Numeric description of long distance propagation of temporal pulses in nonlinear Kerr-like media

Jerzy Jasiński*

Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warszawa

Abstract — In the paper the propagation of temporal pulses through nonlinear Kerr and Kerr-like media is described numerically. The evolution of numerical solutions of the nonlinear Schrödinger equation significantly changing its shape is studied over the distance up to few thousands nonlinear lengths. The influence of two differentiation algorithms and three types of transparent boundary conditions on the accuracy of calculation is discussed. The optimal choice is proposed.

In saturable Kerr-like media the slowly varying envelope $U(z,t)$ propagating along the z-axis satisfies a modified NSE, for cubic-quintic nonlinearity sometimes called Higher Order NSE or the Ginzburg-Landau equation [1-3]:

$$\frac{\partial U}{\partial z} + \frac{ik_2}{2}\frac{\partial^2 U}{\partial t^2} - i\varepsilon_{NL}(|U|^2)U = 0 \qquad (1)$$

In the above equation $\varepsilon_{NL}(|U|^2)$ represent nonlinear permittivity as a function of local intensity. Without a nonlinear term this equation is a version of a parabolic partial differential equation describing the process of diffusion [4-5] – the only difference is an imaginary coefficient of diffusion. This difference follows the necessity to use complex field amplitude, but numerical methods of solving the equation (1) remain the same. An effective algorithm describing field $U(z,t)$ for z between z_0 and z_{max} and t between t_{min} and t_{max} should realize three main tasks: one – perform progress forward, that is calculate field distribution at successive planes $z_0+n\,\Delta z$ for sufficiently large n, two – numerically calculate second-order derivative $\partial^2 U/\partial t^2$ and three – ensure the proper behavior of a field at boundaries t_{min} and t_{max}.

The simplest algorithm performing the first and second task is known as explicit or forward time centered space (FTCS) and is done by the following scheme [5-8]:

$$\frac{U_j^{n+1}-U_j^n}{\Delta z} = -\frac{ik_2}{2}\frac{U_{j+1}^n-2U_j^n+U_{j-1}^n}{\Delta t^2} - i\varepsilon\left(\left|U_j^n\right|^2\right)U_j^n \quad (2)$$

The left-hand expression approximates z-derivative $\partial U/\partial z$ at $t=j\Delta t$ while the quotient $(U_{j+1}^n-2U_j^n+U_{j+1}^n)/\Delta t^2$ - the second order time derivative at the plane $z=z_0+n\Delta z$. Since the field U_j^{n+1} at the plane $z=z_0+(n+1)\Delta z$ calculated by

* E-mail: jasinski@if.pw.edu.pl

means of the above scheme exhibits quite serious errors, one can use more complicated schemes – fully implicit or the Crank-Nicholson. In algorithms based on these schemes we can apply larger step Δz, but because of nonlinearity at each plane $z=const$ we should solve a large set of coupled nonlinear equations [5, 7]. The number of additional operations is very large, so these algorithms are much slower than an algorithm based on an explicit scheme.

The stability of the FTCS scheme can be determined using the von Neumann analysis [5, 7]. Assuming $U_j^n=(1+i\Delta\xi)^n e^{ij\Delta k}$ for $n\to\infty$ we obtain the condition for convergence:

$$\eta = \frac{|k_2|\,\Delta z}{\Delta t^2} < \frac{1}{2} \qquad (3)$$

But even if the FTCS scheme is convergent, its error at each step is of order $(\Delta z)^2$. To effectively apply this scheme at large distances we should take quite a small Δz. However, a much better solution is to adopt the Runge-Kutta 4-th order method in which:

$$U_j^{n+1} = U_j^n + \left(\Delta U_j^{n,1} + 2\Delta U_j^{n,2} + 2\Delta U_j^{n,3} + \Delta U_j^{n,4}\right)\big/6 \quad (4)$$

where $\Delta U_j^{n,1},..\Delta U_j^{n,4}$ are four successive field changes calculated using specific rules [4, 5, 8]. The Runge-Kutta method has errors of the order $(\Delta z)^4$, so the accuracy of calculated values of the field is much better. Applying this method we take into account the values of a field at three additional planes, so the RK method realizes the same aim as the implicit or Crank-Nicholson schemes using much less calculation. In practice including the Runge-Kutta method into an FTCS scheme we can apply even larger Δz than those allowed by condition (3).

