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Difference schemes for second-order ordinary differential equations with corrector and predictor properties

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Abstract — A technique for constructing a sequence of difference schemes with the properties of a corrector and a predictor for integrating systems of the second-order ordinary differential equations is presented. The sequence of schemes begins with the explicit three-point Störmer method of the second order of approximation. Each subsequent scheme also implements the Störmer method corrected with additional terms calculated through the solution of the previous scheme. The stability of the resulting schemes and the increase in the order of convergence for the first of them are carefully substantiated. The results of calculations of the test problem are presented, confirming the increase in the order of accuracy of the constructed methods.

Keywords: Second order ordinary differential equations, explicit difference schemes, Störmer method, predictor–corrector algorithms

MSC 2010: 65L06, 65L20

1. Introduction

In thermodynamics, electrical engineering, celestial mechanics, and other applications, the following Cauchy problem arises:

$$
\begin{aligned}
x''(t) &= f\,(t, x(t))\,, \quad t \in [0,\ T] \\
x(0) &= x_0, \quad x'(0) = x'_0.
\end{aligned}
\tag{1.1}
$$

Here x and f are sufficiently smooth vector functions: $x(t), f\,(t, x(t))$ from R^n with the ‘uniform’ norm

$$
\|y\| = \max_{1 \leqslant i \leqslant n} |y_i|\,, \quad y = (y_1, \ldots, y_n)^T \in R^n. \tag{1.2}
$$

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By introducing additional unknowns, ordinary differential equations (ODEs) of higher order can be reduced to systems of equations of the first order. Therefore, the question of the numerical solution of the Cauchy problem for higher-order equations could be considered settled. However, in some cases, direct integration algorithms without lowering the order of the system are more efficient (see, e.g., [5–8, 11, 14] and the references therein).

At present, both multistep and one-step numerical methods are used to directly solve explicit systems of second-order ODEs. One-step methods include, for example, the Runge–Kutta–Nyström methods [5]. Their advantage is that they allow flexible changing the size of the integration step in contrast to explicit symmetric difference schemes. On the other hand, multistep methods like Störmer–Cowell ones [6–8, 11, 14] allow only one calculation of right-hand side at each time step, in contrast to the multiple calculations in the Runge–Kutta–Nyström methods.

The purpose of this paper is to present an approach for constructing and implementing an algorithm with corrector and predictor properties based on the simplest Störmer method with some corrections in right-hand side, which allows one to calculate approximately the desired solution of problem (1.1) with an arbitrary even order of accuracy.

2. Main idea of the approach

To solve the posed problem, let us introduce a uniform difference grid $t_i = ih$, $i = -0, \pm 1, \pm 2, \ldots$, with a step $h = T/N$ and integer $N \geqslant 2$. We also introduce the notation $g(t) = f(t, x(t))$ and $y(t_i) = y_i$ for an arbitrary vector function $y(t)$.

We approximate the second derivative of the desired solution (1.1) by the central difference

$$\frac{x_{i+1} - 2x_i + x_{i-1}}{h^2} = x_i'' + O(h^2). \tag{2.1}$$

Resolve it for x_{i+1}:

$$x_{i+1} = 2x_i - x_{i-1} + h^2 f(t_i, x_i) + O(h^4). \tag{2.2}$$

Obviously, to start the calculations, it is necessary to set two consecutive values. The value x_0 is given in (1.1), and we will find x_1 as follows. Consider the central difference

$$\frac{x_1 - x_{-1}}{2h} = x_0' + O(h^2). \tag{2.3}$$

Resolve it for x_1:

$$x_1 = x_{-1} + 2hx_0' + O(h^3). \tag{2.4}$$

Take formula (2.2) for the case $i = 0$:

$$x_1 = 2x_0 - x_{-1} + h^2 f(t_0, x_0) + O(h^4). \tag{2.5}$$

Add (2.4) to (2.5) and divide the result by two:

$$x_1 = x_0 + hx_0' + h^2 f(t_0, x_0)/2 + O(h^3).$$

In this case, this expression is the Taylor formula for $x(t_1)$ in the vicinity of the point $t=0$.

