoothness and decay properties for time-frequency localization. This endows the SGWDs with great potential for signal and image processing and solving differential equations. Another convenient property of the SGWDs is that they are given by explicit expressions in both the time and coordinate domains. This makes them very easy to use for signal analysis and computational physics. The SGWDs can be regarded as elements of a generalized delta sequences and as such, are DAFs. Thus, they can be used as $L^2(R)$ kernels for numerically solving ODEs and PDEs. In

Table 1
Eigenvalues of the 2D harmonic oscillator

$k (= k_x + k_y)$	k_d	exact	SGWD calculation
0	1	1	0.99999999999835
1	2	2	1.99999999999952 1.99999999999965
2	3	3	2.99999999999986 2.999999999999838 2.99999999999997
3	4	4	3.99999999999943 3.99999999999947 3.99999999999986 3.99999999999994
4	5	5	4.99999999999907 4.99999999999953 4.99999999999989 5.000000000000674 5.000000000000813
5	6	6	5.99999999999982 6.00000000000018 6.000000000000752 6.000000000000801 6.00000000011972 6.00000000012005

one limit, the SGWDs reduce to the Shannon wavelets. In this limit, our Shannon–Gabor wavelet DAF becomes exact for bandlimited functions. This relation provides a rigorous basis for the use of SGWDs for approximately solving ODEs and PDEs. We note that the present SGWDs are closely related to our previous Lagrange DAFs [24–26] and to the discrete variable representation [27]. These aspects will be explored in detail elsewhere [28]. We have demonstrated the usefulness and the accuracy of the present SGWDs for signal processing (extracting information by impulse response). Because the Gabor-DAF window effectively smoothes the Shannon sampling kernel in Fourier space, our SGWDs, when operating in appropriate window sizes, are much more accurate than the truncated Shannon sampling. Since the accuracy of sampling is fundamental to digital signal and image processing, the SGWDs should be very powerful for such analyses. To demonstrate further the ability of SGWDs for accurately and efficiently representing differential operators, we have used SGWDs to solve the two-dimensional Schrödinger equation. It is found that our SGWDs provide highly accurate numerical solutions for the two-dimensional harmonic oscillator. From the point of view of computational physics, the SGWD matrices are effectively banded; therefore they have great potential for large-scale computations.

Acknowledgements

The authors thank Dr. S.W. Ding of University of British Columbia for stimulating discussions about wavelets. The Ames Laboratory is operated for the Department of Energy by Iowa State University under Contract No 2-7405-ENG82. GWW is supported under an NSERC postdoctoral fellowship of Canada, and is also supported under R.A. Welch Foundation Grant E-0608. DJK is supported in part under National Science Foundation Grant CHE-9700297 and R.A. Welch Foundation Grant E-0608.

References

- [1] Y. Meyer, *Wavelets and Operators*, Cambridge Stud. Adv. Math., vol. 37, Cambridge Univ. Press, Cambridge, 1992.
- [2] C.K. Chui, *An Introduction to Wavelets*, Academic Press, San Diego, 1992.
- [3] I. Daubechies, *Ten Lectures on Wavelets* CBMS-NSF Series in Applied Mathematics, SIAM, Philadelphia, 1992.
- [4] R.L. Schult, H.W. Wyld, *Phys. Rev. A* 46 (1992) 12.
- [5] J. Liandrat, V. Perrier, P. Tchamitchian, in: M.B. Ruskai, G. Beylkin, R. Coifman, I. Daubechies, S. Mallat, Y. Meyer, L. Raphael (Eds.), *Wavelets and Their Applications*, Jones & Bartlett, Boston, 1992.
- [6] B. Jawerth, W. Sweldens, *SIAM Rev.* 36 (1994) 377.
- [7] W.K. Liu, *Int. J. Numer. Methods Fluids* 21 (1995) 901.
- [8] R. Glowinski, T.W. Pan, R.O. Wells Jr., X. Zhou, *J. Comput. Phys.* 126 (1996) 40.
- [9] G. Beylkin, J. Keiser, *J. Comput. Phys.* 132 (1997) 233.
- [10] J. Fröhlich, K. Schneider, *J. Comput. Phys.* 130 (1997) 174.
- [11] G.W. Wei, D.J. Kouri, D.K. Hoffman, *Phys. Rev. Lett.*, submitted.
- [12] G.W. Wei, S.A. Althorpe, D.J. Kouri, D.K. Hoffman, *J. Chem. Phys.*, in press.
- [13] C.E. Shannon, *Proc. IRE* 137 (1949) 10.
- [14] E.T. Whittaker, *Proc. Roy. Soc. Edinburgh Sec. A* 35 (1915) 181.
- [15] J.M. Whittaker, *Proc. Edinburgh Math. Soc.* 1 (1929) 41.
- [16] H.D. Helms, J.B. Thomas, *Proc. IRE* 50 (1962) 179.
- [17] D. Slepian, *Proc. IEEE* 64 (1976) 292.
- [18] A. Bohm, *Quantum Mechanics*, 3rd ed., Springer-Verlag, 1993.
- [19] D. Gabor, *J. IEE (London)* 93, Part III (1946) 429.
- [20] R.L. Stens, *Signal Processing* 5 (1983) 139.
- [21] D.K. Hoffman, N. Nayar, O.A. Sharafeddin, D.J. Kouri, *J. Phys. Chem.* 95 (1991) 8299.
- [22] D.J. Kouri, W. Zhu, X. Ma, B.M. Pettitt, D.K. Hoffman, *J. Phys. Chem.* 96 (1992) 9622.
- [23] D.K. Hoffman, T.L. Marchioro II, M. Arnold, Y. Huang, W. Zhu, D.J. Kouri, *J. Math. Chem.* 20 (1996) 117.
- [24] G.W. Wei, D.S. Zhang, D.J. Kouri, D.K. Hoffman, *Phys. Rev. Lett.* 79 (1997) 775.
- [25] D.K. Hoffman, G.W. Wei, D.S. Zhang, D.J. Kouri *Phys. Rev. E*, in press.
- [26] G.W. Wei, S.A. Althorpe, D.S. Zhang, D.J. Kouri, D.K. Hoffman, *Phys. Rev. A*, in press.
- [27] J.V. Lill, G.A. Parker, J.C. Light, *Chem. Phys. Lett.* 82 (1985) 1400.
- [28] G.W. Wei, D.J. Kouri, D.K. Hoffman, to be published.