As an example let us consider the propagation of a second-order soliton of the initial width 50 fs and initial amplitude 100/3 kV/mm. Its field can be described analytically [3], so the accuracy of a numeric algorithm can be checked directly. The distance of propagation covers about 14 periods of oscillations (about 90 nonlinear lengths [1]), while the central height $|U(0,z)|$ varies between 33.3 and 100 kV/mm. Figure 1 shows the difference between a numerical and analytical solution of Eq. 1 at the point $t_0=1000$ fs. First, comparing the pink

and blue line we can observe that errors diminish with diminishing Δt. As a matter of fact, the blue line represents three coinciding lines obtained for three cases of convergence coefficient η = 0.25, 0.5 and 0.667. The relative difference between these cases is very small – less than 10^{-8}. Therefore one can conclude that we can apply as large Δz as possible – provided only the numerical procedure is convergent.
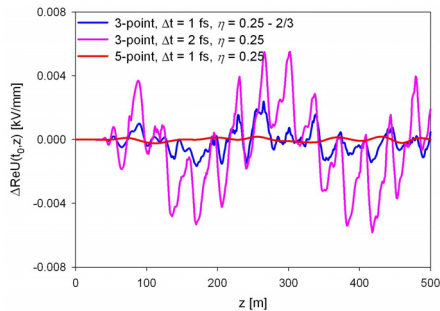

Fig.1. Errors of calculation at t_0=1000 fs as a function of the distance of propagation.

To improve the accuracy of determination of a time derivative one can use a 5-point algorithm:

$$\frac{\partial^2 U_j^n}{\partial t^2} = \frac{\left(-U_{j+2}^n + 16U_{j+1}^n - 30U_j^n + 16U_{j-1}^n - U_{j-2}^n\right)}{12\Delta t^2} \quad (5)$$

instead of a 3-point algorithm used in (2). To check the stability of this algorithm we apply again the von Neumann stability criterion. Introducing the corresponding values approximating fields into (5) and replacing the 3-point difference ratio in (2) by the obtained one, we derive the condition:

$$\eta = \frac{|k_2|\Delta z}{\Delta t^2} < \frac{3}{8} \quad (6)$$

Thus we proved that a 5-point algorithm exhibits a bit smaller convergence than a 3-point one, but nevertheless in many cases it is more precise. The red line in Fig. 1 shows the difference between the numerical and analytical solution of this algorithm. Comparing it with a 3-point algorithm of differentiation (the blue line) we can conclude that for the considered case a 5-point algorithm is much better.

Unfortunately, it is not the general rule concerning all cases. In Fig. 2 we compare the numerical description of propagation of – sequence of two Sech pulses of 50 fs wide with the initial distance of 300 fs. Each of the single pulse is soliton, but because of their interaction pulses attract. As a result pulses periodically oscillate changing their distance from 0 to 300 fs – period of these oscillations is 78.2 m. Since there is no analytical description of pulse propagation, as a measure of accuracy of TBC we take the difference between the values of a field at a certain point while the distance from

boundary t_{max} is changed. a 3-point algorithm of differentiation (2) gives very close results (all of them are given by the pink line) for any width of a calculation window while the results obtained by a 5-point algorithm vary much more. In this case a 3-point algorithm is more reliable.
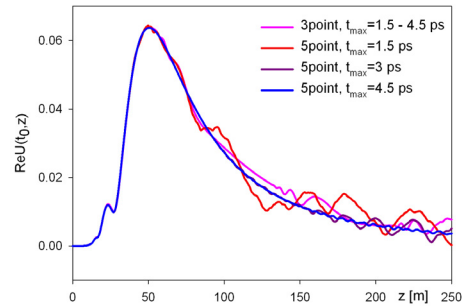

Fig.2. 3-point algorithm of differentiation. Field amplitude at t_0=1000 fs as a function of the distance of propagation

The third factor influencing calculations and being the source of major errors for large distance propagation are proper boundary conditions. There are a few ways to formulate them. Introducing an artificial absorbing layer at both boundaries (Perfectly Matched Layer [8,9]) we can suppress the field beyond the boundaries t_{max} and t_{min}. Another method includes energy conservation law [10, 11]. In fact, to apply effectively scheme (2) we need only one (or two - for a 5-point algorithm of differentiation (5)) value of the field beyond the boundaries. To obtain these values we use Transparent Boundary Conditions (TBCs). It is a method of analytic continuation of the field [9,11]. TBCs are much quicker than other methods and for a smart algorithm of extrapolation TBCs produce very good results.