Discarding the approximation errors, we arrive at the following well-known explicit Störmer difference algorithm [5]:

$$\begin{aligned} x_0^h &= x_0 \\ x_1^h &= x_0 + hx_0' + h^2 f(t_0, x_0)/2 \\ x_{i+1}^h &= 2x_i^h - x_{i-1}^h + h^2 f(t_i,\, x_i^h) \end{aligned} \tag{2.6}$$

where $x_i^h \approx x(t_i), i = 0,1,...,N-1$. It has the second order of convergence [5].

To increase the order of convergence, one can select more accurate approximations of the second derivative by involving higher-order differences on the left side of (2.1), as well as select a linear combination of values $f(t_i, x_i)$ on the right side of (2.1) and (2.2) (see [5–8, 11, 14]).

In this paper, we will leave the left side of (2.1) unchanged, but choose the weights $\alpha_j^{(k)} = \alpha_{-j}^{(k)},\ j = 1,\ldots,\ k-1$, so that the resulting symmetric difference expression has the order of approximation $O(h^{2k})$:

$$\frac{x_{i-1} - 2x_i + x_{i+1}}{h^2} = \sum_{j=-k+1}^{k-1} \alpha_j^{(k)} x''_{i+j} + O(h^{2k}). \tag{2.7}$$

In the left and right sides, we use the expansion in a Taylor series at a point t_i, taking into account the symmetry of the coefficients:

$$\frac{x_{i-1} - 2x_i + x_{i+1}}{h^2} = x_i'' + \frac{h^2}{12} x_i^{IV} + \frac{h^4}{360} x_i^{VI} + \ldots = 2\sum_{s=0}^{k-1} \frac{h^{2s}}{(2s+2)!} x_i^{(2s+2)} + O(h^{2k})$$

$$\sum_{j=-k+1}^{k-1} \alpha_j^{(k)} x''_{i+j} = \alpha_0 x_i'' + \sum_{j=1}^{k-1} 2\alpha_j^{(k)} \sum_{s=0}^{k-1} \frac{(jh)^{2s}}{(2s)!} x_i^{(2s+2)} + O(h^{2k}).$$

Equating the coefficients at the same powers of h, we obtain the following system of linear algebraic equations (SLAE) in the unknowns $\alpha_j^{(k)},\ j = 0,...,k-1$:

$$\begin{cases} \alpha_0^{(k)} + 2\sum\limits_{j=1}^{k-1} \alpha_j^{(k)} = 1 \\ \sum\limits_{j=1}^{k-1} j^{2s} \alpha_j^{(k)} = \dfrac{1}{2(s+1)(2s+1)}, \quad s = 1,...,k-1. \end{cases} \tag{2.8}$$

Its matrix of size $k \times k$ has the form

$$A_k = \begin{pmatrix} 1 & 2 & 2 & 2 & \ldots & 2 \\ 0 & 1 & 4^1 & 9^1 & \ldots & (k-1)^2 \\ 0 & 1 & 4^2 & 9^2 & \ldots & (k-1)^4 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 1 & 4^{k-1} & 9^{k-1} & \ldots & (k-1)^{2k-2} \end{pmatrix}.$$

Since the transposition of a matrix does not change its determinant, we take into account its expansion in the first column:

$$\det A_k = ((k-1)!)^2 \begin{vmatrix} 1 & 1 & \dots & 1 \\ 1 & 2^2 & \dots & 2^{2k-4} \\ 1 & 3^2 & \dots & 3^{2k-4} \\ \dots & \dots & \dots & \dots \\ 1 & (k-1)^2 & \dots & (k-1)^{2k-4} \end{vmatrix}$$
$$= ((k-1)!)^2 \det V_{k-1}\left(1^2, 2^2, \dots, (k-1)^2\right). \tag{2.9}$$

Here $\det V_{k-1}\left(1^2,\, 2^2,\, \dots\,,\, (k-1)^2\right)$ is a Vandermonde determinant [15]:

$$\det V_{k-1}\left(1^2,\, 2^2,\, \dots\,,\, (k-1)^2\right) = \prod_{1\leqslant j<i\leqslant k-1} (i^2-j^2).$$

It is obvious that $\det A_k \neq 0$; therefore system (2.8) is non-degenerate and has a unique solution. To determine it, we employ Cramer's formulas [15] to get the coefficients of these strongly implicit schemes. As a result, we obtained coefficients in the form of irreducible fractions for the first six difference schemes shown in Table 1.

