

A NUMERICAL STUDY FOR IMPROVING TIME STEP METHODS IN PSUDOSPECTRAL SCHEMES APPLIED TO THE KORTEWEG AND DE VRIES EQUATION

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Abstract. The numerical integration of partial differential equations that admit solitons like solutions appears frequently in science as the case of the equation of Korteweg and de Vries (KdV).

The nonlinear behavior and the existence of solitons and interacting solitons constitute an important tool for the study of the propagation of that kind of nonlinear traveling waves. On the other hand, the linear term is the one in which arise the main restriction for the time step setup.

The time expended in the computational running is important in particular when the time integration is done by an explicit method; although implicit schemes exist, the explicit ones are often used, because they are easy to codify in almost every computer language.

To reduce the time required for the numerical integration, one proposal found in the literature is known as the integrating factor (IF), another is based upon the method named exponential time differencing (ETD). The second one represents the state of the art in improving time stepping in explicit methods for non linear differential equations.

In the present work a pseudospectral method was implemented for the KdV equation, and with the aid of the IF and ETD a several numerical experiments was performed.

The numerical study includes an analysis of the global error depending of the time step selection and the variation of results among a few explicit numerical schemes of high order of precision for the time integration.

1 INTRODUCTION

The propagation of several solitons in 1D and the interaction of them is a very interesting problem to study from the theoretic point of view and have many applications in several fields of science and technological research. For example the transmission of information in optical fiber requires the deep understanding of the solitons propagation. The numerical study of the solitons interaction born with the work of Fornberg y Whitham (1978) and was continued after this as can see in Soomere y Engelbrecht (2005).

In a computer laboratory equipped with accessible platforms is easy to generate numerical solitons and design their propagation in many scenarios, so is cheaper to acquire solid knowledge in the behavior of the solitons propagation and all linked concepts.

One way to generate solitons is solving nonlinear wave equations that admit this kind of solitary wave as possible solutions of them.

The nonlinear wave equation of Korteweg and de Vries (Kortweg y de Vries 1895) named as KdV is well known and with the appropriate initial conditions admits solitons as their solutions. The time expended in many computer simulations of solitons propagation and interaction is really high. This is one of the main reasons to investigate alternative numerical schemes to solve it.

The spectral and pseudospectral numerical schemes are recommendable to apply in the spatial numerical integration of the KdV equation for many considerations (Whitham, 1974), (Drazin and Johnson, 1989).

There are a few different ways to integrate spatially the KdV equation, but when the time integration is carried out the time required is the main problem. In this work we used, for the study of propagation of two solitons given as initial condition for the KdV equation, the use of a pseudospectral method for the spatial integration and three different numerical schemes for the time integration. One, the simplest, is based in a Runge-Kutta fourth order scheme (Trefethen, 2000), (Canuto et al., 2007). Other of them is implemented with the aid of the integrating factor (IF) applied to the KdV equation (Trefethen, 2000). The remaining scheme uses the exponential time differentiation method (ETD), which constitutes as the community, cut edge, kind of scheme, or in other words the state of the art (De la Hoz, and Vellido, 2008), (Kassam and Trefethen, 2005), (Cox and Matthews, 2002).

Comparisons among the schemes mentioned above were made including considerations about the stability of each method.

2 NUMERICAL SCHEMES FOR THE SOLUTION OF THE KDV EQUATION

The KdV equation, derived by Kortweg and de Vries in 1895 (Kortweg y de Vries, 1895) in the study of shallow water waves has the form.

$$u_t + 6uu_x + u_{xxx} = 0, \quad (1)$$

where $u(x,t)$ is the amplitude of the wave, and, the sub index t and x refers to partial derivatives respect to time and space respectively.

This equation has a soliton like solution (Martinez et al, 2010). In order to obtain this kind of solutions one needs to have a close relationship between the dispersion and the non-linear term, solitons solutions appear when the nonlinear term compensate the dispersion term and the wave travel without dispersion.

Equations like the KdV that have a high-order linear derivative and a low-order nonlinear term are called stiff. A stiff equation is a differential equation for which certain numerical methods for solving the equation are numerically unstable, unless the step size is extremely

small. It has been proven difficult to formulate a precise definition of stiffness, but the main idea is that the equation includes some terms that can lead to rapid variation in the solution (Emmrich and Wittbold, 2009).

Like we mentioned before there are no universally accepted definition of stiffness. Rather than proposing a precise mathematical definition of “stiffness”, we consider here that “stiff” systems are systems in which “abrupt transition” (discontinuity) are observed in the time series, such abrupt transitions often result from different time scales in the dynamics.

To simulate precisely the abrupt transition, it is required to have a very small time steps, but reducing the time step may drastically increases the computational time. Therefore, algorithms specifically designed to solve such stiff systems have been proposed.

In the case of the KdV the stiffness come from the linear term. So the idea is to eliminate this term for the equation to become less stiff.

We studied three numerical methods for the solution of the KdV equation.