Their simplest formulation uses M+1 field values [9]:

$$U_{j\max+1}^n = \sum_{m=0}^M a_m U_{j\max-m}^n \quad (7)$$

But for propagation over long distance this simple version of TBCs results in quite serious errors. Much better results are obtained by continuation of the modulus and the phase of a field instead of its real and imaginary part. This is because modulus $|U|$ and phase $\mathrm{Arg}(U)$ change slower than $\mathrm{Re}U$ and $\mathrm{Im}U$ in the vicinity of boundaries so extrapolation of a modulus and a phase is more precise. In order to diminish problems appearing because of a very small value of the modulus or periodicity of trigonometric functions let us apply the following rule for analytic continuation:

$$\left|U_{j\max+1}^n\right|^q = \sum_{m=0}^{M_m} a_m \left|U_{j\max-m}^n\right|^q$$

$$\Delta\,\mathrm{Arg}\left(U_{j\max}^n\right) = \sum_{m=0}^{M_f} a_m \Delta\,\mathrm{Arg}\left(U_{j\max-m}^n\right)$$

$$(8)$$

In the first line of the above formula q can be arbitrary. But in order to succeed in extrapolation of small fields we should apply $0.2<q<0.6$. The second line expresses the rule for extrapolation of a difference of phases $\Delta U=U(z,t+\Delta t)–U(t)$ between two adjacent points. Using the phase difference we practically avoid the problems of ambiguity of inverse trigonometric functions. The number of point M_m and M_f used for extrapolation can be different. In practice, using $q=0.5$ and $M_m,M_f=2$-4 we can obtain errors even 100 times smaller than those resulting from the extrapolation of ReU and ImU.

But in many cases one can obtain even better results by extrapolating the quotients of complex field amplitudes at two adjacent points U(z,t)/U$(z,t-\Delta t)$:

$$\frac{U^n_{j\max+1}}{U^n_{j\max}}=\sum_{m=0}^{M}a_m\frac{U^n_{j\max-m}}{U^n_{j\max-m-1}} \qquad (9)$$

For small Δt the quotient $U_j^n/U_{j-1}^n=U(z,t)/U(z,t-\Delta t)$ equals $1+(\partial\ln U(z,t)/\partial t)\Delta t$, so rule (9) is a method of analytic continuation of a time derivative $\partial U(z,t)/\partial t$ and that is why it is so effective. In Fig. 3 we compare two TBC methods defined by relations (8) and (9) for a 3-point algorithm of differentiation and the same initial pulse as in Fig. 2. As we can see, the difference between the results obtained for two calculation window widths is about twice smaller when we use boundary conditions (9) (for boundary conditions (7) the analogous results differ 100 times more, so practically they are not suitable for propagation over large distances). But TBCs in the form (9) fail when field value $|U_j^m|$ appearing in the denominator of any of the right-hand fraction is too small – in such cases TBCs of the form (8) are better.
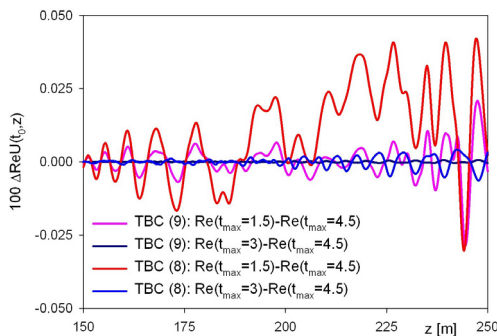

Fig. 3. Influence of Transparent Boundary Conditions on results: differences between fields at $t_0=1$ ps for window width $2t_{\max}=3$, 4.5 and 9 ps.

At last let us apply 3-point algorithm with TBC given by (9) to describe propagation over a distance much greater. In Fig. 4 we see the central amplitude of an oscillating two-soliton pulse over the distance between 4500 and 5000 m for $j_{\max}=1000$, $\Delta t=1$ fs and $\Delta z=4/3$ mm ($\eta=2/3$). However, there are no distinguishable differences in the shape of oscillation (the solid line

shows an imposed curve from the very beginning of propagation), the total intensity of the pulse diminished by 0.01%, the minimum field height decreased by 0.2% (compared to the amplitude of oscillation), the maximum field height decreased by 0.4% while the oscillation period decreased by 0.06%. Despite these changes, the applied algorithm of TBCs and a 3-point algorithm of differentiation yield quite reliable results.
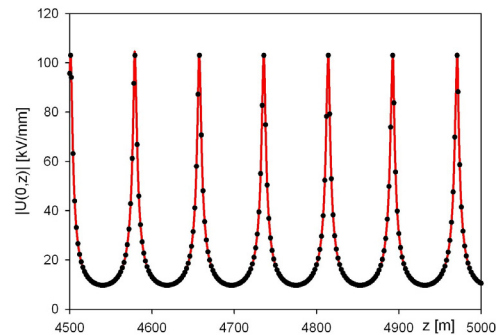

Fig. 4. Calculated values of a field at the distance from 4500 m to 5000m (dots) and a shifted plot of oscillations at the beginning (solid line)

The explicit scheme of the solution of NSE combined with the Runge-Kutta method is quite effective in the description of light propagation over a long distance. Two different transparent boundary conditions applied to this scheme yield very good results – modified extrapolation of amplitude and phase (8) and extrapolation of complex quotients of field (9). However, the last one is more accurate and the first one - more stable. There is no need to improve a 3-point algorithm of differentiation – a 5-point algorithm is much stronger influenced by boundary conditions.

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