Compact first-order differential approximations: a case study of the Korteweg-de Vries equation

Yury A. Blinkov[1]

[1]Mechanics and Mathematics Department
Saratov State University, Saratov, Russia

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On the example of the first-order differential approximation, a qualitative study was conducted for the Crank-Nicolson-type scheme for the Korteweg-de Vries equation. This made it possible to qualitatively assess the method's truncation error and propose simple criteria for selecting the time step and spatial step during calculations. The presented methods make it possible to carry out effective calculations using computer algebra systems. For the research, author's programs for working with the first-order differential approximation, implemented in the computer algebra system SymPy, were used.

FDA

In the 1960s of the last century, N. N. Yanenko and Yu. I. Shokin [1] formulated the method of differential approximations for the difference scheme. First-order differential approximation (FDA) for partial differential equations of evolutionary type and, in particular, the Korteweg-de Vries equation using computer algebra systems is considered in [2], and for the Navier-Stokes equations in [3].

In this work, the Korteweg-de Vries equation (1)

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

is chosen as a demonstrator of FDA for investigating difference schemes. Soliton solutions of the Korteweg-de Vries equation are those that describe wave propagation in nonlinear media. The soliton solution (2) represents a traveling wave $\xi = k(x - 4k^2 t)$ depending on the parameter k, which propagates without changing its shape and amplitude

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

In this work, we will investigate a second-order scheme with respect to h [2]

$$\frac{u_j^{n+1} - u_j^n}{\tau} + \frac{3}{4h}\left(\left({u^2}_{j+1}^{n+1} - {u^2}_{j-1}^{n+1}\right) + \left({u^2}_{j+1}^{n} - {u^2}_{j-1}^{n}\right)\right) +$$
$$+ \frac{1}{4h^3}\left(\left(u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + 2u_{j-1}^{n+1} - u_{j-2}^{n+1}\right) + \right.$$
$$\left. + \left(u_{j+2}^{n} - 2u_{j}^{n+1} + 2u_{j-1}^{n} - u_{j-2}^{n}\right)\right) = 0. \quad (3)$$

Constructing FDA uses only algebraic operations and can be effectively implemented algorithmically using computer algebra tools. The author's program is implemented in the open-source computer algebra system SymPy (`https://www.sympy.org`) and can be downloaded at `https://github.com/blinkovua/sharing-blinkov/blob/master/KDV_FDA_Crank-Nicolson.ipynb`.

Algorithmically, the application of the Gröbner basis construction algorithm for constructing FDA can be represented as working with an infinite module with the *POT* ordering (*position over term* - ordering first by dependent variables and then by independent variables), where the role of *position* is played by time steps τ and space steps h. In this case, calculations are carried out up to the first non-zero members of the series in τ and h.

Lexicographic ordering

Initially, the FDA method was a decomposition of the difference scheme (3) into a Taylor series expansion in the central point of the difference scheme template at the point $(\tau/2, 0)$ which would have the following form

$$6uu_x + u_t + u_{xxx} + h^2\left(uu_{xxx} + \frac{u_{xxxxx}}{4} + 3u_{xx}u_x\right) + \\ + \tau^2\left(\frac{3uu_{ttx}}{4} + \frac{u_{ttt}}{24} + \frac{u_{ttxxx}}{8} + \frac{3u_{tt}u_x}{4} + \frac{3u_{tx}u_t}{2}\right) + \ldots = 0 \quad (4)$$

Since the formal Taylor series (4) is equal to zero, its linear combination with itself and its differential consequences will also be equal to zero. This can be taken advantage of and brought to a canonical form that can be used to study the properties not only of difference schemes for linear equations but also for nonlinear ones [1].

