Finite Difference Solution Methods for a System of the Nonlinear Schrödinger Equations [*]

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Abstract. This paper investigates finite difference schemes for solving a system of the nonlinear Schrödinger (NLS) equations. Several types of schemes, including explicit, implicit, Hopscotch-type and Crank-Nicholson-type are defined. Cubic spline interpolation is used for solving time-shifting part of equations. The numerical results of the different solution methods are compared using two analytical invariant properties.

Keywords: finite-difference, scheme comparison, numerical simulation, nonlinear, Schrödinger equation, second harmonics generation.

1 Introduction

The nonlinear Schrödinger (NLS) equations describe many important physical phenomena and have applications in fluid dynamics, plasma physics and nonlinear optics [1]. Recently considerable attention has been paid to the analysis of different finite difference methods for solution of the NLS equations [2]–[4]. The comparison of various methods for specific applications of the NLS equation was performed in [5]–[7].

In this paper we investigate a system of NLS equations widely used to describe the nonlinear effects of the type II second harmonics generation and optical parametrical amplification of laser pulses in a nonlinear medium [8]. The system

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consists of three nonlinear differential equations involving complex functions A_1, A_2 and A_3:

$$\frac{\partial A_1}{\partial z} + a_1 \frac{\partial A_1}{\partial t} + ib_1 \frac{\partial^2 A_1}{\partial t^2} + \frac{ic_1}{r} \frac{\partial}{\partial r}\left(r\frac{\partial A_1}{\partial r}\right) = id_1 A_2^* A_3 e^{-i\kappa z}, \qquad (1)$$

$$\frac{\partial A_2}{\partial z} + a_2 \frac{\partial A_2}{\partial t} + ib_2 \frac{\partial^2 A_2}{\partial t^2} + \frac{ic_2}{r} \frac{\partial}{\partial r}\left(r\frac{\partial A_2}{\partial r}\right) = id_2 A_1^* A_3 e^{-i\kappa z}, \qquad (2)$$

$$\frac{\partial A_3}{\partial z} + a_2 \frac{\partial A_3}{\partial t} + ib_2 \frac{\partial^2 A_3}{\partial t^2} + \frac{ic_3}{r} \frac{\partial}{\partial r}\left(r\frac{\partial A_3}{\partial r}\right) = id_3 A_1 A_2 e^{i\kappa z}. \qquad (3)$$

Here $A_l(r, t, z)$ are complex-valued functions, a_l, b_l, c_l, d_l and κ_l are real constants; l=1, 2, 3; $d_3 = d_1 + d_2$.

The system of equations (1)–(3) should be solved in a rectangular domain $Q = [0, R] \times [0, T] \times [0, Z] \subset \mathbb{R} \times \mathbb{R} \times \mathbb{R}$, where $r \in [0, R], t \in [0, T], z \in [0, Z]$, with the following initial condition:

$$A_l(r, t, z = 0) = A_l^0 \cdot e^{-\frac{r^{2S}}{w_l^{2S}}} \cdot e^{-2ln2 \cdot \frac{(t-t_l)^2}{\tau_l^2}}, \quad A_l^0 \in \mathbb{C}. \qquad (4)$$

The functions $A_l(r, t, z)$ also satisfy the following boundary conditions:

$$\begin{aligned} &A_l(r = R, t, z) = 0, \quad A_l(r, t = -\infty, z) = 0, \\ &\frac{\partial A_l(r = 0, t, z)}{\partial r} = 0, \quad A_l(r, t = +\infty, z) = 0. \end{aligned} \qquad (5)$$

Note, that the terms, containing partial derivatives by r in the equations (1)–(3), correspond to the second-order Laplacians, expressed in polar coordinates. The equations (1)–(3) do not contain the polar angle variable, because we are assuming radial symmetry. This assumption is also used in the derivation of the invariants, where all the integration in r domain is performed in polar coordinates, premultiplying all the integrated expressions by r.