The first method, called the “direct method”, which does not takes into account the stiffness of the equation, find the solution directly applying a pseudospectral scheme with a Fourier basis in space and a Runge-Kutta of fourth order in time (called DRK4).

The second introduced the use of the integrating factor (IF) formulation in the problem helping to eliminate the stiffness of the equation.

The latter represents the state of the art for stiff problems which conducts a semi change of variables, and is known as ETD as mentioned above.

2.1 Standard Methods.

The direct method to find the numerical solution is to evaluate the derivatives of $u(x,t)$ in Fourier space (Trefethen, 2000) and then go back to spatial space to find the solution in the original domain.

This scheme for equation (1) stands as follow

$$u_x = u_x = \mathcal{F}^{-1}(ik * \mathcal{F}(u)), \quad (2)$$

$$u_{xxx} = u_{xxx} = \mathcal{F}^{-1}((ik)^3 * \mathcal{F}(u)), \quad (3)$$

where \mathcal{F} and \mathcal{F}^{-1} are the direct and inverse Fourier transform, k are the Fourier nodes, and i is the imaginary unit.

Then solution is found replacing u_x and u_{xxx} in (1) by u_x and u_{xxx} respectably.

$$u_t = -6u * u_x - u_{xxx}. \quad (4)$$

The integral of the left side of the equation was made with a Runge-Kutta scheme of fourth-order (RK4) (Yang et al., 2005).

The program written was able to compute the solution successful but needed a very small time step for stability.

2.2 Improved Method: Integrating Factor

Since the linear term in equation (1) is the one involving high frequencies, providing the stiff characteristic that constrains the stability and requires very small time steps, the method of integrating factor is based on the idea that the problem can be transformed so that the linear (stiff) part of the partial differential equation (PDE) is solved exactly.

One of the needs of the IF method is that the equation can be written as following.

$$u_t + L(u) + N(u) = 0, \quad (5)$$

where L is a linear operator and N is a nonlinear operator, with periodic boundary conditions. Following the development done by Trefethen (2000), one way to proceed is to write equation (1) as

$$u_t + 3(u^2)_x + u_{xxx} = 0, \quad (6)$$

which Fourier transform is

$$\hat{u}_t + 3ik\widehat{u^2} - ik^3\hat{u} = 0. \quad (7)$$

Taking $L = -3ik^3$ as the integrating factor and making a change of variables

$$\widehat{U} = e^{Lt}\hat{u}, \quad (8)$$

where \hat{u} is the Fourier transform of u . Replacing (8) in (7) we obtain an equation where the linear term is gone

$$\widehat{U}_t = -3ike^{Lt}\widehat{u^2}, \quad (9)$$

and the problem is no longer stiff.

Working in Fourier space, the problem can be discretized in the form

$$\widehat{U}_t = -3ike^{Lt}\mathcal{F}(\mathcal{F}^{-1}(e^{-Lt}\widehat{U}))^2. \quad (10)$$

Now that the linear part is effectively removed from the evolution equation, the stability is expected to hinge on the less stiff nonlinear operator, allowing larger time steps and thus reduce the computation time.

It can be found that the method does not eliminate the total stiffness from the problem. However, it does change the nature of the instability that we see, now has a rapidly varying coefficient and ensures that the instability barrier is much softer in a sense than the time step restriction in the direct pseudospectral method (Krogstad, 2005) (Tang, 2009).

In both the direct method and the integrating factor method we used a fourth-order Runge-Kutta method for time-stepping (called DRK4 and IFRK4 respectively). The fourth-order Runge-Kutta algorithm used to perform the time integration for these implementations was the classical one (Yang et al., 2005) which is the following.

$$\begin{aligned} a_n &= hf(u_n, t_n) \\ b_n &= hf(u_n + a_n/2, t_n + h/2) \\ c_n &= hf(u_n + b_n/2, t_n + h/2) \\ d_n &= hf(u_n + c_n, t_n + h) \\ u_{n+1} &= u_n + \frac{1}{6}(a_n + 2b_n + 2c_n + d_n) \end{aligned}$$

where h is the time step and f is the nonlinear functional on the right side of (4) and (10). The next value (u_{n+1}) is determined by the present value (u_n) plus the weighted average of four deltas (Figure 1), where each delta is the product of the size of the interval ($h=\Delta t$) and an estimated slope: $h(\text{slope}) = \Delta t (du/dt) = \Delta u$. Then

a is the delta based on the slope at the beginning of the interval, using Euler's method.

b is the delta based on the slope at the midpoint of the interval, using $u_n + a/2$.

c is again the delta based on the slope at the midpoint, but now using $u_n + b/2$.

d is the delta based on the slope at the end of the interval using $u_n + c$.

The RK4 method is a fourth-order method, meaning that the error per step is on the order of h^5 , while the total accumulated error has order h^4 .

