

THE INTERPOLATORY WAVELETS FOR THE NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

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ABSTRACT

In this work we present a hybrid scheme combining the method-of-line with interpolatory wavelets and central finite differences to solve numerically some nonlinear evolution partial differential equations, (PDEs), with soliton type solutions. The employment of the interpolatory wavelets permits, in this case, to significantly reduce the number of nodes of the non-uniform moving grid. Consequently an important reduction of the order of the resulting stiff ODE system is obtained. Some numerical tests are presented solving the Schrödinger equation, which models important physical phenomena nowadays.

Key words: wavelets, numerical approximations, Schrödinger equation.

MCS: 65M20

RESUMEN

En este trabajo se presenta un esquema híbrido basado en el método de líneas, las funciones wavelets de interpolación y un esquema en diferencias finitas centradas para la solución de ecuaciones diferenciales parciales, (EDPS), no-lineales de evolución con soluciones tipo solitón. El empleo de los wavelets interpolatorios permite, en este caso, reducir significativamente el número de nodos de la malla adaptativa no-uniforme y por consiguiente se reduce el número de ecuaciones diferenciales ordinarias de tipo stiff resultantes de aplicar la técnica de semidiscretización. Se presentan ejemplos con la solución numérica de la ecuación no-lineal de Schrödinger, la cual modela importantes problemas de la Física.

Palabras clave: wavelets, aproximaciones numéricas, ecuación de Schrödinger.

1. INTRODUCTION

Finding effective computational techniques to solve hyperbolic systems of conservation laws has encouraged researches in this field during the last 20 years. As a result, a variety of methods are now available that can compute accurate numerical approximations of the physically relevant solutions. Most of these methods are the so-called high resolution shock-capturing schemes, typically with second or third order approximation in the smooth regions and maintaining sharp and oscillations free, numerical profiles at the discontinuities, [Donat, R. and A. Marquina, 1999]. The pioneer in the area with a set of techniques to reduce computational efforts was Ami Harten [1995].

In this paper we present a hybrid technique, which has the above-mentioned properties. It is based on interpolatory wavelets as the previous works of David Donoho [1992], and Mats Holmström [1996], but using a semidiscrete technique, the method-of-lines, and an efficient ODE solver for the resulting stiff ODE system.

We show the main advantages in using this technique, which brings also the possibility to construct an adaptive non-uniform moving mesh.

As far as the author know, this is the paper presenting the solution of the nonlinear Schrödinger equation using interpolatory wavelets.

This work is a continuation of earlier papers of the first author [Alvarez, L. and Cunha, C., 1997] and [Alvarez, L. and Navarro, J., 1999].

In section 2, some relevant concepts on wavelets are given, showing their capabilities for compression or sparse function representation, in particular the Daubechies and interpolatory wavelets are presented.

The employment of the method-of-lines in two particular PDEs and the relationships between finite difference grid refinement and wavelets methods are discussed in section 2.

Finally, in section 3 some interesting numerical solutions of the nonlinear Schrödinger equation with soliton type behavior, computed with an efficient ODE solver, are presented.

2. DAUBECHIES AND INTERPOLATORY WAVELETS

The most famous wavelets in the literature are the Daubechies wavelets, [Daubechies, I., 1992] and [Cohen, A. and Daubechies, I., 1993]. We introduce them here, because they illustrate well all the main properties that have fulfill "good wavelets". They satisfy the following equations:

$$\phi(x) = \sqrt{2} \sum_{k=0}^{L-1} h_k \phi(2x - k), \quad \psi(x) = \sqrt{2} \sum_{k=0}^{L-1} g_k \phi(2x - k) \quad (2.1)$$

where $\phi(x)$ are the scaling function and $\psi(x)$ are the wavelets. We assume that $\phi(x)$ is normalized, that is

$$\int_{-\infty}^{\infty} \phi(x) dx = 1 \quad (2.2)$$

Taking these two functions as:

$$\phi_k^j(x) = 2^{-\frac{j}{2}} \phi_k^j(2^{-j}x - k) \quad (2.3)$$

and

$$\psi_k^j(x) = 2^{-\frac{j}{2}} \psi_k^j(2^{-j}x - k) \quad (2.4)$$

where j, k are integers denoting the dilations and translations of the arguments or in other words, j denotes the scale and k denotes the position, we have that the coefficients

$$H = \{h_k\}_{k=0}^{L-1} \quad \text{and} \quad G = \{g_k\}_{k=0}^{L-1}$$

are related by

$$g_k = (-1)^k h_{L-k}, \quad k = 0, 1, \dots, L-1 \quad (2.5)$$

These coefficients are called filters.

