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СИМВОЛЬНОЕ И ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ РАЗНОСТНЫХ СХЕМ С ИСПОЛЬЗОВАНИЕМ ПЕРВОГО ДИФФЕРЕНЦИАЛЬНОГО ПРИБЛИЖЕНИЯ НА ПРИМЕРЕ УРАВНЕНИЯ КОТРЕВЕГА ДЕ ВРИЗА

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SYMBOLIC AND NUMERICAL INVESTIGATION OF FINITE DIFFERENCE SCHEMES USING THE FIRST DIFFERENTIAL APPROXIMATION: THE CASE OF THE KORTEWEG-DE VRIES EQUATION

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Аннотация. В работе проводится символьное и численное исследование разностных схем для уравнения Кортвега де Вриза с использованием первого дифференциального приближения (FDA). Основное внимание уделено качественному анализу разностных схем, аналогичных схеме Кранка–Николсона, и оценке их невязки. Предложены критерии выбора шагов по времени и пространству для численных расчетов, что позволяет улучшить точность и эффективность вычислений.

Рассматриваются одно- и двух-солитонные решения уравнения КДВ, а также исследуются две разностные схемы второго и четвертого порядка точности. Показано, что выбор допустимого упорядочения при построении FDA влияет на объем вычислений и компактность результата.

Предложен интегральный метод оценки погрешности разностных схем, основанный на вычислении FDA, что позволяет оценить глобальную погрешность при проведения вычислительных экспериментов. Результаты подтверждены численными расчетами для одно- и двух-солитонных решений, демонстрирующими хорошее качественное совпадение глобальной ошибки с ошибкой, вычисленной с помощью FDA.

Результаты работы могут быть полезны для повышения точности и эффективности численных методов решения нелинейных уравнений в частных производных.

Ключевые слова: разностные схемы, первое дифференциальное приближение, уравнения Котревега де Вриза, компьютерная алгебра, базисы Грёбнера.

Abstract. The paper presents a symbolic and numerical investigation of finite difference

schemes for the Korteweg-de Vries (KdV) equation using the first differential approximation (FDA). The main focus is on the qualitative analysis of finite difference schemes similar to the Crank–Nicolson scheme and the evaluation of their residual errors. Criteria for selecting time and space steps for numerical calculations are proposed, which improve the accuracy and efficiency of computations.

The method of differential approximations, introduced by N. N. Yanenko and Yu. I. Shokin, is used to analyze the properties of finite difference schemes through the approximation of the original differential equations. The paper considers one- and two-soliton solutions of the KdV equation and investigates two finite difference schemes of second and fourth-order accuracy. It is shown that the choice of ordering in the construction of the FDA affects the volume of computations and the compactness of the result.

An integral method for estimating the error of finite difference schemes based on the computation of the FDA is proposed, which allows for the evaluation of the global error without conducting computational experiments. The results are confirmed by numerical calculations for one- and two-soliton solutions, demonstrating good qualitative agreement between the global error and the error computed using the FDA.

The results of this work can be useful for improving the accuracy and efficiency of numerical methods for solving nonlinear partial differential equations.

Keywords difference schemes, first-order differential approximation, Korteweg-de Vries equations, computer algebra, Gröbner bases.

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Introduction

In the article [1], a qualitative study of finite difference schemes of the Crank–Nicolson type for the Korteweg-de Vries (KdV) equation is conducted using the first

differential approximation (FDA). The main goal of the work is to evaluate the residual error of the method and propose criteria for selecting time and space steps for numerical calculations.

The method of differential approximations, proposed by N. N. Yanenko and Yu. I. Shokin [2, 3, 4], allows for the investigation of the properties of finite difference schemes through the analysis of differential equations approximating the original problem.

Currently, for partial differential equations of evolutionary type, and in particular for the KdV equation, the use of computer algebra systems has been considered in [5], and for the Navier–Stokes equations in [6].

In [7], the FDA for finite difference schemes describing ordinary differential equations is considered. The connection between the singular perturbation of the original system and the concept of FDA is discussed. The issues of computing FDA in computer algebra systems, Sage and SymPy, are also considered.

In [1], the propagation of waves in nonlinear media is considered for the KdV equation, along with its one- and two-soliton solutions. Two finite difference schemes of second and fourth-order accuracy, similar to the Crank–Nicolson scheme for the heat equation, are investigated. The construction of the FDA is performed using computer algebra systems (SymPy), which allows for the verification of the consistency of the finite difference schemes and the original differential equations. It is shown that the choice of ordering in the construction of the FDA affects the volume of computations and the compactness of the result. Numerical calculations for one- and two-soliton solutions confirm the theoretical conclusions. It is shown that as the parameter k increases, it is necessary to reduce the time and space steps.

The application of the FDA allows for both qualitative and quantitative investigation of finite difference schemes, and the choice of ordering reduces the volume of computations. The results are confirmed by numerical experiments for soliton solutions of the KdV equation.

The main idea of this method is to replace the study of the properties of a finite difference scheme with the study of a problem involving differential equations that occupy an intermediate position between the original differential problem and the approximating finite difference scheme.