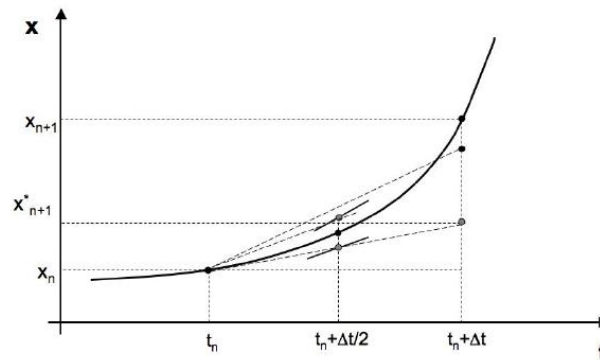


Figure 1. Points used by RK4 for solving the time integral.

2.3 Exponential Time Differencing

In this paper we used the modified ETDRK4 proposed by (Kassam and Trefethen, 2005). Algebraically ETD is similar to IF method but the difference is that ETD does not make a complete change of variables. If we proceed as in the IF approach and apply the same integrating factor and then integrate over a *single* time step of length h , we get

$$u_{n+1} = e^{Lh}u_n + \int_0^h e^{-L\tau}N(u(t_n + \tau), t_n + \tau)d\tau . \tag{11}$$

The expression (11) is exact, and the various order ETD schemes come from how one approximate the integral.

In the work (Cox and Mathews 2002) first present a sequence of recurrence expressions that provide higher and higher-order approximations of a multistep type. They also derived a set of ETD methods based on Runge-Kutta time-stepping, which they call ETDRK schemes.

The Cox and Mathews ETDRK4 formulation are:

$$\begin{aligned} a_n &= e^{Lh/2}u_n + L^{-1}(e^{Lh/2}u_n - I)N(u_n, t_n) \\ b_n &= e^{Lh/2}u_n + L^{-1}(e^{Lh/2}u_n - I)N(a_n, t_n + h/2) \\ c_n &= e^{Lh/2}u_n + L^{-1}(e^{Lh/2}u_n - I)(2N(b_n, t_n + h/2) - N(u_n, t_n)) \\ u_{n+1} &= e^{Lh}u_n + h^{-2}L^{-3}\{[4 - Lh + e^{Lh}(4 - 3Lh + (Lh)^2)]N(u_n, t_n) \\ &\quad + 2[2 + Lh + e^{Lh}(-2 + Lh)](N(a_n, t_n + h/2) + N(b_n, t_n + h/2)) \\ &\quad + [-4 - 3Lh - (Lh)^2 + e^{Lh}(4 - Lh)]N((c_n, t_n + h))\} \end{aligned} . \tag{12}$$

In the expansion (12) is useful to define the following coefficients

$$\begin{aligned} \alpha &= [4 - Lh + e^{Lh}(4 - 3Lh + (Lh)^2)] \\ \beta &= [2 + Lh + e^{Lh}(-2 + Lh)] \\ \gamma &= [-4 - 3Lh - (Lh)^2 + e^{Lh}(4 - Lh)] \end{aligned} . \tag{13}$$

Unfortunately, in this form (12), the ETDRK4 proposed by Cox and Mathews (2002) suffer from numerical instability.

All three coefficients in (13) suffer disastrous cancellation errors when L has eigenvalues close to zero. This vulnerability to cancellation errors in the high-order ETD and ETDRK schemes can render them effectively useless for problems which have small eigenvalues in the discretized linear operator (Klein, 2008).

The coefficients in expression (13) have the form of a function of complex variables, $f(z)$, which are analytic except for a removable singularity at $z = 0$, this is the main mathematical reason that ruins the stability of the method.

The solution found by Kassam and Trefethen (2005) was to evaluate the function $f(z)$ via an integral over a contour in the complex plane that encloses z and is well separated from zero. Contour integrals of analytic functions in the complex plane are easy to evaluate by means of the trapezoidal rule.

In the special case of KdV in 1D the contour integral reduces to a simply mean of $f(z)$ over a contour, that was approximated by a mean over equally spaced points along the contour.

3 NUMERICAL IMPLEMENTATION

The numerical implementation was made in MATLAB® 2010b version, on a platform ASUS N82JQ notebook with an Intel I7-720QM processor with 4GB of ram memory

For all the experiments we solve the KdV equation with initial condition

$$u(x, t) = \frac{a^2}{2} \operatorname{sech}\left(\frac{a}{2}(x - x_0)\right)^2 + \frac{b^2}{2} \operatorname{sech}\left(\frac{b}{2}(x - x_1)\right)^2,$$

with $a=10$, $b=20$, $x_0=0$ and $x_1=-\pi/2$, which is similar to (Martinez et al, 2010).