Along with increasing the order of approximation of the difference equation (2.1), we increase the order of approximation for the initial condition (2.3). For this purpose, we use an approximation with antisymmetric coefficients:

$$\frac{x_1 - x_{-1}}{2h} = x_0' + h\sum_{j=1}^{k-1} \beta_j^{(k)}\left(x_j'' - x_{-j}''\right) + O(h^{2k}). \tag{2.10}$$

In the left and right sides, we use the Taylor formula at the point $t=0$, taking into account the antisymmetry of the coefficients:

$$\frac{x_1 - x_{-1}}{2h} = x_0' + \sum_{j=1}^{k-1} \frac{h^{2j} x_0^{(2j+1)}}{(2j+1)!} + O(h^{2k}) \tag{2.11}$$

$$h\sum_{j=1}^{k-1} \beta_j^{(k)}\left(x_j'' - x_{-j}''\right) = 2\sum_{l=1}^{k-1} \beta_l^{(k)} \sum_{j=1}^{k-1} \frac{l^{2j-1}h^{2j}}{(2j-1)!} x_0^{(2j+1)} + O(h^{2k}). \tag{2.12}$$

Equating the coefficients at the same powers of h, we obtain the following SLAE in the unknowns $\beta_l^{(k)}$, $l = 1, \dots, k-1$:

$$\sum_{l=1}^{k-1} \beta_l^{(k)} l^{2s-1} = \frac{1}{2\cdot(2s+1)\cdot 2s}, \quad s = 1, \dots, k-1. \tag{2.13}$$

Table 1. Coefficients $\alpha_j^{(k)}$ of strongly implicit symmetric methods similar to Störmer–Cowell ones for 2-12 orders of approximation.

Order of approximation	Coefficients
2	$\alpha_0^{(1)} = 1$
4	$\alpha_0^{(2)} = \frac{5}{6}, \quad \alpha_1^{(2)} = \alpha_{-1}^{(2)} = \frac{1}{12}$
6	$\alpha_0^{(3)} = \frac{97}{120}, \quad \alpha_{-1}^{(3)} = \alpha_1^{(3)} = \frac{1}{10}, \quad \alpha_{-2}^{(3)} = \alpha_2^{(3)} = -\frac{1}{240}$
8	$\alpha_0^{(4)} = \frac{12067}{15120}, \quad \alpha_{-1}^{(4)} = \alpha_1^{(4)} = \frac{2171}{20160}$ $\alpha_{-2}^{(4)} = \alpha_2^{(4)} = -\frac{73}{10080}, \quad \alpha_{-3}^{(4)} = \alpha_3^{(4)} = \frac{31}{60480}$
10	$\alpha_0^{(5)} = \frac{57517}{72576}, \quad \alpha_{-1}^{(5)} = \alpha_1^{5} = \frac{101741}{907200}$ $\alpha_{-2}^{(5)} = \alpha_2^{(5)} = -\frac{8593}{907200}, \quad \alpha_{-3}^{(5)} = \alpha_3^{(5)} = \frac{149}{129600}$ $\alpha_{-4}^{(5)} = \alpha_4^{(5)} = -\frac{289}{3628800}$
12	$\alpha_0^{(6)} = \frac{31494553}{39916800}, \quad \alpha_{-1}^{(6)} = \alpha_1^{(6)} = \frac{9186203}{79833600}$ $\mathrm{v}\alpha_{-2}^{(6)} = \alpha_2^{(6)} = -\frac{222331}{19958400}, \quad \alpha_{-3}^{(6)} = \alpha_3^{(6)} = \frac{40489}{22809600}$ $\alpha_{-4}^{(6)} = \alpha_4^{(6)} = -\frac{17453}{79833600}, \quad \alpha_{-5}^{(6)} = \alpha_5^{(6)} = \frac{317}{22809600}$