The Daubechies wavelets are orthonormals, i.e.,

$$\int_{-\infty}^{\infty} \psi_k^j(x) \psi_l^m(x) dx = \delta_{kl} \delta_{lm} \quad (2.6)$$

and also $\psi(x) = \psi_0^0(x)$ satisfies that:

$$\int_{-\infty}^{\infty} \psi(x) x^m dx = 0, \quad m = 0, \dots, M-1 \quad (2.7)$$

That means that $\psi(x)$ has M vanishing moments, property, which will be relevant in the compression or in the sparse function representation.

The space spanned by $\phi(x)$ and $\psi(x)$ over k with fixed j are usually denoted by

$$V_j = \text{span}_{k \in \mathbb{Z}} \phi_k^j(x), \quad W_j = \text{span}_{k \in \mathbb{Z}} \psi_k^j(x), \quad (2.8)$$

In the reference [Jameson, L., 1994], is shown that Daubechies wavelets satisfy the following properties:

a) The space V generate a ladder of spaces:

$$\dots \subset V_1 \subset V_0 \subset V_{-1} \subset \dots$$

So, we can move the function from coarser to finer grids, (different scale j) and in opposite direction.

b) We say that these wavelets form an orthonormal basis of L^2 :

$$L^2(\mathbb{R}) = \bigoplus_{j \in \mathbb{Z}} W_j$$

and also that,

$$\bigcap_{j \in \mathbb{Z}} V_j = \{0\} \quad \text{and} \quad \bigcup_{j \in \mathbb{Z}} V_j = L^2(\mathbb{R})$$

c) So, there exists a set of coefficients $\{d\}_k^j$ such that any function

$$f(x) \in L^2(\mathbb{R})$$

can be written as:

$$f(x) = \sum_{j \in \mathbb{Z}} \sum_{k \in \mathbb{Z}} d_k^j \psi_k^j(x), \quad d_k^j = \int_{-\infty}^{\infty} f(x) \psi_k^j(x) dx$$

Using the properties a) and b) and knowing that in a computer we perform a finite number of operation, we will have a limit scale number J , we can write that:

$$V_0 = W_1 \oplus W_2 \oplus \dots \oplus W_J \oplus V_J$$

and also that any projection of the function $f(x)$ can be written as:

$$P_{V_0} f(x) = \sum_{j \in \mathbb{Z}} s_k^j \phi_k^j(x) + \sum_{j=1}^J \sum_{k \in \mathbb{Z}} d_k^j \psi_k^j(x) \quad (2.10)$$

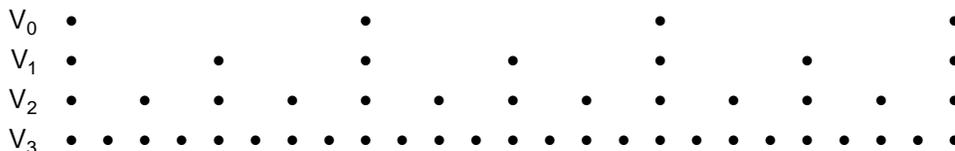
The above equation says that we can represent any function in terms of some coefficients of smoothness, s_k^j in the space of the scaling functions plus the combination of all the details in J scales.