In this work, using the results of [1], an integral method for estimating the error of finite difference schemes is proposed. This allows for the use of the local error provided by the computation of the FDA to obtain an estimate of the global error of the finite difference scheme.

1. First Differential Approximation

The Korteweg-de Vries equation [8] is one of the main tools in the theory of nonlinear waves and is used to model various physical phenomena, such as the propagation of sound waves, surface water waves, and plasma waves.

$$u_t + 6uu_x + u_{xxx} = 0 \tag{1}$$

One- and two-soliton solutions of the Korteweg-de Vries equation are solutions that describe the propagation of waves in nonlinear media. The one-soliton solution (2) represents a traveling wave $\xi = k(x-4k^2t)$, depending on the parameter k, which propagates without changing its shape and amplitude [9]:

$$u = \frac{2k^2}{\cosh^2 \xi} \tag{2}$$

The two-soliton solution (3) describes the interaction of two waves $\xi_1 = k_1(x-4k_1^2t)$ and $\xi_2 = k_2(x-4k_2^2t)$, depending on the parameters k_1 and k_2, in which they retain their shape and amplitude during further motion [9, p. 294]:

$$u = \frac{\left(8k_1^2 - 8k_2^2\right)\left(k_1^2 \cosh^2 \xi_2 + k_2^2 \sinh^2 \xi_1\right)}{\left((k_1 - k_2)\cosh(\xi_1 + \xi_2) + (k_1 + k_2)\cosh(\xi_1 - \xi_2)\right)^2} \tag{3}$$

In this work, two schemes similar to the Crank–Nicolson scheme [10] for the heat equation will be investigated. The following second-order scheme in h is considered in [5]:

$$\begin{aligned} &\frac{u_j^{n+1} - u_j^n}{\tau} + \frac{3}{4h}\left(\left(u^{2\,n+1}_{j+1} - u^{2\,n+1}_{j-1}\right) + \left(u^{2\,n}_{j+1} - u^{2\,n}_{j-1}\right)\right) + \\ &+ \frac{1}{4h^3}\left(\left(u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + 2u_{j-1}^{n+1} - u_{j-2}^{n+1}\right) + \right. \\ &\left. + \left(u_{j+2}^{n} - 2u_{j}^{n+1} + 2u_{j-1}^{n} - u_{j-2}^{n}\right)\right) = 0. \end{aligned} \tag{4}$$

The finite difference scheme (4) has an order of $O(\tau^2, h^2)$. We also consider a higher-order scheme $O(\tau^2, h^4)$:

$$\begin{aligned} &\frac{u_j^{n+1} - u_j^n}{\tau} - \frac{3}{24h}\left(\left(u^{2\,n+1}_{j+2} - 8u^{2\,n+1}_{j+1} + 8u^{2\,n+1}_{j-1} - u^{2\,n+1}_{j-2}\right) + \right. \\ &\left. + \left(u^{2\,n}_{j+2} - 8u^{2\,n}_{j+1} + 8u^{2\,n}_{j-1} - u^{2\,n}_{j-2}\right)\right) + \\ &- \frac{1}{16h^3}\left(\left(u_{j+3}^{n+1} - 8u_{j+2}^{n+1} + 13u_{j+1}^{n+1} - 13u_{j-1}^{n+1} + 8u_{j-2}^{n+1} - u_{j-3}^{n+1}\right) + \right. \\ &\left. \left(u_{j+3}^{n} - 8u_{j+2}^{n} + 13u_{j+1}^{n} - 13u_{j-1}^{n} + 8u_{j-2}^{n} - u_{j-3}^{n}\right)\right) = 0 \end{aligned} \tag{5}$$

The construction of the first differential approximation (FDA) is based on algebraic operations and can be effectively implemented using computer algebra systems [12, 13, 14]. If the finite difference scheme is inconsistent or has a smaller solution space compared to the original system of differential equations, then extra equations will be obtained during the construction of the FDA, which allows for stopping the computations. This check is simpler and requires fewer resources than checking consistency in the finite difference case.

The paper proposes the use of the Gröbner basis algorithm [15, 16] to verify the consistency of the original system of differential equations and the approximating finite difference scheme, both directly and through the FDA. Although the Gröbner algorithm is built into most computer algebra systems, it has limitations when working with differential equations, finite difference schemes, and formally infinite Taylor series required for the FDA.

The author's program is implemented in the SymPy system (https://www.sympy.org) and is available for download at https://github.com/blinkovua/sharing-blinkov/blob/master/KDV. Algorithmically, the construction of the FDA using Gröbner bases can be represented as working with an infinite module, where ordering is first performed by dependent variables and then by independent variables *POT* (*position over term* — ordering first by dependent variables and then by independent variables). In this case, the computations are performed up to the first non-zero terms of the series in time steps τ and space steps h.