The purpose of this work is to investigate four finite different schemes for solving the system of NLS equations (1)–(3) and to evaluate their performance and conservation of known analytical invariants. Some of these schemes were used to solve similar problems in [9] and we apply them to the system of equations (1)–(3) here.

The paper is organized as follows. In the next Section 2 we describe, how the presented difference schemes will be compared. Four finite difference schemes

will be introduced in Section 3. The conservation properties used for the comparison, will be presented in Section 4. Sections 5 and 6 describe the chosen model problem and the performed numerical simulation. The discussion and analysis on the obtained numerical results will be given in Section 7.

2   Comparison of finite difference methods

One of the problems when solving a system of differential equations is the large requirement on the computational resources. We can try to decrease the time of the numerical computations by decreasing the number of the grid points. But some of finite difference methods (usually explicit) have some analytical requirements on the ratio of the grid steps. If we break these requirements, or come near to their limit, the precision of the resulting solution may suffer.

In the case of the presented system of equations (1)–(3), it is difficult to derive the analytical restrictions on grid step ratios for a particular finite difference scheme. Furthermore, we do not know the precise solution of the considered system of equations. So we are comparing different finite difference schemes by performing a series of numerical experiments with different grid step sizes and comparing the invariant properties which we are able to derive analytically.

We chose to perform the comparison by using the numerical simulation of the laser pulse compression using the type II second harmonics generation phenomenon [10]. First we choose some fixed number of temporal and radial steps, required for this application. These steps will be common for all experiments. Then, we perform a series of experiments with increasing number of spatial steps. In total, four series of experiments were performed, one for each finite difference scheme: explicit, Hopscotch-type, implicit and Crank-Nicholson type. At the end we try to compare three quantitative characteristics of each finite difference scheme: computation time, total energy and the movement integral.

3   Finite difference schemes

We consider four types of finite difference schemes for the solution of the system of NLS equations (1)–(3): explicit, implicit, Hopscotch-type and Crank-Nicholson-type. First, let us introduce a uniform grid with the steps Δr, Δt and

Δz in the domain Q and the following notations on this grid:

$$\Delta r = R/N_r, \quad r_i = i\Delta r, \quad i = 0 \dots N_r, \tag{6}$$

$$\Delta t = T/N_t, \quad t_j = j\Delta t, \quad j = 0 \dots N_t, \tag{7}$$

$$\Delta z = Z/N_z, \quad z_k = k\Delta z, \quad k = 0 \dots N_z. \tag{8}$$

Let us also define the set of notations for the grid functions on two subsequent grid layers by z. All grid functions are defined equally for all functions A_1, A_2 and A_3, therefore in the following definitions we will omit the index $l = 1, 2, 3$. The index will also be omitted in constants b_l, c_l and d_l. So please keep in mind that every grid function and constant symbol denotes three different functions or constants corresponding to the equations (1)–(3).

$$p = p^{ij} = p^{ij}(z) = A_l(r_i, t_j, z), \tag{9}$$

$$p^e = p^{ij}, \quad \text{if} \quad i + j \quad \text{is an even number}, \tag{10}$$

$$p^o = p^{ij}, \quad \text{if} \quad i + j \quad \text{is an odd number}, \tag{11}$$

$$\widehat{p} = \widehat{p}^{ij} = p^{ij}(z + \Delta z), \tag{12}$$

$$p_{\bar{t}t} = \frac{p^{j+1} - 2p + p^{j-1}}{\Delta t^2}, \tag{13}$$

$$p_{\dot{r}r} = \frac{r_{i+\frac{1}{2}}(p^{i+1} - p) - r_{i-\frac{1}{2}}(p - p^{i-1})}{\Delta r^2}, \tag{14}$$

$$\varphi = \varphi^{ij} = \varphi_l\big(A_1(r_i, t_j, z), A_2(r_i, t_j, z), A_3(r_i, t_j, z)\big). \tag{15}$$

Here φ_l are nonlinear functions, representing the nonlinear terms of the l-th equation:

$$\varphi_1 = A_2^* A_3 e^{-i\kappa z}, \quad \varphi_2 = A_1^* A_3 e^{-i\kappa z}, \quad \varphi_3 = A_1 A_2 e^{i\kappa z}. \tag{16}$$

We will also need grid functions on the intermediate layer: $\widetilde{p} = \widetilde{p}^{ij} = p^{ij}(z + \Delta z/2)$.