2.2. Interpolatory wavelets

The interpolatory wavelets, first established by Donoho in 1993, are constructed following the interpolating subdivision scheme of Deslauries and Dubuc, [1989]. Starting with a set of dyadic grids in the real line:

$$V^j = \{x_{j,k} \in \mathbb{R} : x_{j,k} = 2^{-j}k, k \in \mathbb{Z}\}, \quad j \in \mathbb{Z} \quad (2.11)$$

The localization of the nodes in these grids in different scales are showed in the following picture:



Formally, we define one step in the subdivision scheme as:

$$\begin{cases} f_{j+1,2k} = f_{j,k} \\ f_{j+1,2k+1} = P_{j+1,2k+1} \end{cases} \quad \forall k \in \mathbb{Z}$$

Here $f_{j,k}$ are the functional values to be represented in the grid, with scale j and position k , (where for simplicity we avoid the superindex) and $P_{j+1,2k+1}(x)$ will be an interpolation polynomial. So, the last equation means that we set the same functional values in the odd nodes and interpolate the values in the even nodes.

For example, we can construct the function in the next scale using the functional values from the coarser grid as follows:

$$f_{j+1,2k+1} = (f_{j,k} + f_{j,k+1})/2 \quad \text{if } p = 2$$

$$f_{j+1,2k+1} = (-f_{j,k-1} + 9f_{j,k} + 9f_{j,k+1} - f_{j,k+2})/16 \quad \text{if } p = 4$$

Of course, $p - 1$ will be the order of the approximation in the interpolating subdivision scheme.

Backing again to the interpolatory wavelets of Donoho, they are constructed starting with a sequence $\{\delta_{0,k}\}_{k \in \mathbb{Z}}$ on V_0 and applying the interpolating subdivision scheme subsequently, in the limit grid, $V_l, l \rightarrow \infty$ we get what Donoho calls his scaling function or the fundamental function of Deslauries and Dubuc, $\varphi(x)$.

From the construction it is established that $\varphi(x)$ has compact support on the interval $[-p + 1, p - 1]$, and is symmetric and cardinal.

Performing dilations and translations of $\varphi(x)$ by the equation

$$\varphi_{j,k}(x) = \varphi(2^j x - k)$$

a basic of interpolatory wavelets have polynomial reproduction and for $p > 2$ they are not piecewise polynomial. All of the mentioned properties are shown in [4].

By introducing the spaces W_j , such that

$$V_{j+1} = V_j \oplus W_j$$

We can represent a function in the next scale by

$$P_{j+1}f(x) = \sum_k f_{j+1,k} \phi_{j+1,k}(x) \quad (2.13)$$

Or in another way, by introducing now the interpolatory wavelets $\{\psi_{j,k}\}_{k \in \mathbb{Z}}$ in the spaces W_j , where they are represented as $\psi_{j,k}(x) = \psi(2^j x - k)$. These wavelets fulfill the properties a) and b) of the Daubechies wavelets. Then we can represent any function in these two forms:

$$\sum_k f_{j+1,k} \phi_{j+1,k}(x) \text{ or } \sum_k f_{j,k} \phi_{j,k}(x) + \sum_k d_{j,k} \psi_{j,k}(x) \quad (2.14)$$

So, the difference of the functional values from one scale to another can be computed by:

$$P_{j+1}f(x) - P_j f(x) = \sum_k d_{j,k} \psi_{j,k}(x) \quad (2.15)$$

This last equation gives two important facts:

- The wavelet coefficient encode the interpolation error when the function is moved from one scale j to another $j+1$.

- The position in the grid of the coefficient coincides with the physical position of the functional value being interpolated.

The first fact is that the equation (2.15) gives the formula to compute the wavelet coefficients and the second one gives us the possibility to perform all the operations that we need to solve numerically the PDEs, that means, discretization, multiplication, computing all the nonlinearities in the physical functional space.

2.3. Sparse function representation

For a given threshold ε we truncate to zero all the non-significant wavelet coefficients:

$$d_{j,k} = 0 \quad \text{if} \quad |d_{j,k}| < \varepsilon \quad (2.16)$$

We will represent $f(x)$ only with the significant coefficients.

In other words, we truncate the linear combination to represent the function in the wavelet basis, taking only a few numbers of terms. So, a smooth function will be represented with a small number of significant coefficients and only the region where a given function has sharp behavior we will need to add terms in the series with significant coefficients $d_{j,k}$.