In the works [1], evolutionary type equations were studied. This allowed the transformation of the formal Taylor series (4) by replacing all derivatives with respect to time through spatial derivatives

$$
\begin{aligned}
&6uu_x + u_t + u_{xxx} + h^2\left(uu_{xxx} + \frac{u_{xxxxx}}{4} + 3u_{xx}u_x\right) + \\
&\quad + \tau^2\left(18u^3u_{xxx} + 9u^2u_{xxxxx} + 162u^2u_{xx}u_x + \frac{3uu_{xxxxxxx}}{2} + \right. \\
&+63uu_{xxxx}u_x + 99uu_{xxx}u_{xx} + 108uu_x^3 + \frac{u_{xxxxxxxxx}}{12} + 6u_{xxxxxx}u_x + \\
&\left. + \frac{27u_{xxxxx}u_{xx}}{2} + 21u_{xxxx}u_{xxx} + 81u_{xxx}u_x^2 + 99u_{xx}^2u_x\right) + \ldots = 0 \quad (5)
\end{aligned}
$$

The canonical form (5) obtained by replacing all derivatives with respect to time through spatial derivatives allows, firstly, to precisely determine the order of the difference scheme, and secondly, it allows to draw certain conclusions about such properties of difference schemes as stability, approximation, accuracy, monotonicity, conservativeness, group properties, etc. [1].

Replacing all derivatives with respect to time through spatial derivatives corresponds to the construction of Groebner basis with lexicographical ordering first by t and then by x ($t \succ x$).

Since knowing the Taylor series expansion in a selected point, one can use it to *formally* recalculate the derivatives of the sought function (in this case, the differential equation) in another selected point. Therefore, the choice of the point for the FDA expansion does not matter, which is required for the canonical representation.

For example, let us consider the expansion of the difference scheme (3) into a Taylor series at the point $(\tau, -h)$

$$6uu_x + u_t + u_{xxx} + h\left(6uu_{xx} + u_{tx} + u_{xxxx} + 6u_x^2\right) + \\ + h^2\left(4uu_{xxx} + \frac{u_{txx}}{2} + \frac{3u_{xxxxx}}{4} + 12u_{xx}u_x\right) + \\ + \tau\left(-3uu_{tx} - \frac{u_{tt}}{2} - \frac{u_{txxx}}{2} - 3u_t u_x\right) + \\ + \tau h\left(-3uu_{txx} - \frac{u_{ttx}}{2} - \frac{u_{txxxx}}{2} - 6u_{tx}u_x - 3u_t u_{xx}\right) + \\ + \tau^2\left(\frac{3uu_{ttx}}{2} + \frac{u_{ttt}}{6} + \frac{u_{ttxxx}}{4} + \frac{3u_{tt}u_x}{2} + 3u_{tx}u_t\right) + \ldots = 0 \quad (6)$$

In the expansion (6), it is seen that the members of the series at τ, τh are simple differential consequences of the original equation (1).

At higher-order terms of the expansion, besides the original equation, the lower-order members of the original expansion may also be involved. The construction of the Groebner basis reduces the series (6) to the form (5).

The choice of the point for the expansion affects only the amount of calculations, taking into account the nonlinearity of the equations, the high order of the applied derivatives, and symbolic parameters of the problem. A much greater reduction in the amount of calculations can be achieved by performing the calculation not in lexicographical ordering, but in ordering by total degree, and then in reverse lexicographical (degrevlex – degree reverse lexicographic).

Degrevlex ordering

The initial Taylor series expansion does not depend on the ordering, but depends only on the point of expansion. Therefore, using expansion (4) or expansion (6) in the degrevlex ordering, we obtain a more compact, compared to (5), version of FDA.

$$6uu_x + u_t + u_{xxx} + h^2\left(3u^2u_x + \frac{uu_t}{2} - \frac{u_{txx}}{4} - \frac{3u_{xx}u_x}{2}\right) + \\ + \tau^2\left(-\frac{u_{ttt}}{12}\right) + \ldots = 0 \quad (7)$$

In this specific case, we can obtain this form even in lexicographical ordering by swapping the order of variables $x \succ t$, but the approach based on the use of degrevlex ordering in most cases gives the most compact form of FDA or close to it, and it is less dependent on the choice of variable order.

Symbolic experiments

Despite their very cumbersome appearance, especially in lexicographical ordering, the first differential approximations can be effectively checked against exact solutions. More precisely, FDA, when substituted with the exact solution, allows us to evaluate the scheme itself without programming it and conducting computational experiments to check it.

Let's substitute the exact solution (2) into FDA (5) or (7) to get the following form of FDA

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

Since ξ represents a running wave, and the value of hyperbolic tangent lies in the interval from -1 to 1, the main contribution to the truncation error of the difference scheme (3) on the exact solution (2) can be represented in the form of $\mathcal{O}(\tau^2k^{11}, h^2k^7)$.