The FDA for the finite difference scheme (4) in the *degrevlex* ordering takes the following form:

$$6uu_x + u_t + u_{xxx} + h^2\left(3u^2u_x + \frac{uu_t}{2} - \frac{u_{txx}}{4} - \frac{3u_{xx}u_x}{2}\right) + \\ + \tau^2\left(-\frac{u_{ttt}}{12}\right) + \ldots = 0. \tag{6}$$

For further use, we introduce the following notation:

$$\mathrm{FDA} = h^2\left(3u^2u_x + \frac{uu_t}{2} - \frac{u_{txx}}{4} - \frac{3u_{xx}u_x}{2}\right) + \\ + \tau^2\left(-\frac{u_{ttt}}{12}\right) = \mathrm{FDA}_{h^2} + \mathrm{FDA}_{\tau^2}. \tag{7}$$

For the scheme (5) in the same ordering:

$$6uu_x + u_t + u_{xxx} + h^4\left(\frac{27u^3u_x}{5} + \frac{9u^2u_t}{10} - \frac{uu_{txx}}{2} - \frac{81uu_{xx}u_x}{5} - \right.$$
$$\left. - \frac{7u_{ttx}}{120} - \frac{29u_{tx}u_x}{20} - \frac{37u_tu_{xx}}{20} - \frac{9u_x^3}{2}\right) + \tau^2\left(-\frac{u_{ttt}}{12}\right) + \ldots = 0. \quad (8)$$

Similarly, we introduce the following notation:

$$\mathrm{FDA} = h^4\left(\frac{27u^3u_x}{5} + \frac{9u^2u_t}{10} - \frac{uu_{txx}}{2} - \frac{81uu_{xx}u_x}{5} - \frac{7u_{ttx}}{120} - \right.$$
$$\left. - \frac{29u_{tx}u_x}{20} - \frac{37u_tu_{xx}}{20} - \frac{9u_x^3}{2}\right) + \tau^2\left(-\frac{u_{ttt}}{12}\right) = \mathrm{FDA}_{h^4} + \mathrm{FDA}_{\tau^2}. \quad (9)$$

Checking the FDA on exact solutions allows for the evaluation of the accuracy of the numerical scheme without programming and conducting computational experiments [1]. Substituting the exact solution into the FDA shows that the residual error of the scheme depends on the grid steps h and τ, as well as on the parameter k.

Substituting the exact solution (2) into the FDA (4) yields the following form of the FDA:

$$h^2\left(8k^7\left(\tanh\xi - 1\right)\left(\tanh\xi + 1\right)\times\right.$$
$$\times\left(15\tanh^4\xi - 16\tanh^2\xi + 3\right)\tanh\xi\left.\right) + \tau^2\left(-256k^{11}\left(\tanh\xi - 1\right)\times\right. \quad (10)$$
$$\left.\times\left(\tanh\xi + 1\right)\left(3\tanh^2\xi - 2\right)\tanh\xi/3\right) + \ldots = 0$$

Substituting the exact solution (2) into the FDA (5), the term with τ^2 coincides with the corresponding term in (10), while the term with h^4 takes the following form:

$$-32k^9\left(\tanh\xi - 1\right)\left(\tanh\xi + 1\right)\left(945\tanh^6\xi - 1800\tanh^4\xi + \right.$$
$$\left. + 1014\tanh^2\xi - 152\right)\tanh\xi/15 \quad (11)$$

The analysis of the residual error for the one-soliton solution (2) for formulas (10) and (11) showed [1] that for $0 < k < 1$, the error depends more on the step h, while for $k > 1$, it depends more on the step τ. For the scheme (4), the residual error is of the form $O(\tau^2k^{11}, h^2k^7)$, while for the scheme (5), it is of the form $O(\tau^2k^{11}, h^2k^9)$.

Substituting the two-soliton solution (3) into the FDA leads to complex symbolic expressions, making analysis difficult. It can be assumed that the constraints obtained for the one-soliton solution remain valid for the two-soliton case.

Thus, the FDA allows for the effective evaluation of the accuracy of numerical schemes based on exact solutions, even for complex nonlinear problems.

2. Accumulation Function for Estimating Global Error

The error accumulates at each time step since the finite difference scheme approximates the original system of differential equations with an accuracy up to the FDA. Thus, the FDA defines the local error. To estimate the global error, the following accumulation function can be proposed, which characterizes the growth of the error over time steps:

$$\mathrm{acc}_{t_i} = \mathrm{acc}_{t_{i-1}} + \frac{1}{2}\left(1 + \frac{\|\mathrm{FDA}(t_{i-1})\|}{\|\mathrm{FDA}(t_i)\|}\right)(t_i - t_{i-1}). \qquad (12)$$

In formula (12), the additional term represents the numerical value of the integral using the trapezoidal method, normalized by the value $\|FDA(t_i)\|$:

$$\frac{1}{2}\left(\|\mathrm{FDA}(t_i)\| + \|\mathrm{FDA}(t_{i-1})\|\right)(t_i - t_{i-1}).$$

Using the values from formula (12), we can write the function for the upper estimate of the global error at the i-th step as:

$$\mathrm{error}_{\mathrm{FDA}}(x, t_i) = \mathrm{acc}_{t_i}\mathrm{FDA}(x, t_i) \qquad (13)$$

The program for numerical experiments is implemented in the open-source packages SciPy (https://scipy.org) and Matplotlib (https://matplotlib.org/) and can be downloaded at https://github.com/blinkovua/sharing-blinkov/blob/master/KDV.