When defining the finite difference schemes for the solution of the system of NLS equations (1)–(3), we will replace differential operators of the equations by the corresponding finite-difference approximations, except the term with the first derivative by t: $a_l\frac{\partial A_l}{\partial t}$.

The terms $a_l\frac{\partial A_l}{\partial t}$ represent the time-shifting components of the equations (1)–(3). Many implementations of the NLS equation solvers use the fast Fourier

transform (FFT) to solve the time-shifting equation $\frac{\partial A}{\partial z} + a\frac{\partial A}{\partial t} = 0$. We found that FFT method does not work well when combined with some finite difference schemes [10]. Instead of FFT, we chose to approximate the time-shifting using a the cubic spline interpolation [11]. To incorporate the time-shifting component into the solution of the system of equations (1)–(3), we will perform cubic spline interpolation after each step of finite-difference calculations.

3.1 Explicit finite difference scheme

We will consider the following explicit finite-difference scheme:

$$\frac{\widehat{p} - p}{\Delta z} + ibp_{\bar{t}t} + \frac{ic}{r}p_{\dot{r}r} = id\varphi. \tag{17}$$

When applying this scheme to the system of equations, we compute the values of the grid functions $\widehat{p}$ on the next layer by z using the values of the grid functions p which are already known.

3.2 Implicit finite difference scheme

The implicit scheme looks quite similar:

$$\frac{\widehat{p} - p}{\Delta z} + ib\widehat{p}_{\bar{t}t} + \frac{ic}{r}\widehat{p}_{\dot{r}r} = id\widehat{\varphi}. \tag{18}$$

To compute the values of the grid functions $\widehat{p}$, we need to solve a system of nonlinear equations, because the grid functions $\widehat{p}$ are used as arguments of the nonlinear functions $\widehat{\varphi}$.

3.3 Crank-Nicholson-type scheme

The Crank-Nicholson-type scheme is also an implicit finite difference scheme which uses the average approximations compared to the simple implicit scheme (18):

$$\frac{\widehat{p} - p}{\Delta z} + \frac{ib}{2}(\widehat{p}_{\bar{t}t} + p_{\bar{t}t}) + \frac{ic}{2r}(\widehat{p}_{\dot{r}r} + p_{\dot{r}r}) = \frac{id}{2}(\widehat{\varphi} + \varphi). \tag{19}$$

3.4 Hopscotch-type scheme

Hopscotch-type difference scheme splits the computation of new values into four steps:

$$2\frac{\widetilde{p}^e - p^e}{\Delta z} + ibp_{\bar{t}t}^e + \frac{ic}{r}p_{\dot{r}r}^e = id\varphi^e, \tag{20}$$

$$2\frac{\widetilde{p}^o - p^o}{\Delta z} + ib\widetilde{p}_{\bar{t}t}^o + \frac{ic}{r}\widetilde{p}_{\dot{r}r}^o = id\widetilde{\varphi}^o, \tag{21}$$

$$2\frac{\widehat{p}^o - \widetilde{p}^o}{\Delta z} + ib\widetilde{p}_{\bar{t}t}^o + \frac{ic}{r}\widetilde{p}_{\dot{r}r}^o = id\widetilde{\varphi}^o, \tag{22}$$

$$2\frac{\widehat{p}^e - \widetilde{p}^e}{\Delta z} + ib\widehat{p}_{\bar{t}t}^e + \frac{ic}{r}\widehat{p}_{\dot{r}r}^e = id\widehat{\varphi}^e. \tag{23}$$

According this scheme, even and odd grid points are computed separately. First, using known values of p, the values at even grid points on the intermediate layer ($\widetilde{p}^e$) are computed. This system of difference equations (20) is explicit, since it uses only the known values on the previous layer p and the grid function $\widetilde{p}$ occurs only in linear expressions. After solving this system of equations, we know all the even values and the values on the border of the intermediate layer $\widetilde{p}$.