Its $(k-1)\times(k-1)$-matrix has the form

$$B_k = \begin{pmatrix} 1 & 2 & \dots & k-1 \\ 1 & 2^3 & \dots & (k-1)^3 \\ \dots & \dots & \dots & \dots \\ 1 & 2^{2k-3} & \dots & (k-1)^{2k-3} \end{pmatrix}.$$

As was already mentioned, transposing a matrix does not change its determinant. Therefore it equals

$$\begin{aligned} \det B_k =& (k-1)! \begin{vmatrix} 1 & 1 & \dots & 1 \\ 1 & 4^1 & \dots & 4^{k-2} \\ \dots & \dots & \dots & \dots \\ 1 & (k-1)^2 & \dots & (k-1)^{2k-4} \end{vmatrix} \\ =& (k-1)!\, V_{k-1}\left(1^2, 2^2, \dots, (k-1)^2\right). \end{aligned}$$

Since $\det B_k \neq 0$, system (2.14) is non-degenerate and has a unique solution. To solve it, we again employ Cramer's formulas to obtain coefficients for these strongly implicit approximations. Coefficients written in the form of irreducible rational fractions are given for refining the first derivative of the solution with 4–12 orders of approximation in Table 2.

The question arises about the algorithmic use of this strongly implicit difference scheme. We will implement it in the form of a sequence of difference schemes of increasing order of accuracy up to $2p$.

First, we use the explicit Störmer difference scheme of the second order of approximation:

$$x_0^{h,1} = x_0 \tag{2.14}$$

$$\frac{x_1^{h,1} - x_{-1}^{h,1}}{2h} = x_0' \tag{2.15}$$

$$\frac{x_{i+1}^{h,1} - 2x_i^{h,1} + x_{i-1}^{h,1}}{h^2} = f(t_i, x_i^{h,1}),\ i = -p+1, ..., N+p-1. \tag{2.16}$$

Calculations (2.1)–(2.6) demonstrate how to obtain a computational algorithm for sequentially finding $x_i^{h,1},\ i = 0,1,2,\ldots$. Note that the use of expression (2.16) allows the calculation of (several) values to the left of the segment $[0,T]$.

Then we use the second scheme, the right-hand side of which is supplemented by an expression in terms of the solution of the first scheme:

$$x_0^{h,2} = x_0 \tag{2.17}$$

$$\frac{x_1^{h,2} - x_{-1}^{h,2}}{2h} = x_0' + \frac{h}{12}\left(f(t_1, x_1^{h,1}) - f(t_{-1}, x_{-1}^{h,1})\right) \tag{2.18}$$

$$\frac{x_{i+1}^{h,2} - 2x_i^{h,2} + x_{i-1}^{h,2}}{h^2} = f(t_i, x_i^{h,2}) + \frac{1}{12}\left(f(t_{i-1}, x_{i-1}^{h,1}) - 2f(t_i, x_i^{h,1}) + f(t_{i+1}, x_{i+1}^{h,1})\right) \tag{2.19}$$

$$i = -p+1, ..., N+p-1.$$

If we replace the superscript 1 by 2 in these corrections, then we get the implicit Numerov scheme of the fourth order of approximation [12, 13]. Here we get an explicit difference scheme with respect to $x_i^{h,2}$, for which we will later prove also the fourth order of convergence.

Subsequent schemes have a larger template size for solutions of the previous level of accuracy, so we will use several values that go beyond the interval $[0,T]$ since the difference operator in Störmer method allows one to find values at nodes to the left of zero. So let the solution $x_i^{h,k-1},\ i = -p+1, ..., N+p-1$, be already

Table 2. Coefficients $\beta_j^{(k)}$ for the approximation of the initial condition (2.10).