After this thresholding operation we will have a locally cubic function, (if $p = 4$), well represented with only N_s coefficients or, which is the same, the function will be represented taking only N_s nodes in the grid, that will be a sparse non-uniform grid.

If, for example, the function moves in the space, its sharpness also moves, and so the grid, so we are able to construct an adaptive non-uniform grid.

The steps to get the sparse point representation, (spr), of a function and the computation of the discrete spatial derivatives by central finite difference are shown in [Holmström, M., 1996], and [Alvarez, L. and Navarro, J., 1999].

As it is remarked in [Jameson, L., 1994], when wavelet methods are considered in the physical space, where the function lives:

- they are equivalent to use explicit finite difference methods.
- strictly speaking wavelet methods correspond to central finite difference operators.
- one important fact is that there exists superconvergence in the chosen nodes.
- the refinement is accomplished only by adding wavelets basis in the series where the function has singular behavior.

3. SOLVING THE SCHRÖDINGER EQUATION

The non-linear evolution PDEs that we have solved are those with soliton type solutions. In a previous work we have presented this technique for the KdV equation, [Alvarez, L. and Navarro, J., 1999], which describes wave trains with weak dispersion. This equation replaces the Burger's equation, in models with extremely weak dispersions [Witham, G.B., 1974].

Now we are presenting in this paper the numerical solution of the nonlinear Schrödinger, (NLS), equation [Zakharov, V. and Shabat, A.B., 1972]:

$$iu_t + u_{xx} \pm v u|u|^2 = 0 \quad (3.1)$$

This equation describes the modulation of quasi-monochromatic wave trains and also is a model which arises in various branches of physics, as for example, to describe the nonideal Bose gas of the attracting particles of the propagation of light beams in a nonlinear dispersive media (the propagation of *bright solitons*), etc.

To find efficient numerical techniques to solve the NLS equation is still a challenging researching area [Kholmujdorov, I., V. Puzynin and Yu S. Smirnov, 2000].

3.1. The Method-of-lines

The method of lines is a semidiscrete technique, that transforms the scalar PDE to an ODE system [Le Veque, R., 1992] and [Alvarez, L. and Cunha, C., 1997].

Discretizing the second order spatial derivatives of (3.1), using a central finite difference scheme with filter coefficients coming from the Lagrange interpolation polynomials and denoting it by:

$$V2(x_i, t) \approx (u_{xx})|_{x=x_i}$$

Then we transform the Schrödinger equation to the following ODE system:

$$u'(x_i, t) = V2(x_i, t) \pm |u(x_i, t)|^2 u(x_i, t), \quad (3.2)$$

This ODE system is completed with N_s initial conditions from the evaluation of the initial condition of the PDE in the N_s sparse nodes.

The treatment of the boundary point for the interpolation of the function values and for the centered difference schemes for the discretization of the derivatives are well explained in [Holmström, M., 1996] and [Alvarez, L. and Navarro, J., 1999].

It is important to remark that the number of the resulting ordinary differential equations is exactly the same quantity of the sparse point representation of the solution, because the discretization of the PDE is done only in the nodes of the non-uniform grid.

The final step of the procedure will be to solve the ODE system with an efficient technique for stiff problems, taking into account that we can have small parameters in the denominator of the right hand sides of the systems (Δx_j , v , etc.).

In each temporal step, (taken automatically by the code), we need to compute the sparse wavelet representation, (spr), of the solution, constructing thus, the moving grid.

The method of lines has the advantage that decouples the spatial and temporal issues in the ODE system.

4. NUMERICAL SIMULATIONS

Test 1. NLS equation:

$$i u_t + u_{xx} \pm |u|^2 u = 0$$

with a complex initial condition:

$$u(x, 0) = a \operatorname{sech} \left(\frac{ax}{\sqrt{2}} \right) \exp \left(\frac{ix}{2} \right)$$

and parameters values:

$$\alpha = 2, v = 1, a = 2(\alpha - v^2/4)$$

The exact solution reported in Ref. (Vvdensky, D., 1993), is:

$$u(x, t) = a \operatorname{sech} \left[\frac{1}{\sqrt{2}} a(x - vt) \right] \exp \left\{ \left[\frac{1}{2} v(x - vt) + \alpha t \right] \right\}$$

The following pictures show the accuracy and well correspondence of the exact and numerical solutions, which error has been $0(10^{-4})$ in both, spatial and temporal issues.