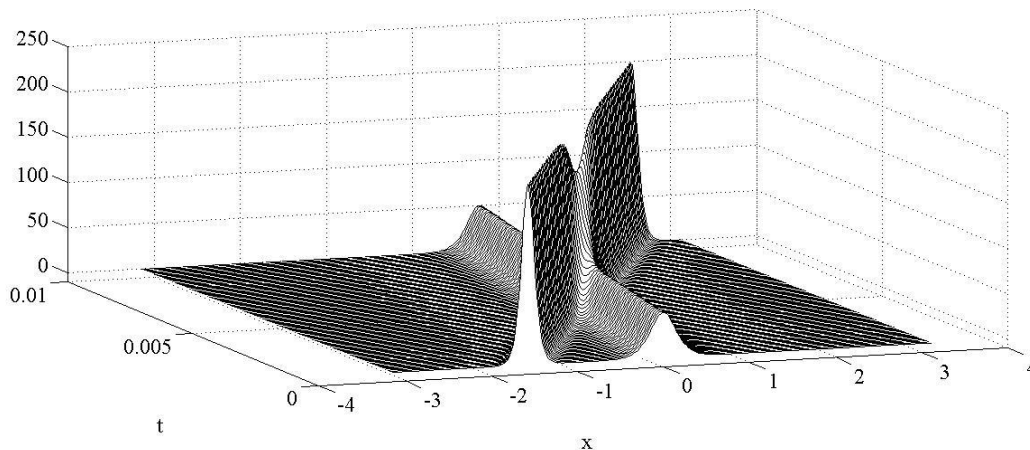


Figure 2. Example of propagation of solitons. As one can see the waves, after colliding, continue with only a phase shift.

3.1 Flow chart of the code

To solve the soliton KdV equation with the schemes mentioned above, several Matlab® scripts were made. The scripts of the three methods, `drk4.m`, `if_drk4.m` and `etd_drk4.m`, have a flow code similar to Figure 3. The difference within each method is made in the third gray term of Figure 3.

Others scripts were made especially for the evaluation of time performance and error estimation. To help reduce the time spent on the simulations, we performed a parallel implementation using the Matlab® parallel toolbox, in with using the multicore functionality of the computer, 8 scripts with different conditions (length, N and time steps, h) were processed at the same time, reducing significantly the duration of the numerical experiments.

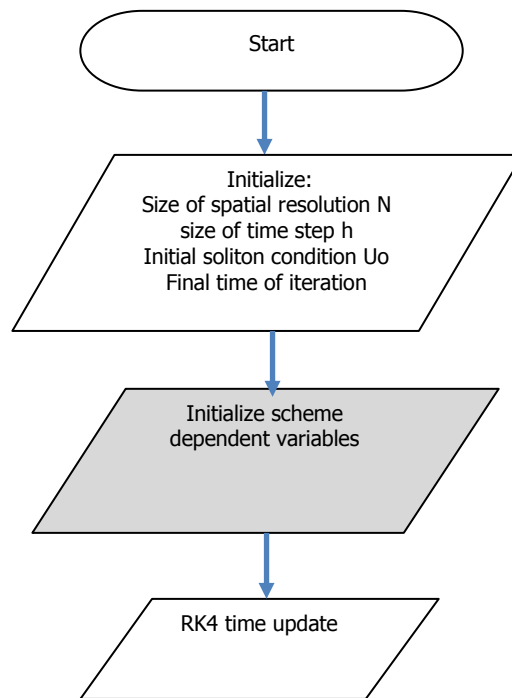


Figure 3. General Flow code of implemented scripts.

3.2 Numerical examples of the integration scheme

Some of the numerical experiments done are presented here as an example of solitons solutions. Figure 4 shows the propagation and collision of two solitons moving on an interval of length 2π .

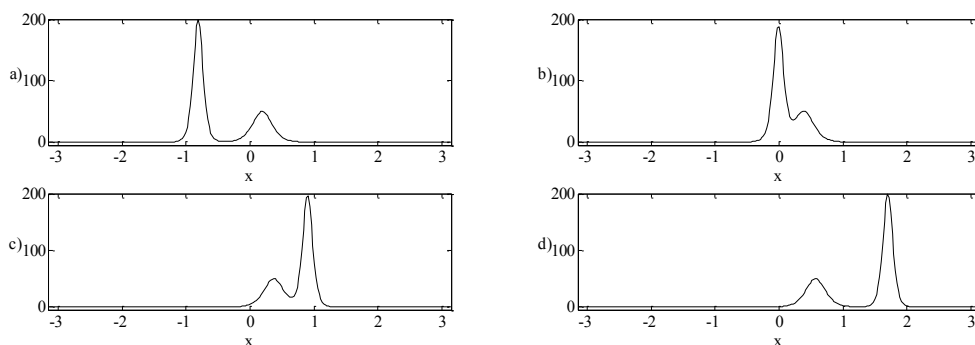


Figure 4. In this figure we can see four states of the travelling solitons. (a) is a state before colliding, (b) and (c), before and after while colliding and (d) after the collision. The shape and velocity maintain, only a phase shift has occurred

The amplitude and velocity of a soliton are linked, so the higher and faster soliton catch the smaller one and pass over him.

Figure 5 shows the same example as previous depicted in 3D, the horizontal axis represents the time and space respectively and the vertical axis is the soliton amplitude. Here we can see the phase shift for each soliton after colliding.