Order of approximation	Coefficients
4	$\beta_{-1}^{(2)} = \beta_1^{(2)} = -\frac{1}{12}$
6	$\beta_{-1}^{(3)} = \beta_1^{(3)} = -\frac{37}{360}, \quad \beta_{-2}^{(3)} = \beta_2^{(3)} = \frac{7}{720}$
8	$\beta_{-1}^{(4)} = \beta_1^{(4)} = -\frac{2257}{20160}, \quad \beta_{-2}^{(4)} = \beta_2^{(4)} = \frac{43}{2520}$
	$\beta_{-3}^{(4)} = \beta_3^{(4)} = -\frac{37}{20160}$
10	$\beta_{-1}^{(5)} = \beta_1^{(5)} = -\frac{212881}{1814400}, \quad \beta_{-2}^{(5)} = \beta_2^{(5)} = \frac{40711}{1814400}$
	$\beta_{-3}^{(5)} = \beta_3^{(5)} = -\frac{2503}{604800}, \quad \beta_{-4}^{(5)} = \beta_4^{(5)} = \frac{199}{518400}$
12	$\beta_{-1}^{(6)} = \beta_1^{(6)} = -\frac{3216337}{26611200}$
	$\beta_{-2}^{(6)} = \beta_2^{(6)} = \frac{528463}{19958400}, \quad \beta_{-3}^{(6)} = \beta_3^{(6)} = -\frac{341227}{53222400}$
	$\beta_{-4}^{(6)} = \beta_4^{(6)} = \frac{126611}{119750400}, \quad \beta_{-5}^{(6)} = \beta_5^{(6)} = -\frac{40321}{479001600}$

defined. Then the next solution is determined from the difference system

$$x_0^{h,k} = x_0 \tag{2.20}$$

$$\frac{x_1^{h,k} - x_{-1}^{h,k}}{2h} = x_0' + h\sum_{j=1}^{k-1} \beta_j^{(k)} \left(f(t_j, x_j^{h,k-1}) - f(t_{-j}, x_{-j}^{h,k-1}) \right) \tag{2.21}$$

$$\begin{aligned} \frac{x_{i+1}^{h,k} - 2x_i^{h,k} + x_{i-1}^{h,k}}{h^2} &= f\left(t_i, x_i^{h,k}\right) + \left(\alpha_0^{(k)} - 1\right) f\left(t_i, x_i^{h,k-1}\right) \\ &+ \sum_{j=1}^{k-1} \alpha_j^{(k)} \left(f\left(t_{i-j}, x_{i-j}^{h,k-1}\right) + f\left(t_{i+j}, x_{i+j}^{h,k-1}\right) \right) \\ & i = -p+1, \ldots, N+p-1. \end{aligned} \tag{2.22}$$

So, each time an explicit difference scheme with a difference operator of the second order of approximation is used. But due to the use of the previous solution for correcting the right-hand side, new solution has a higher order of convergence. This process continues until the use of the difference scheme (2.20)–(2.22) with the number $k = p$.

3. Justification of the convergence of difference schemes

Justification of the convergence of approximate solutions of the presented grid problems we begin with the derivation of the expansion in powers of h^2 for the solution of the first problem (2.14)–(2.16). Let the following smoothness conditions be satisfied for the differential problem (1.1):

$$
\begin{aligned}
&x(t) \in \boldsymbol{C}^{(2p+2)}([0,T]) \\
&f(t,x) \in \boldsymbol{C}^{(2p)}([0,T]\times R^n)
\end{aligned}
\tag{3.1}
$$

where $\boldsymbol{C}^{(r)}(\Omega)$ means the class of vector functions each component of which is continuous on the set Ω. And let vector function $f(t,x)$ satisfies the Lipschitz condition in the second argument:

$$
\|f(t,\bar{x}) - f(t,\widetilde{x})\| \leqslant L\|\bar{x}-\widetilde{x}\| \quad \forall \bar{x},\widetilde{x} \in R^n. \tag{3.2}
$$

Let us prove that there is an expansion

$$
x_i^{h,1} = x_i + \sum_{j=1}^{p-1} h^{2j} z_j(t_i) + h^{2p}\xi_i^h, \quad i = 0,\dots,N \tag{3.3}
$$

where $z_j(t)$ are vector functions with components $z_{j,s}(t)$ independent of h; and ξ_i^h are the values of grid vector functions depending on the choice of h but uniformly bounded with respect to h:

$$
\max_{0\leqslant i\leqslant N} \left\|\xi_i^h\right\| \leqslant c \tag{3.4}
$$