The second system of difference equation (21) defines the way the odd grid points $\widetilde{p}^o$ are computed using odd points of the lower layer and already known even points of the intermediate layer. Here we have to solve the system of non-linear equations with three variables, because the unknown variables occur in nonlinear expressions φ. We solve this system of equations using the method of simple iterations.

The third and the fourth system of difference equations are used to compute grid points of the upper layer ($\widehat{p}$). They are equivalent to the first ones with the exception to the order the grid points are computed: first the odd and then the even ones.

Let us note that the finite difference scheme (20–23) leaves out the approximation of the time-shifting terms $a_l\frac{\partial A_l}{\partial t}$. So we should keep in mind that after the numerical application of each of the steps (20–23) we should perform the approximation of the time-shifting terms.

4   Analytical invariants

Now that we have described different solution methods, let us define the analytical invariants which will be used for comparison of these methods.

4.1   Total energy conservation law

Energy conservation law can be obtained from the system of differential equations (1)–(3). First we multiply every l'th equation by the corresponding conjugate function A_l^*, then add the corresponding conjugate equation multiplied by A_l. Then, by adding three resulting equations and integrating the sum in the following domain: $r \in [0, R]$, $t \in [-\infty, \infty]$, polar angle $\in [0, 2\pi]$, we get the expressions which are constant for all values of z. Let us denote: $I_l = \int\limits_{-\infty}^{\infty} \int\limits_{0}^{R} |A_l|^2 r\,dr\,dt$. Then we get the following total energy conservation law:

$$I = I_1 + I_2 + I_3 = const. \tag{24}$$

4.2   The movement integral

The movement integral can be obtained performing similar procedures to those used to get energy conservation law. If we multiply every l'th equation by the corresponding conjugate function's first derivative by $t \, \frac{\partial A_l^*}{\partial t}$ and then add the corresponding conjugate equation multiplied by $\frac{\partial A_l}{\partial t}$, then after integration we get the following invariant:

$$J = \int\limits_{-\infty}^{\infty} \int\limits_{0}^{R} \sum_l \left(\frac{|A_l|^2}{d_l} \frac{\partial \phi_l}{\partial t} \right) r\,dr\,dt = const. \tag{25}$$

Here ϕ_l is an argument of the complex function: $A_l = |A_l| e^{i\phi_l}$. Also note that for real-valued initial conditions (4), $const = 0$.

5   The model problem

To see how the precision of the particular method depends on the grid steps, we chose to perform a numerical simulation of the second harmonic generation using

ultrashort laser pulses with inter-pulse delay (see [10]). The following parameters in equations (1)–(3) correspond to this particular model problem:

$$
\begin{aligned}
&a_1 = 1.02665, &&a_2 = 1.0, &&a_3 = 1.01544, \\
&b_1 = 1.1455 \cdot 10^{-6}, &&b_2 = -1.148 \cdot 10^{-6}, &&b_3 = -6.9125 \cdot 10^{-6}, \\
&c_1 = -2.83146 \cdot 10^{-8}, &&c_2 = -2.89722 \cdot 10^{-8}, &&c_3 = -1.43866 \cdot 10^{-8}, \\
&d_1 = 0.2425, &&d_2 = 0.2481, &&d_3 = 0.4906, \\
&\kappa = 0.0.
\end{aligned}
$$

The initial values (4) were chosen as follows:

$$
\begin{aligned}
&A_1^0 = 0.3, &&A_2^0 = 0.3, &&A_3^0 = 0.0, \\
&t_1 = 2.0, &&t_2 = 2.7, &&t_3 = 2.7, \\
&\tau_1 = 1.0, &&\tau_2 = 1.0, &&\tau_3 = 1.0, \\
&w_1 = 0.3, &&w_2 = 0.3, &&w_3 = 0.3, \\
&S = 2.
\end{aligned}
$$