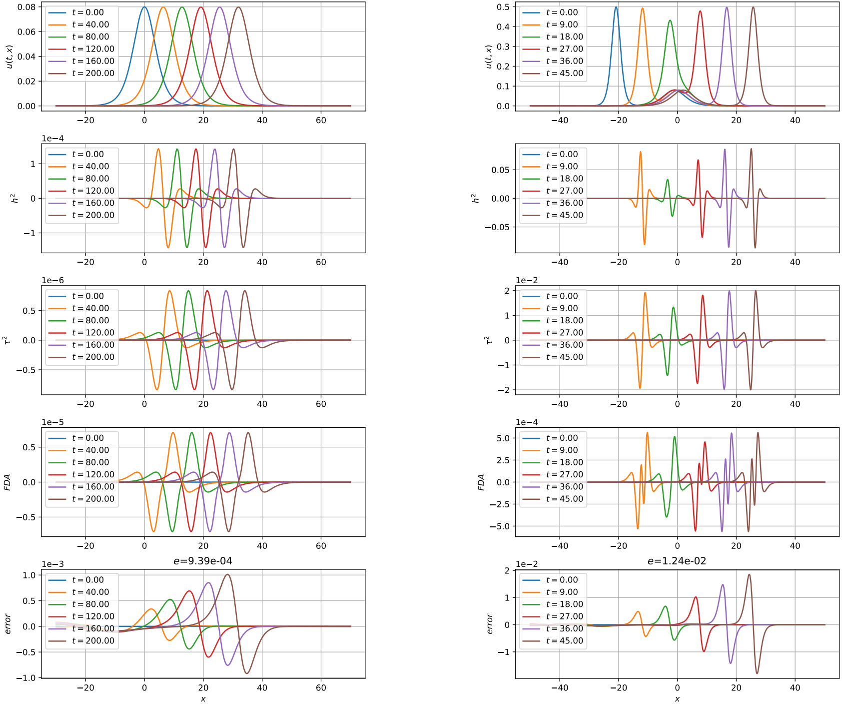
As a result, it can be concluded that, for $0 < k < 1$, the error of performing equation (1) on the grid will be more influenced by the step size h than τ, and vice versa for $k > 1$. Of course, it is necessary to take into account that the difference scheme (3) is, in a sense, an approximation of the desired solution by a polynomial, and the solution (2) is exponential, and in addition, the amplitude and the steepness of the kink of the soliton depend on the value of k.

The numerical experiment program is implemented in 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_FDA_Crank-Nicolson.ipynb`.

In FDA with lexicographical ordering (5), the term τ^2 involves the 9th derivative with respect to x. Calculating the discrete derivative of the 9th order on a symmetric template requires 10 points, and with a large step it will cause strong oscillations. With the compact representation of FDA in degrevlex ordering (7), at most the third derivative is encountered, as in the original equation itself (1). All numerical experiments below were carried out using the compact representation of FDA.

The two-soliton solution (9) describes the interaction of two waves $\xi_1 = k_1(x - 4k_1^2 t)$ and $\xi_2 = k_2(x - 4k_2^2 t)$, depending on parameters k_1 and k_2, in which they retain their shape and amplitude as they move further

$$u = \frac{\left(8k_1^2 - 8k_2^2\right)\left(k_1^2 \cosh^2 \xi_2 + k_2^2 \sinh^2 \xi_1\right)}{\left((k_1 - k_2)\cosh(\xi_1 + \xi_2) + (k_1 + k_2)\cosh(\xi_1 - \xi_2)\right)^2} \tag{9}$$



u(t, x)
h^2
τ^2
FDA
error
x
1e−4
1e−6
1e−5
1e−3
1e−2
t = 0.00
t = 40.00
t = 80.00
t = 120.00
t = 160.00
t = 200.00
t = 9.00
t = 18.00
t = 27.00
t = 36.00
t = 45.00
e=9.39e-04
e=1.24e-02