with a constant c. Here and below, we denote by c various constants independent of h and i. We take functions $z_j(t)$ as solutions of systems of linear ODEs

$$
z_{1,j}(0) = 0 \tag{3.5}
$$

$$
z_j'(0) = -\frac{x_0^{(2j+1)}}{(2j+1)!} - \sum_{r=1}^{j-1} \frac{z_r^{(2j-2r+1)}(0)}{(2j-2r+1)!} \tag{3.6}
$$

$$
\begin{aligned}
z_j'' - J(t,x)z_j = {} & -\frac{2}{(2j+2)!}x^{(2j+2)} - \sum_{r=1}^{j-1}\frac{2z_r^{(2j-2r+2)}}{(2j-2r+2)!} \\
& + \sum_{r_1+\ldots+r_n=j} \frac{1}{r_1!\cdots r_n!}\frac{\partial^j f(t,x(t))}{\partial x_1^{r_1}\cdots\partial x_n^{r_n}} \times \sum_{s_1+\ldots+s_n=j}\left(\left(\sum_{j_1+\ldots+j_{r_1}=s_1} z_{j_1,1}\cdots z_{j_{r_1},1}\right)\right. \\
& \left.\cdots\left(\sum_{j_1+\ldots+j_{r_n}=s_n} z_{j_1,n}\cdots z_{j_{r_n},n}\right)\right), \quad t\in[0,\ T].
\end{aligned}
\tag{3.7}
$$

Here $J(t,x)$ is the Jacobi matrix:

$$
J(t,x) = \begin{pmatrix} \partial f_1/\partial x_1 & \dots & \partial f_n/\partial x_1 \\ \dots & \dots & \dots \\ \partial f_1/\partial x_n & \dots & \partial f_n/\partial x_n \end{pmatrix}.
$$

Note that these systems uniquely determine solutions $z_j(t) \in \boldsymbol{C}^{(2p-2j+2)}([0,T])$ sequentially in increasing index j, since each problem contains functions of sufficient smoothness with smaller indices $r < j$ in the right-hand side.

Theorem 3.1. *Let the smoothness conditions* (3.1), (3.2) *be satisfied for problem* (1.1). *Then expansion* (3.3) *with estimate* (3.4) *holds for the solution* $x_i^{h,1}$ *of the difference scheme* (2.14)–(2.16).

Proof. Since the vectors $x_i^{h,1}, x_i$ and $z_j(t_i)$ are uniquely defined in expansion (3.3), then ξ_i^h is uniquely determined from this expansion. Thus, it remains to prove estimate (3.4). We use the initial conditions (1.1), (2.14), (3.5) in expansion (3.3) for $i = 0$. As a result, we arrive at the equality

$$\xi_0^{h,1} = 0. \tag{3.8}$$

Now we substitute (3.1) into (2.15). Using the Taylor formula at the point $t = 0$, we have the expansion

$$\sum_{r=0}^{p-1} \frac{h^{2r}}{(2r+1)!} x_0^{(2r+1)} + \sum_{j=1}^{p-1} h^{2j} \sum_{r=0}^{p-1-j} \frac{h^{2r}}{(2r+1)!} z_j^{(2r+1)}(t_0) + h^{2p}\varphi_0^h \\ + h^{2p}\frac{\xi_1^h - \xi_{-1}^h}{2h} = x_0', \quad \left\|\varphi_0^h\right\| \leqslant c. \tag{3.9}$$

Taking into account the initial conditions (3.6), the terms with degrees of h less than $2p$ are cancelled:

$$\frac{\xi_1^h - \xi_{-1}^h}{2h} = \varphi_0^h. \tag{3.10}$$

Now substitute (3.3) into the left-hand side of (2.19):

$$\frac{x_{i+1}^{h,1} - 2x_i^{h,1} + x_{i-1}^{h,1}}{h^2} = 2\sum_{r=0}^{p-1} \frac{h^{2r}}{(2r+2)!} x_i^{(2r+2)} + 2\sum_{j=1}^{p-1} h^{2j} \sum_{r=0}^{p-1-j} \frac{h^{2r}}{(2r+2)!} z_j^{(2r+2)}(t_i) \\ + h^{2p}\eta_i^h + h^{2p}\frac{\xi_{i+1}^h - 2\xi_i^h + \xi_{i-1}^h}{h^2}, \quad \left\|\eta_i^h\right\| \leqslant c. \tag{3.11}$$