6 Results of the numerical simulation

The finite domain with the upper ranges $R = 1.0$, $T = 40.0$ and $Z = 40.0$ was used (see definitions (6)–(8)). Since the functions with the initial condition (4) form Gaussian-like structures, their absolute values outside some range $[T_0, T_N]$ are very small and do not need to be taken into account. Therefore we do the computations only in a fixed-sized range: $T_N - T_0 = 5.0$ and we shift that range $[T_0, T_N]$ accordingly when moving to the next step by z. Thus when computing we use the following temporal step:

$$
\Delta t' = (T_N - T_0)/N_t', \quad t_j' = T_0 + k\Delta z + j\Delta t', \quad j = 0 \ldots N_t'. \tag{26}
$$

The radial and temporal step numbers of the performed simulations were chosen accordingly $N_r = 100$ and $N_t' = 1000$. These were the minimum numbers to be able to analyze the obtained solution of the particular application (the compressed pulse). The simulation was performed along the spatial axis z. For every differential scheme we performed 6 experiments with different number

of steps along the axis z: with $N_z = 200$, $N_z = 400$, $N_z = 600$, $N_z = 1000$, $N_z = 2000$ and $N_z = 4000$. Figs. 1–4 show the conservation of the total energy and the movement integral for each finite-difference method.
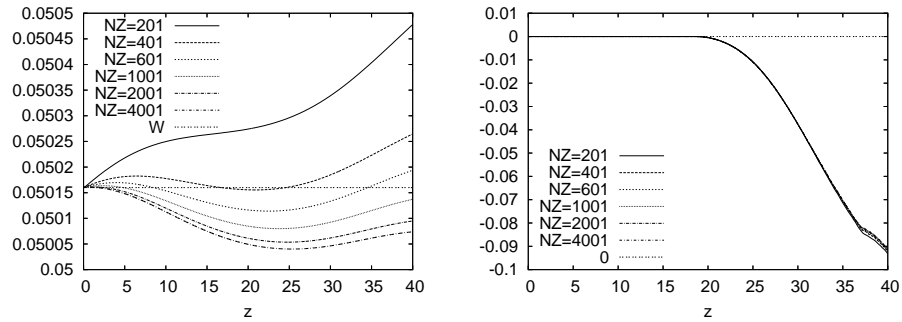

Fig. 1. Explicit finite difference method: total energy (left) and movement integral (right) with different step numbers.
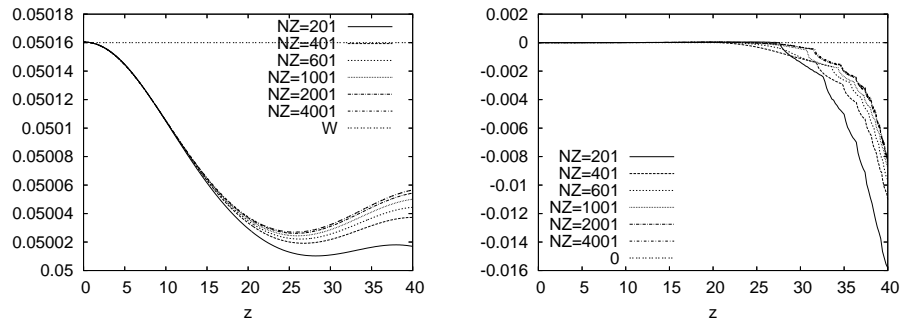

Fig. 2. Hopscotch-type finite difference method: total energy (left) and movement integral (right) with different step numbers.