$h\backslash\tau=*h$	16.0	8.0	4.0	2.0	1.0	0.5	0.25
$\max_{n,j}\|FDA\|_j^n$							
2.500e-01	7.1e-06	5.7e-06	8.1e-06	8.7e-06	8.9e-06	8.9e-06	9.1e-06
1.250e-01	1.8e-06	1.4e-06	2.0e-06	2.2e-06	2.2e-06	2.2e-06	2.3e-06
6.250e-02	4.7e-07	3.6e-07	5.1e-07	5.5e-07	5.6e-07	5.6e-07	5.6e-07
3.125e-02	1.2e-07	8.9e-08	1.3e-07	1.4e-07	1.4e-07	1.4e-07	1.4e-07
$\max_{n,j}\|u_j^n-(2)_j^n\|/(1+\|(2)\|_j^n)$							
2.500e-01	9.4e-04	3.2e-04	1.7e-04	1.3e-04	1.2e-04	1.2e-04	1.2e-04
1.250e-01	2.4e-04	8.1e-05	4.2e-05	3.3e-05	3.1e-05	3.0e-05	3.0e-05
6.250e-02	5.9e-05	2.0e-05	1.0e-05	8.3e-06	7.7e-06	7.6e-06	7.6e-06
3.125e-02	1.5e-05	5.0e-06	2.6e-06	2.1e-06	1.9e-06	1.9e-06	1.9e-06
τ^2k^{11}							
2.500e-01	3.3e-07	8.2e-08	2.0e-08	5.1e-09	1.3e-09	3.2e-10	8.0e-11
1.250e-01	8.2e-08	2.0e-08	5.1e-09	1.3e-09	3.2e-10	8.0e-11	2.0e-11
6.250e-02	2.0e-08	5.1e-09	1.3e-09	3.2e-10	8.0e-11	2.0e-11	5.0e-12
3.125e-02	5.1e-09	1.3e-09	3.2e-10	8.0e-11	2.0e-11	5.0e-12	1.3e-12
h^2k^7							
2.500e-01	8.0e-07	8.0e-07	8.0e-07	8.0e-07	8.0e-07	8.0e-07	8.0e-07
1.250e-01	2.0e-07	2.0e-07	2.0e-07	2.0e-07	2.0e-07	2.0e-07	2.0e-07
6.250e-02	5.0e-08	5.0e-08	5.0e-08	5.0e-08	5.0e-08	5.0e-08	5.0e-08
3.125e-02	1.3e-08	1.3e-08	1.3e-08	1.3e-08	1.3e-08	1.3e-08	1.3e-08

$h\backslash\tau = *h$	2.0	1.0	0.5	0.25	0.125
$\max_{n,j} \lvert FDA\rvert_j^n$					
1.250e-01	5.6e-04	1.0e-03	1.3e-03	1.3e-03	1.4e-03
6.250e-02	1.4e-04	2.6e-04	3.2e-04	3.4e-04	3.4e-04
3.125e-02	3.6e-05	6.6e-05	8.1e-05	8.5e-05	8.6e-05
$\max_{n,j} \lvert u_j^n - (9)_j^n\rvert/(1+\lvert(9)\rvert_j^n)$					
1.250e-01	1.2e-02	5.0e-03	3.1e-03	2.7e-03	2.6e-03
6.250e-02	3.1e-03	1.2e-03	7.8e-04	6.7e-04	6.4e-04
3.125e-02	7.8e-04	3.1e-04	2.0e-04	1.7e-04	1.6e-04
$\tau^2 k_1^{11}$					
1.250e-01	3.1e-05	7.6e-06	1.9e-06	4.8e-07	1.2e-07
6.250e-02	7.6e-06	1.9e-06	4.8e-07	1.2e-07	3.0e-08
3.125e-02	1.9e-06	4.8e-07	1.2e-07	3.0e-08	7.5e-09
$h^2 k_1^7$					
1.250e-01	3.3e-03	3.3e-03	3.3e-03	3.3e-03	3.3e-03
6.250e-02	8.2e-04	8.2e-04	8.2e-04	8.2e-04	8.2e-04
3.125e-02	2.0e-04	2.0e-04	2.0e-04	2.0e-04	2.0e-04

Conclusion

The use of the first differential approximation allows for a qualitative and, in some cases, quantitative investigation of the difference scheme. By choosing the ordering when constructing the first differential approximation, it is possible to significantly reduce both the volume of symbolic calculations and obtain a more compact form that contains derivatives of much lower order. On the example of Crank-Nicolson-type schemes for the Korteweg-de Vries equation, not only an analytical study of the applicability of the soliton solution depending on the parameters was carried out, but also, using the compact form and numerical calculations. The results were confirmed by numerical calculations for single- and two-soliton solutions.

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