When substituting into the right side of (2.19), we first use the increment formula for the second argument:

$$f\left(t_i,\, x_i + \sum_{j=1}^{p-1} h^{2j} z_j(t_i) + h^{2p}\xi_i^h\right) = f\left(t_i,\, x_i + \sum_{j=1}^{p-1} h^{2j} z_j(t_i)\right) + h^{2p} J(t_i, \rho_i^h)\, \xi_i^h \tag{3.12}$$

where the components of vector ρ_i^h belong to intervals which ends are determined by the components of vectors $x_i^{h,1}$ and $x_i + \sum_{j=1}^{p-1} h^{2j} z_j(t_i)$. And then we use the Taylor formula for the second argument at the point x_i:

$$f\left(t_i,\, x_i + \sum_{j=1}^{p-1} h^{2j} z_j(t_i)\right) = f(t_i,x_i) + \sum_{r=1}^{p-1} \sum_{r_1+\ldots+r_n=r} \frac{1}{r_1!\cdots r_n!} \frac{\partial^r f}{\partial x_1^{r_1}\cdots\partial x_n^{r_n}}(t_i,x_i)$$
$$\times \left(\sum_{j=1}^{p-1} h^{2j} z_{j,1}(t_i)\right)^{r_1} \cdots \left(\sum_{j=1}^{p-1} h^{2j} z_{j,n}(t_i)\right)^{r_n} + h^{2p}\sigma_i^h \tag{3.13}$$
$$\left\|\sigma_i^h\right\| \leqslant c.$$

Raise the expressions in brackets to their powers:

$$\left(\sum_{j=1}^{p-1} h^{2j} z_{j,1}(t_i)\right)^{r_1} \cdots \left(\sum_{j=1}^{p-1} h^{2j} z_{j,n}(t_i)\right)^{r_n}$$
$$= \left(\sum_{j_1=1}^{p-1}\cdots\sum_{j_{r_1}=1}^{p-1} h^{2j_1+\ldots+2j_{r_1}} z_{j_1,1}(t_i)\cdots z_{j_{r_1},1}(t_i)\right)$$
$$\cdots\left(\sum_{j_1=1}^{p-1}\cdots\sum_{j_{r_1}=1}^{p-1} h^{2j_1+\ldots+2j_{r_1}} z_{j_1,n}(t_i)\cdots z_{j_{r_n},n}(t_i)\right). \tag{3.14}$$

In the last equality, we leave only the terms of the order of degree no higher than h^{2p-2} and combine the rest into a remainder term:

$$\left(\sum_{j=1}^{p-1} h^{2j} z_{j,1}(t_i)\right)^{r_1} \cdots \left(\sum_{j=1}^{p-1} h^{2j} z_{j,n}(t_i)\right)^{r_n}$$
$$= \sum_{s=1}^{p-1} h^{2s} \sum_{s_1+\ldots+s_n=s} \left(\sum_{j_1+\ldots+j_{r_1}=s_1} z_{j_1,1}(t_i)\cdots z_{j_{r_1},1}(t_i)\right)$$
$$\cdots\left(\sum_{j_1+\ldots+j_{r_n}=s_n} z_{j_1,n}(t_i)\cdots z_{j_{r_n},n}(t_i)\right) + h^{2p}\pi_i^{h,1}, \quad \left\|\pi_i^{h,1}\right\| \leqslant c. \tag{3.15}$$