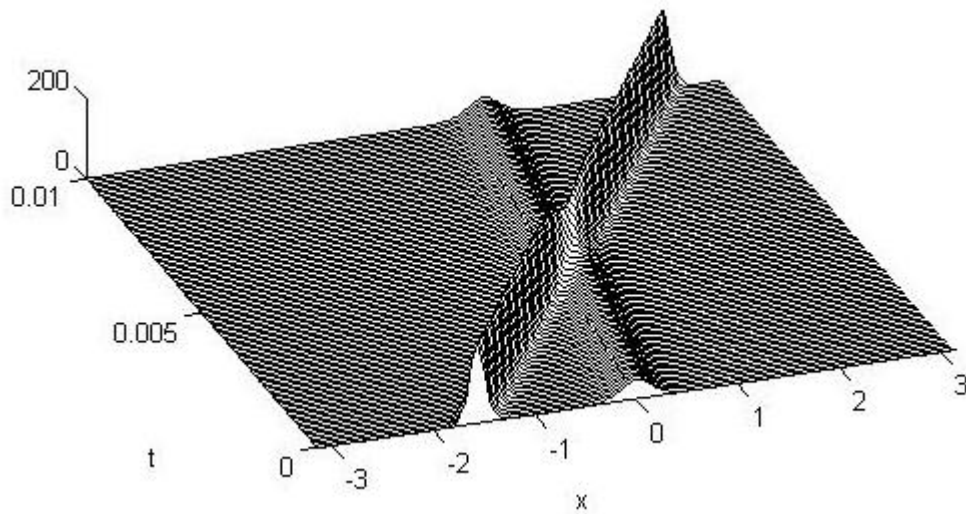


Figure 5. Collision of two soliton. Here we can notice the backward phase shift for the slow soliton and the forward phase shift on the bigger one

4 NUMERICAL EXPERIMENTS

A series of numerical experiments were performed. First we found the performance and stability of the ETDRK4 scheme, later we compare this relative new method with the method of integrating factor that is well known in the area (Krogstad, 2005).

The experiments were performed with size of grid from 64 to 2048 points. The time steps used were from 10^{-5} to 10^{-8} .

4.1 Computational performance of ETDRK4 schemes

Table 1 shows the relative error of ETDRK4 scheme for different values of the time step (h) with 512 nodes of spatial resolution at the end of one period of iteration.

The error was calculated with two-norm and the infinity-norm

<i>Time Step</i>	$\frac{\ u - u_0\ _2}{\ u_0\ _2}$	$\frac{\ u - u_0\ _\infty}{\ u_0\ _\infty}$
4,00E-06	2,36E+02	6,26E+02
2,00E-06	9,08E-04	2,40E-04
1,00E-06	3,72E-05	9,75E-06
8,00E-07	1,23E-05	3,23E-06
4,00E-07	1,84E-06	4,91E-07
2,00E-07	2,55E-06	6,79E-07
1,00E-07	2,62E-06	6,97E-07

Table 1. Errors for ETDRK method with 512 grid points.

The following figures show the time performance of the ETDRK4 method. Figure 6 shows the total time required to integrate the KdV equation vs time step for different values of N . Figure 7 shows time of running vs the size of grid (N).

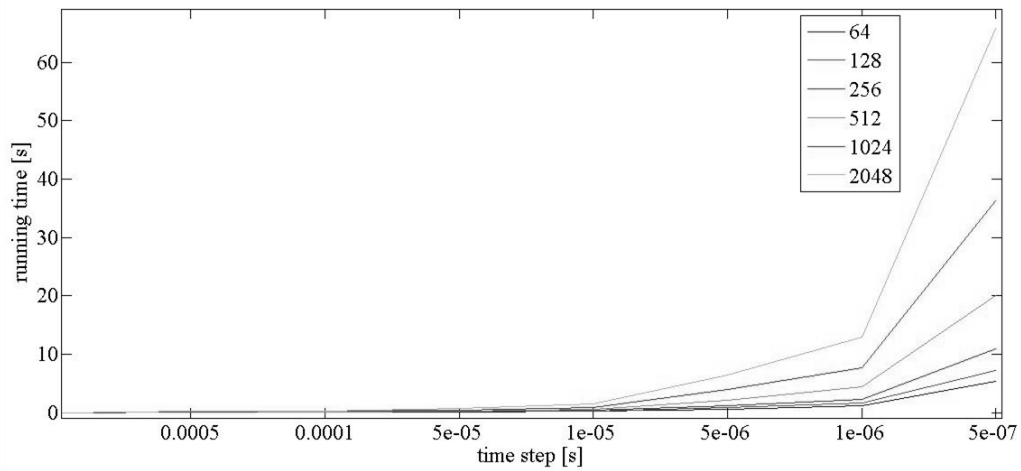


Figure 6. Time required for running the scrip with different time steps for different values of N