The plotted quantity is $|u(x, t)|$.

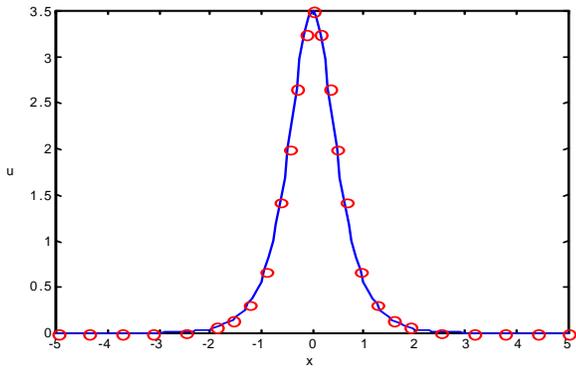


Figure 1. Initial condition. The circle are the sparse nodes from the spr.

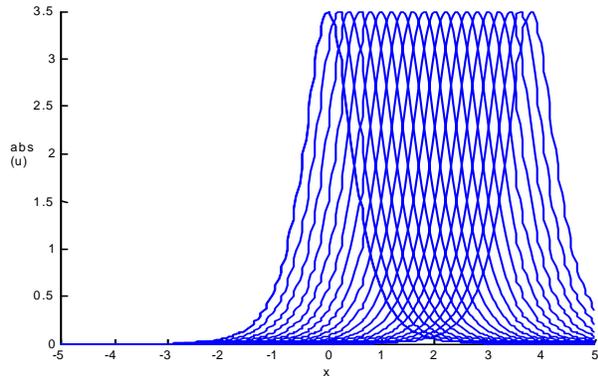


Figure 2. Numerical solution showing the travelling soliton in different time steps.

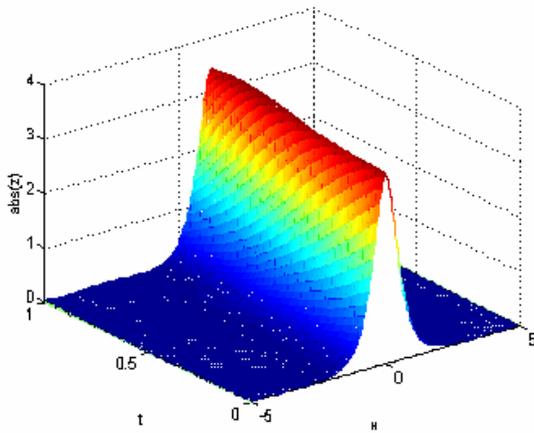


Figure 3. 3D numerical solution, $t \in [0,1]$.

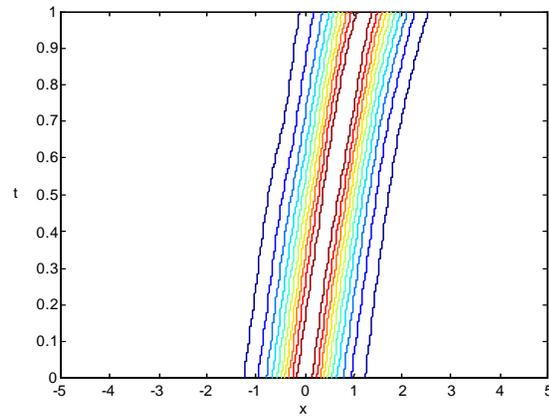


Figure 4. 2D contour of the soliton position.