When performing calculations using both finite difference schemes (4) and (5), the boundary conditions $u_x = 0$ were set. Since the schemes are nonlinear with respect to the next time layer, the system of nonlinear equations was solved using the simple iteration method. The number of iterations until the difference in iterations reached the Frobenius norm of 10^{-12} did not exceed 3.

Figures 1 and 2 show the calculations for the exact solution (2) with $k = 0.2$, $h = 0.25$, and $\tau = 1.0h$ using both finite difference schemes (4) and (5). The notations FDA, $\mathrm{FDA}_{FDA\tau^2}$, FDA_{h^2} for the finite difference scheme (4) and FDA_{h^4} exactly correspond to the notations (7) and (9).

These were computed numerically using formulas (10) and (11), respectively. The additional label "numeric" indicates calculations using formulas (6) and (8), applying numerical differentiation formulas using 5 time layers to compute u_{ttt}.

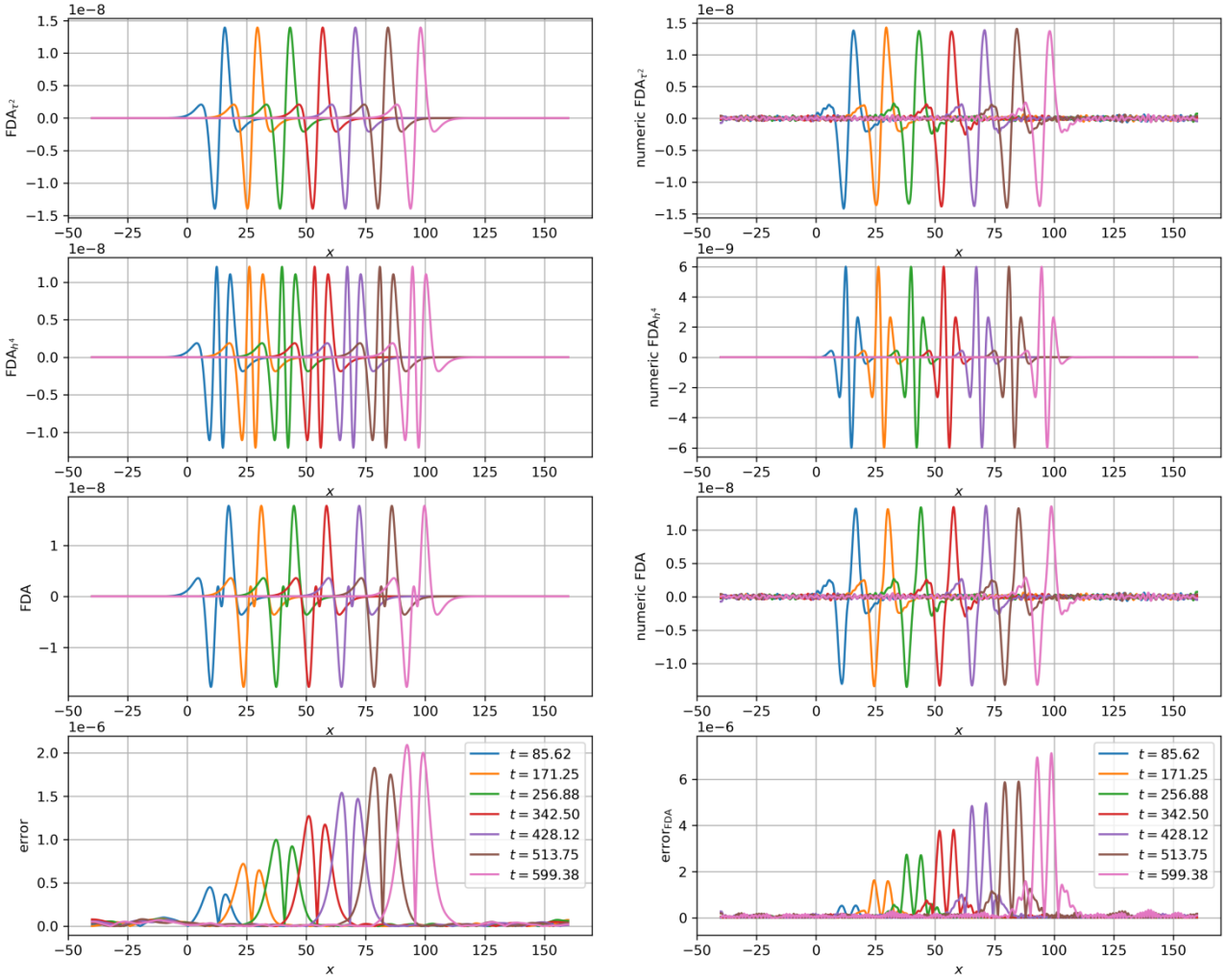

Fig. 1

The notations "error" indicate the relative error. Let u denote the numerical solution and $\bar{u}$ denote the exact solution, then:

$$\begin{aligned} \text{error}(x,t_i) &= \frac{|\bar{u}(x,t_i)-u(x,t_i)|}{1+|u(x,t_i)|} \\ \text{error}_{FDA}(x,t_i) &= \frac{|\text{acc}_{t_i}\text{FDA}(x,t_i)|}{1+|u(x,t_i)|} \end{aligned} \qquad (1)$$