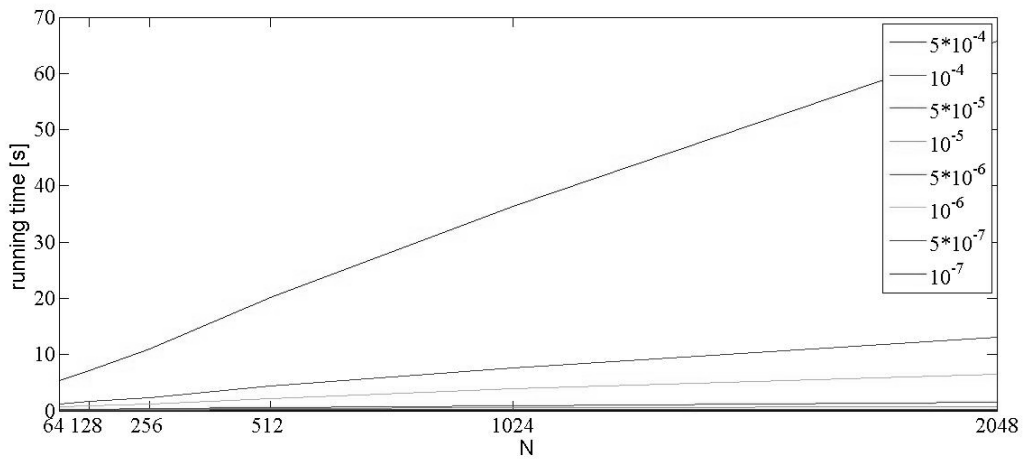


Figure 7. Time required for running the scrip with different values of N for different time steps

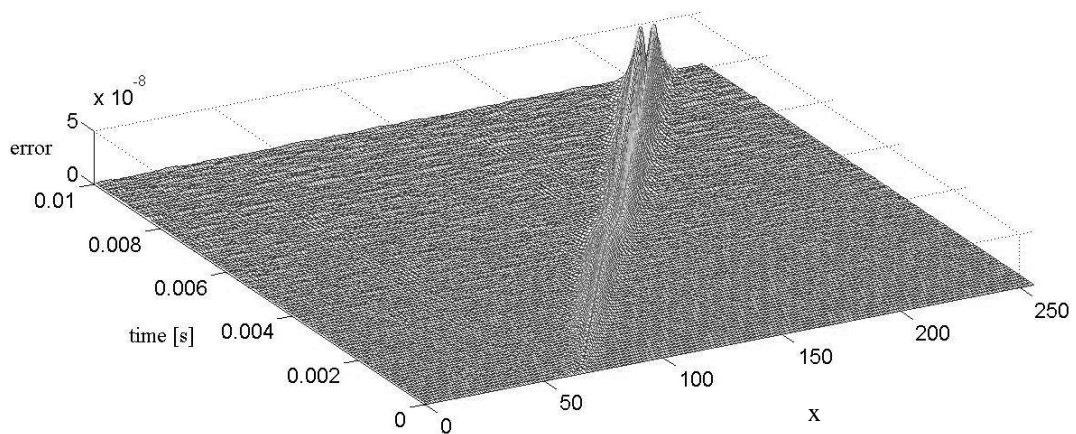


Figure 8. Shows the error at each point for the entire running. With time step= 10^{-6} and $N=256$.

As can be seen in Figure 8, the highest error values are found in the time and region of the soliton interaction. The study of the soliton interaction was one the main aims of our research, in particular the possibility to keeping the error lowest as possible in the integration during the

soliton interaction was an important goal of the research.

4.2 Comparison with FI and the standard scheme

Time, relative error, stability and size of time steps were taken into account for the comparison between the Integrating Factor, and Exponential Time Differencing methods. The direct method was left behind because most of the simulations diverged.

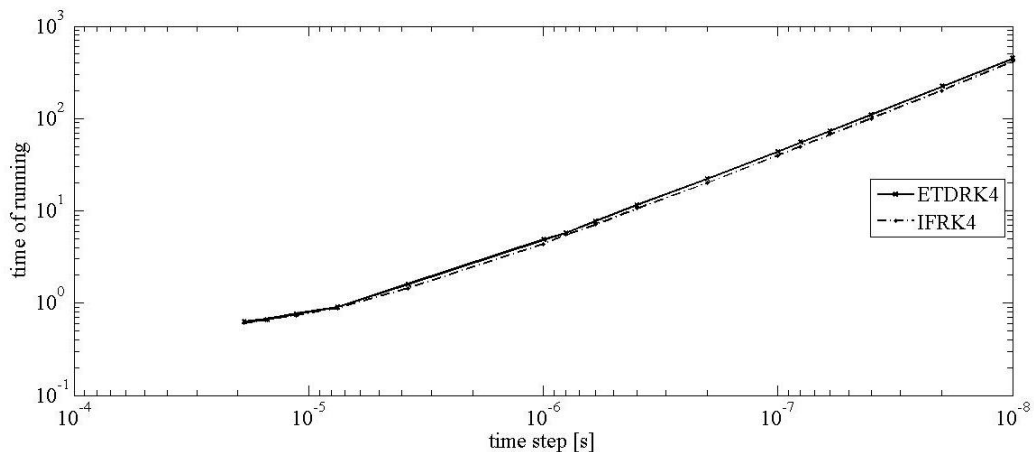


Figure 9. Comparison of running time for the IF and ETDRK schemes with 512 grid points.