Although the number of grid points between the different experiment series was equal, there were also huge differences in computation times required to perform the computations. Table 1 shows the computation time in seconds for each performed experiment. The computations were performed on a 2.4 MHz, Intel Pentium 4 processor based workstation. The algorithm for solution of the equations was programmed in programming language C++ using Blitz [12] – a library for arrays in C++.
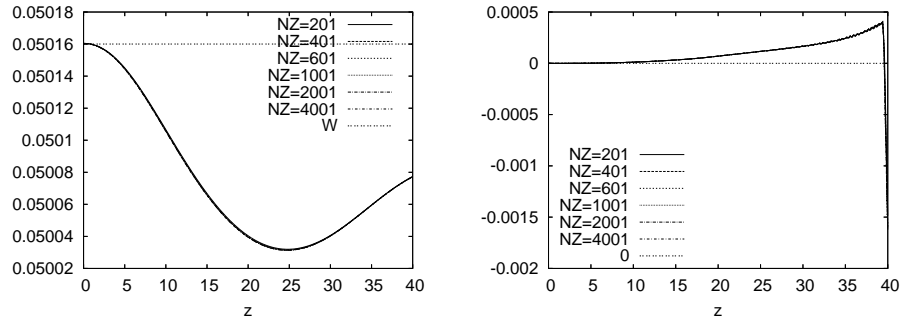
255

Fig. 3. Crank-Nicholson-type finite difference method: total energy (left) and movement integral (right) with different step numbers.
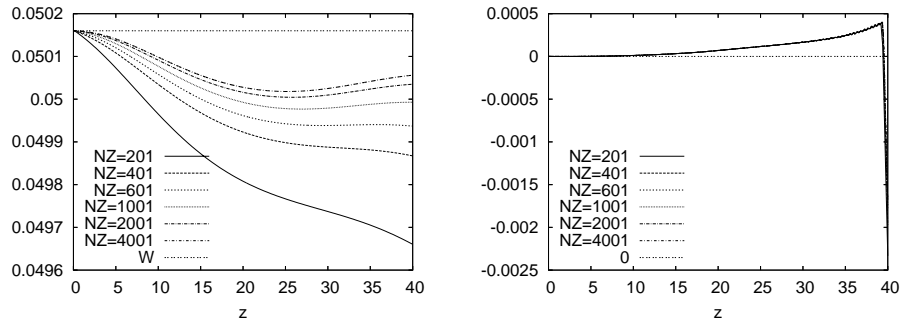

Fig. 4. Implicit finite difference method: total energy (left) and movement integral (right) with different step numbers.

7 Analysis and discussion

According to the data in Table 1, the explicit finite-difference method is the fastest method for the solution of the system of equations (1)–(3). Its drawback is that it has the worst conservation of the movement integral (Fig. 1, right) in comparison with all other methods in consideration. The conservation of total energy is also not very good at low number of grid points, but it gets better at higher numbers (Fig. 1, left).

The Hopscotch-type finite difference method is a mixed method. It uses both explicit and implicit steps in the computation process. Therefore it is slightly more computationally-intensive than the explicit method. But it conserves the total energy and the movement integral much better (Fig. 2). With the high numbers

Table 1. Computation times in seconds

N_z	Explicit	Hopscotch	Crank-Nicholson	Implicit
200	903	1483	6622	4691
400	1805	2893	9952	7082
600	2722	4241	13571	9261
1000	4610	6723	19335	13719
2000	9171	11838	35793	23783
4000	18300	23117	60263	43341

of grid points ($NZ = 4000$) it even comes near to the precision of the implicit methods (Figs. 3 and 4).

The computations using the Crank-Nicholson finite difference scheme are most computationally intensive, but they are also most precise according both considered invariants. They are equally conserved even at the lowest values of the grid point numbers (Fig. 3).

The implicit-type method is faster than the Crank-Nicholson-type. But when decreasing number of grid points, the solution starts to lose its total energy (Fig. 4, left).

8 Conclusions

As the summary of the characteristics of the considered difference schemes we can say that:

- Methods which use explicit computations (explicit and Hopscotch-type) are generally faster, but provide considerably worse precision for our particular application. Because of their speed they could be successfully used for proto-typing and testing of the simulation programs. The fastest one is the explicit method.

- If the precision is of major concern, the implicit methods should be used. The Crank-Nicholson-type method is the most precise one.

- The other two methods (Hopscotch and implicit) can be recommended for other cases with special requirements. They are in the middle according to the precision and speed scale.

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