The analysis of numerical experiments in Figures 1 and 2 shows that numerical differentiation yields results that agree well with symbolic computations on the exact solution. When the time and space steps are significantly reduced, small oscillations may occur, which is explained by the number of digits for floating-point operations and rounding errors. Since numerical differentiation operations are defined through the difference of close values, the error in floating-point computations is greatest in these cases.

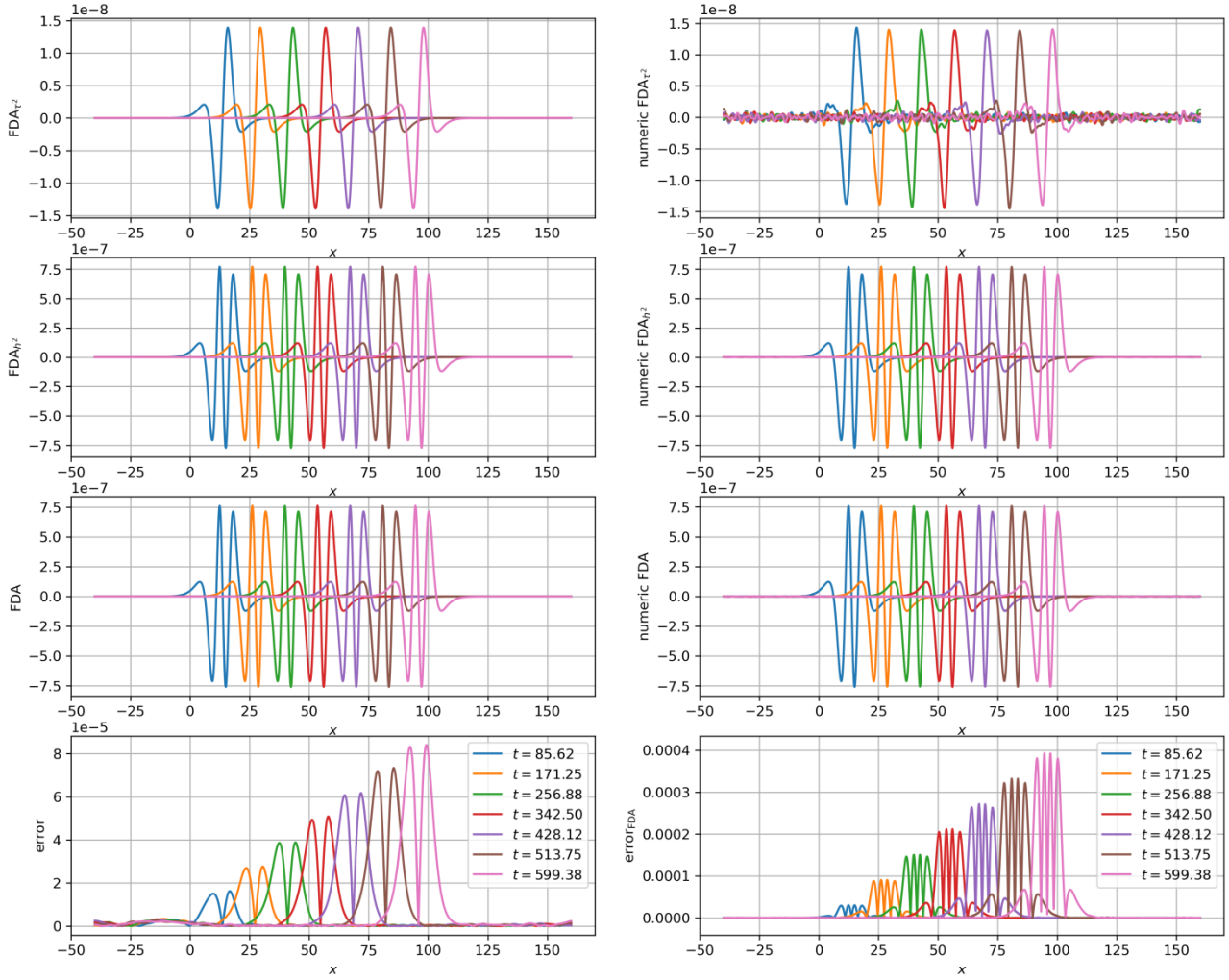

Fig. 2

Figures 3a and 3b show the calculations for the exact solution (3) with $k_1 = 0.5$, $k_2 = 0.2$, $h = 0.25$, and $\tau = 1.0h$ using both finite difference schemes (4) and (5). The notations in Figures 3a and 3b repeat those in Figures 1 and 2.