Like expected the time needed to solve the equation between the IF and ETD was almost equal using the same numerical conditions. This was expected because of the similitude of the algorithms. Both needed to perform eight Fourier transform for each time step, against the direct method that used twelve. The operation of multiplication by the coefficients within the brackets (13) is what gave the advantage to IF.

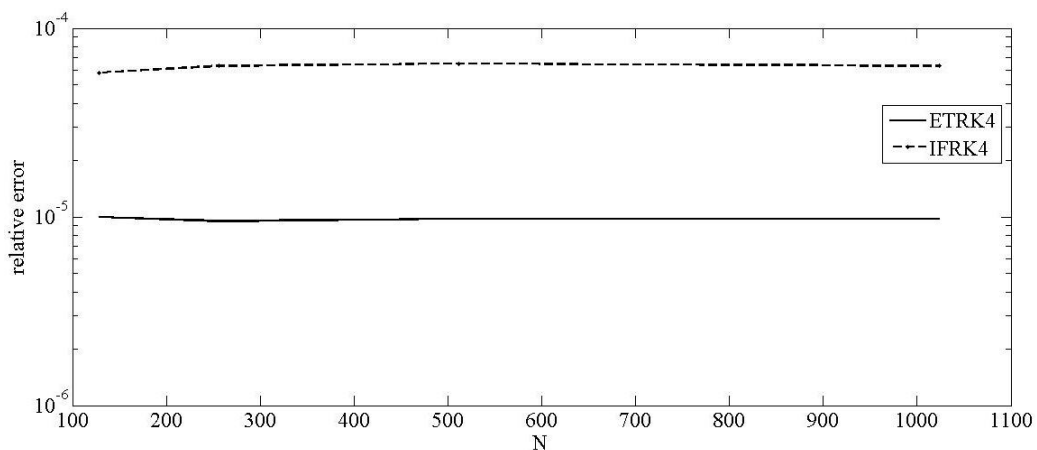


Figure 10. Comparison of the error produced at the end of a period with different grid point while having a time step of 10^{-6} .

As can see en Figure 10 for the same time step but with different number of grid points the ETDRK4 method does better than IFRK4 by a factor of 10.

The same occurs while having the same number of nodes but changing the time step (Figure 11). ETDRK4 method was ten times more efficient with in the same conditions this was because that instead of change the nature of the stiffness likes IFRK4; ETDRK4 finds a

nearly exact solution of the problem and almost eliminate the stiffness.

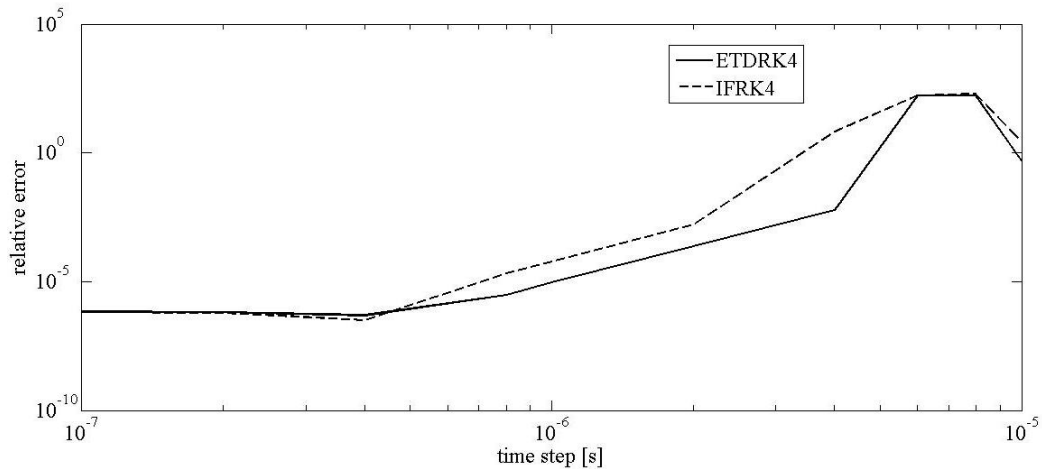


Figure 11. Relative error for 256 nodes of grid calculated and the end of one period.