Test 2. NLX equation with $v = 2$:

$$i u_t + u_{xx} \pm 2 u|u|^2 = 0$$

With a real initial condition:

$$u(x,0) = \pi \sqrt{2(1 + 0.1 \cos \pi x)}$$

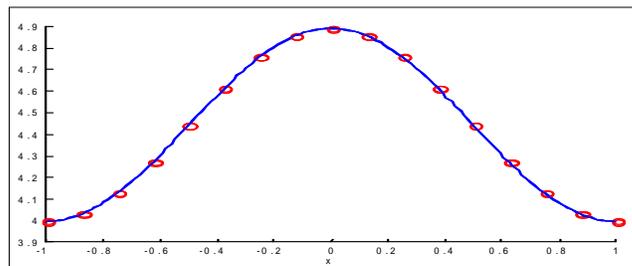


Figure 5. Initial condition for test 2.

In this case the exact solution is unknown and we have only numerical results reported in [Fornber, B., 1998] using spectral methods.

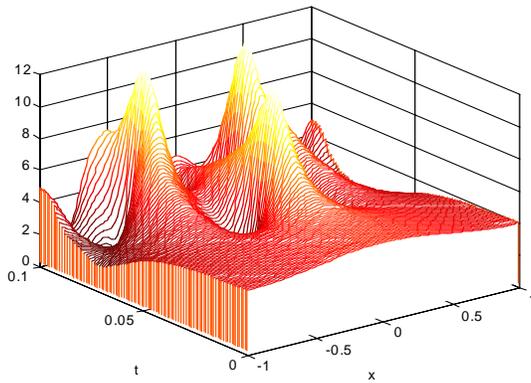


Figure 6. 3D numerical solution for Test 2.

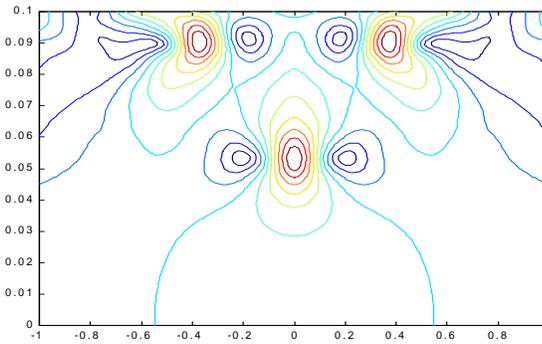


Figure 7. 2D contour of the numerical solution.

Notice that, starting from a smooth initial condition, the solution evolves to a soliton and after certain time steps it evolves to two travelling solitons.

To have certainty of the numerical results, we have computed one of the conserved quantities for the NLS equation:

$$Q(t) \approx i \int |u(x,t)|^2 dx$$

Computing the errors with respect to the initial conserved quantity Q_0 from the initial condition:

$$\text{Error} = \frac{|Q_{\text{num}} - Q_0|}{\max |Q_{\text{num}}|}$$

We obtained the following behavior for the numerical errors:

This figure shows that after certain time value ($t \approx 0.05$), the error increase rapidly due to the accumulation of numerical errors from the ODE solverm showing the complexity of thgis Test 2.

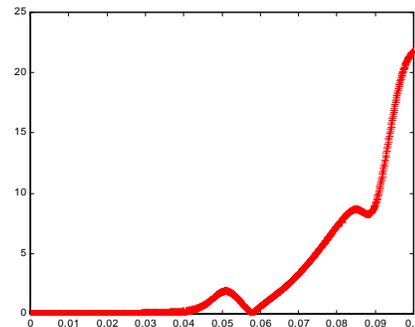


Figure 8.

5. CONCLUSIONS

In this work we have developed an efficient tool to solve the nonlinear evolution 1D PDEs. We have discussed in some details the basic principles of wavelet functions starting from the Daubechies wavelets to introduce the Donoho's interpolary wavelets. For more details in the use of centered finite difference scheme to approximate the spatial derivatives, the reader is submitted to [Holmström, M., 1996] and [Alvarez, L. and Navarro, J., 1999].

The correct results and the little computational effort (only a few minutes in a PC) solving complex PDEs, showed the possibility to extend this technique to solve 2D nonlinear PDEs. The authors continue working in this subject for systems of 1D nonlinear conservation laws and 2D problems.

We think that hybrid methods using wavelets is the future in all branches of the numerical analysis.

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