The results presented in Figures 3a, 3b, 1, and 2 allow us to conclude that there is good qualitative agreement between the global error and the error computed using the FDA and the accumulation function (12). Moreover, the error computed using the FDA and the accumulation function (12) provides an upper bound for the global error. This allows the FDA to be used for the effective selection of time and space steps depending on the problem parameters, as well as for the effective control of computational accuracy.

The results presented in Figures 4a and 4b for the exact solution (2) with $k = 0.2$, $h = 0.25$, and various ratios of τ and h using both finite difference schemes (4) and (5) demonstrate good qualitative behavior. In Figure 4b for scheme (5), with a small ratio of τ and h, a sharp increase in computational accuracy is observed for sufficiently large h. This is related to the high order h^4 of the finite difference scheme (5).

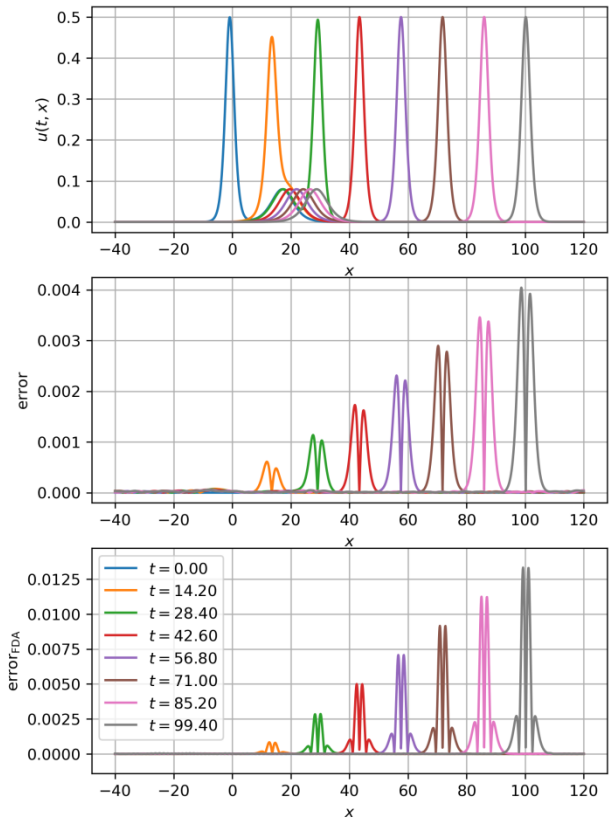

Fig. 2a

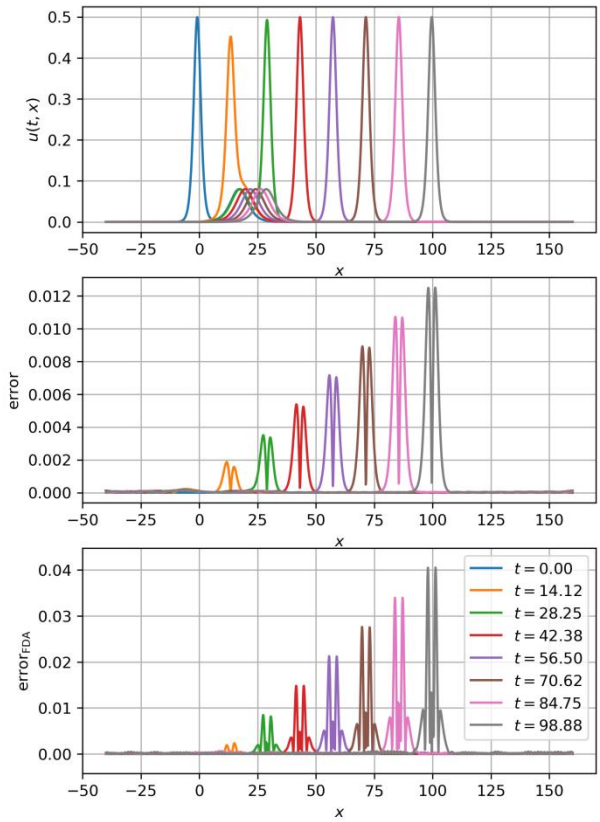

Fig. 2b

"Calculation time" denotes the computation time and allows us to conclude the optimality of computations for the chosen k with $1 \le \tau/h \le 2$, both in terms of computation volume and required accuracy.

The results presented in Figures 5a and 5b for the exact solution (3) with $k_1 = 0.5$, $k_2 = 0.2$, $h = 0.25$, and various ratios of τ and h using both finite difference schemes (4) and (5) demonstrate behavior similar to that in Figures 4a and 4b.

"Calculation time" allows us to conclude the optimality of computations for the chosen k with $1.2 \le \tau/h \le 1$, both in terms of computation volume and required accuracy. This is related to the larger value of $k_1 = 0.5$ compared to $k = 0.2$ and fully corresponds to the conclusions drawn in [1] based on formulas (10) and (11).