4.3 Stability of the ETDRK4 scheme

One of the things concerning stability was that ETDRK4 appears to have no stretch relation with the size of the grid. While IFRK4 have the stability region bounded with the grid size. Figure 12 shows that for small size nodal points the method converge, but for larger size the solution diverge. ETDRK4 however converges for all number of nodal points used. This experiment was done with a time step of 10^{-5} , which is very large for direct method

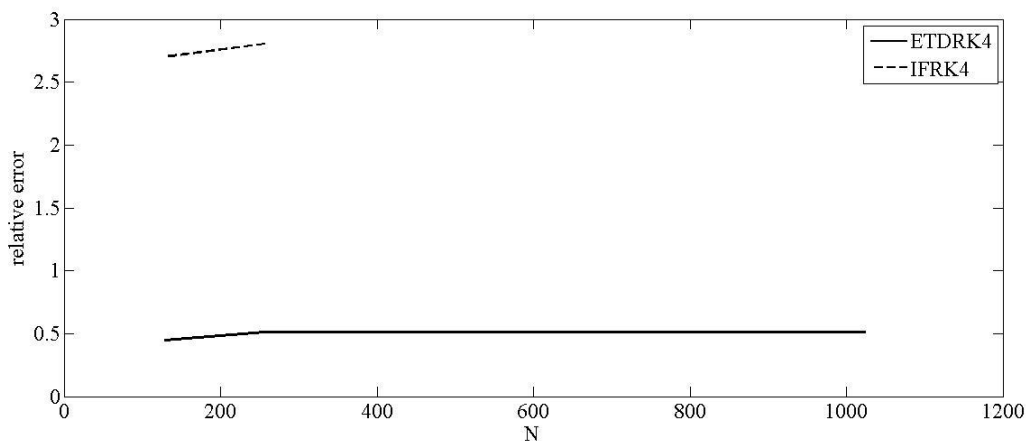


Figure 12. The graphic shows the convergence of the two methods for a time step of 10^{-5} . While ETD perform correctly for all sizes of the grid, IF can only perform with small size.

The evolution of the error was also checked. For different time steps and number of nodal points. An example can be seen in Figure 13, which shows the divergence of the error for ETDRK4 and IFRK4 after one complete propagation of the solitons in the computational spatial domain.

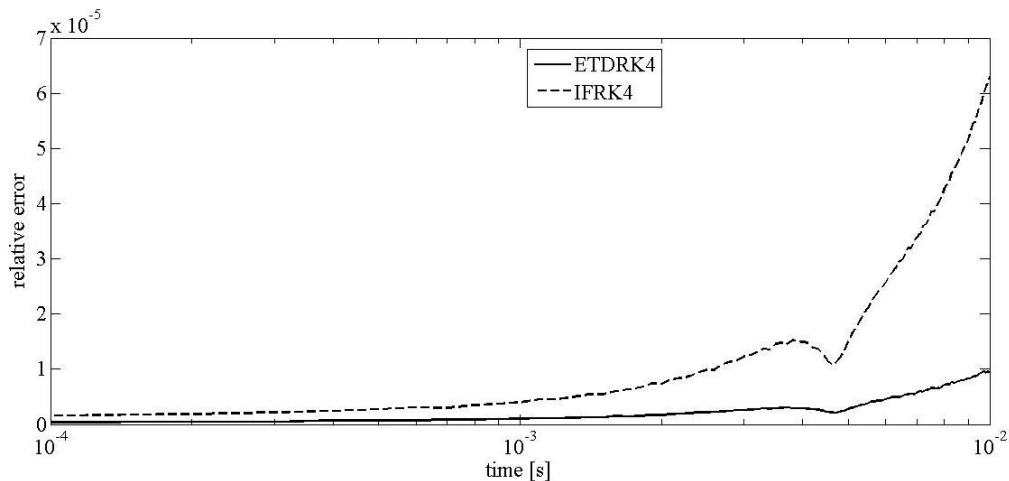


Figure 13. Evolution of the error during one ride of the solitons along the spatial computational domain for the different schemes, with $N=256$ and $h=10^{-6}$.

5 CONCLUSION

From a historic point of view the IF method was the first in the beginning of the XXI century with a clear conceptual way to improve the application of spectral methods to integrate nonlinear wave equations. In the middle of the first decade of the XXI century a few number of researchers work to optimize the IF method and in that way found the ETD in general.

The ETDRK4 scheme arises as the best method for numerical study of soliton like solutions of the KdV. While IFRK4 do from five to ten times better than the direct method, the ETDRK4 method outperformed IFRK4 in stability in an order of ten. Allowing the use of higher time steps while maintaining the same bounds of error.

The error in all situations was calculated in the worst case in which the accumulation done by the spectral method was taken into account.

The independence of ETDRK4 to the size of the grid (over 64 nodal points) is another improvement. We can have a very good spatial resolution while having bigger time steps.

It is noteworthy that this study was done in 1D+1D dimension (time and 1D space). The extrapolation to 2D+1D and 3D+1D will made use of more expensive calculus and time. Choosing the best method in matter of time improvement and stability need to be a well evaluated choice.

The performance of the ETDRK4 method is without any kind of doubt the best choice when the KdV for soliton interactions (at least with two solitons) is under consideration.

6 FUTURE LINES OF RESEARCH

For our research project the passing to 2D+1D dimension is the obvious next step and with the results acquired in this work this could contribute without doubts.

Another way to take in the next future is the implementation of a wavelet based algorithm that can lead to reduce further the time of computations making use of smaller basis space, maintaining the spatial accuracy. That is one of the Fourier problems.

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