Conclusion

The application of the first differential approximation allows for qualitative and, in some cases, quantitative investigation of finite difference schemes. By choosing the ordering in the construction of the first differential approximation, it is possible to significantly reduce the volume of symbolic computations and obtain a more compact form containing derivatives of much lower order. Using the example of Crank–Nicolson-type finite difference schemes for the Korteweg-de Vries equation, it was possible not only to conduct an analytical investigation of the

applicability of soliton solutions depending on the parameters but also to use the compact form for numerical computations.

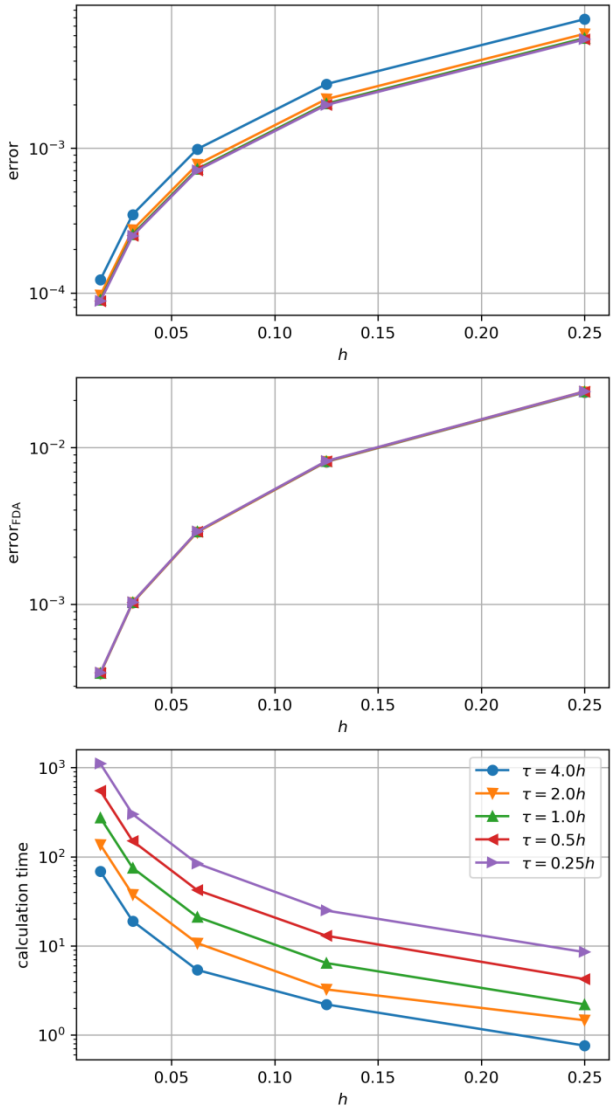

Fig. 3a

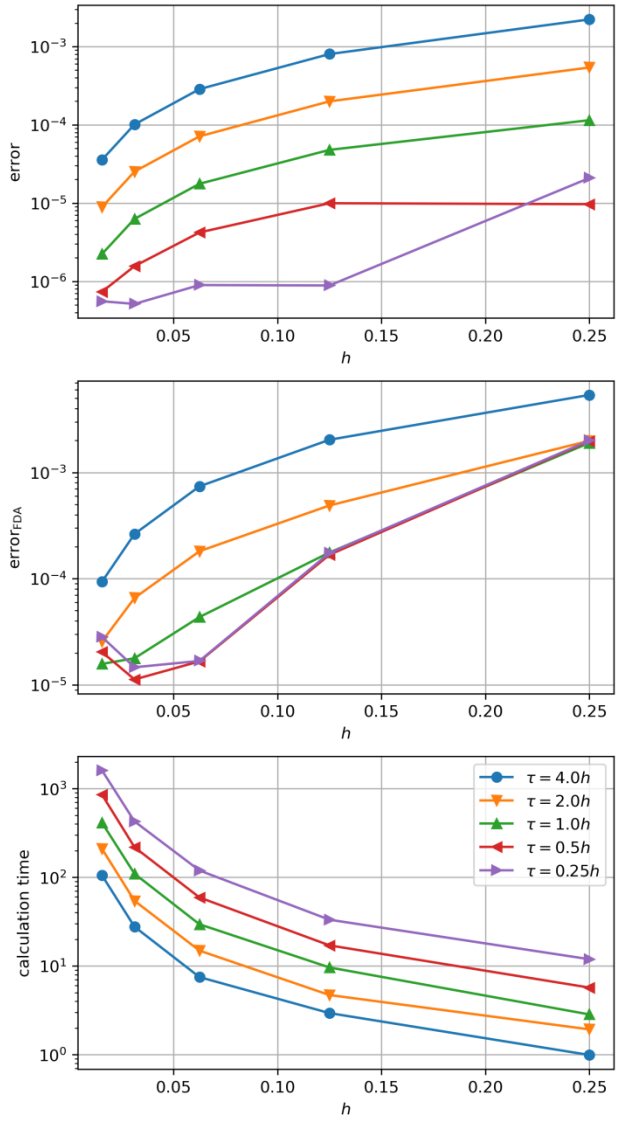

Fig. 3b

The analysis of numerical experiments shows that numerical differentiation yields results that agree well with symbolic computations on the exact solution. When the time and space steps are significantly reduced, small oscillations may occur, which is explained by the number of digits for floating-point operations and rounding errors. Since numerical differentiation operations are defined through the difference of close values, the error in floating-point computations is greatest in these cases.

The results allow us to conclude that there is good qualitative agreement between the global error and the error computed using the FDA and the accumulation function. Moreover, the error computed using the FDA and the accumulation function provides an upper bound for the global error. This allows the FDA to be used for the effective selection of time and space steps depending on the problem parameters, as well as for the effective control of computational accuracy.

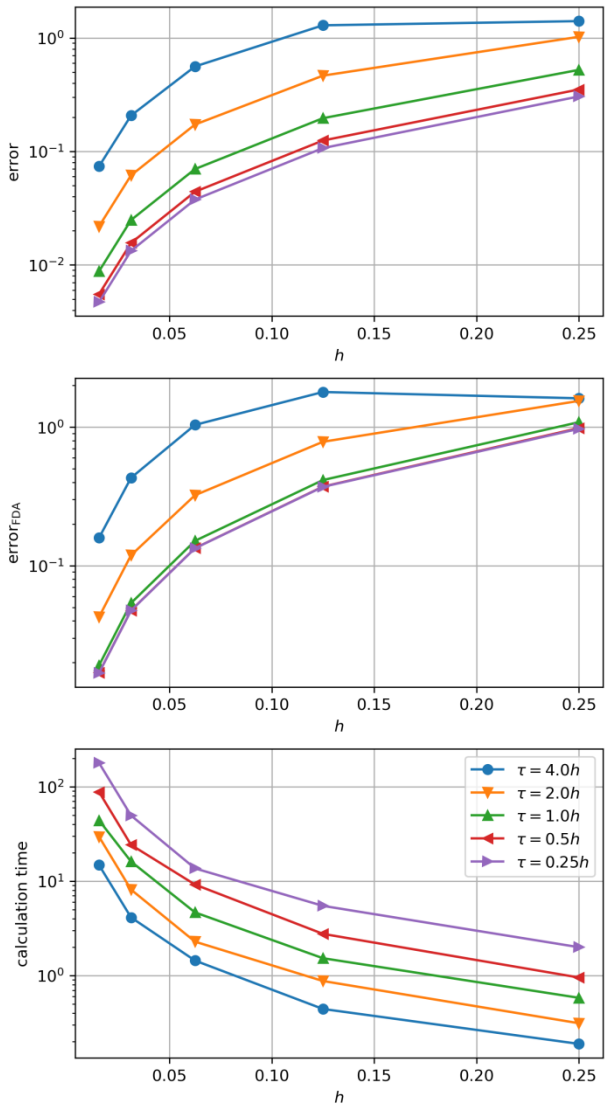

Fig. 4a

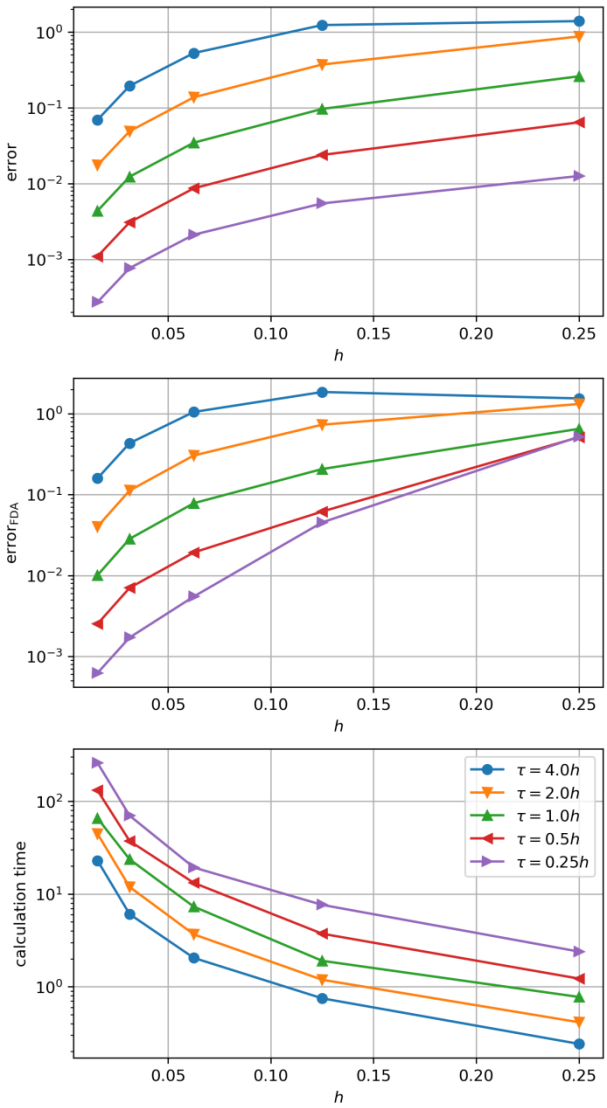

Fig. 4b

The results are confirmed by numerical calculations for one- and two-soliton solutions.

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