Now we use expansions (3.11)–(3.13) and (3.15) in equality (2.19):

$$2\sum_{r=0}^{p-1} \frac{h^{2r}}{(2r+2)!} x_i^{(2r+2)} + 2\sum_{j=1}^{p-1} h^{2j} \sum_{r=0}^{p-1-j} \frac{h^{2r}}{(2r+2)!} z_j^{(2r+2)}(t_i) + h^{2p}\tau_i^h + h^{2p}\frac{\xi_{i+1}^h - 2\xi_i^h + \xi_{i-1}^h}{h^2} =$$

$$= f(t_i,x_i) + h^{2p}J(t_i,\rho_i^h)\,\xi_i^h + \sum_{r=1}^{p-1}\sum_{r_1+\ldots+r_n=r}\frac{1}{r_1!\cdots r_n!}\frac{\partial^r f(t_i,x_i)}{\partial x_1^{r_1}\cdots\partial x_n^{r_n}}$$

$$\times\sum_{s=1}^{p-1}h^{2s}\sum_{s_1+\ldots+s_n=s}\left(\sum_{j_1+\ldots+j_{r_1}=s_1} z_{j_1,1}(t_i)\cdots z_{j_{r_1},1}(t_i)\right)$$

$$\cdots\left(\sum_{j_1+\ldots+j_{r_n}=s_n} z_{j_1,n}(t_i)\cdots z_{j_{r_n},n}(t_i)\right), \quad \|\,\tau_i^h\,\|\leqslant c. \tag{3.16}$$

In this equality, we cancel the terms of order $1, h^2, \ldots, h^{2p-2}$ due to defining the vector functions $x(t)$ and $z_{1,j}(t)$ in problems (1.1) and (3.7):

$$\frac{\xi_{i+1}^h - 2\xi_i^h + \xi_{i-1}^h}{h^2} - J(t_i,\rho_i^h)\,\xi_i^h = \tau_i^h, \quad i = 0,...,N. \tag{3.17}$$

As a result, we have obtained the difference problem (3.8), (3.10), (3.17) for determining the grid function ξ_i^h with estimates from (3.9) and (3.17) for the right-hand sides. To estimate this grid function, we prove the following result.

Lemma 3.1. *Let the smoothness conditions* (3.1)–(3.2) *be satisfied for the grid problem* (3.8)*,* (3.10)*,* (3.17) *with estimates from* (3.9) *and* (3.17) *for the right-hand sides. Then*

$$\max_{0\leqslant i\leqslant N}\left\|\xi_i^h\right\| \leqslant c, \quad \max_{1\leqslant i\leqslant N}\left\|\left(\xi_i^h - \xi_{i-1}^h\right)/h\right\| \leqslant c. \tag{3.18}$$

Proof. Put $z_i^h = \left(\xi_i^{h,1} - \xi_{i-1}^{h,1}\right)/h$. From here

$$\xi_i^{h,1} = \xi_{i-1}^{h,1} + hz_i^h \tag{3.19}$$

$$\xi_i^{h,1} - 2\xi_{i-1}^{h,1} + \xi_{i-2}^{h,1} = h(z_i^h - z_{i-1}^h).$$

Then it follows from (3.17) that

$$z_i^h - z_{i-1}^h = hJ(t_{i-1},\rho_{i-1}^h)\,\xi_{i-1}^{h,1} + h\tau_{i-1}^{h,1}.$$

Move the term z_{i-1}^h to the right side:

$$z_i^h = z_{i-1}^h + hJ(t_i,\rho_{i-1}^h)\,\xi_{i-1}^{h,1} + h\tau_{i-1}^{h,1}. \tag{3.20}$$

Let us introduce into consideration the vector with twice the number of components

$$v_i = \begin{pmatrix} \xi_i^{h,1} \\ z_i^h \end{pmatrix}.$$

Relations (3.19) and (3.20) can be written in matrix form

$$v_i = v_{i-1} + hDv_i + hB_i v_{i-1} + q_{i-1} \qquad (3.21)$$

with the matrices and the vector

$$B_i = \begin{pmatrix} 0 & 0 \\ J(t_{i-1}, \rho^h_{i-1}) & 0 \end{pmatrix}, \qquad D = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad q_{i-1} = h \begin{pmatrix} 0 \\ \tau^{h,1}_{i-1} \end{pmatrix}$$

respectively.

Let us resolve equation (3.21) with respect to v_i. For this purpose, we subtract from the left and right parts of this equation the expression hDv_i:

$$v_i - hDv_i = Ev_{i-1} + hB_i v_{i-1} + q_{i-1}$$

where E is identity matrix. Multiply the resulting equation by $(E-hD)^{-1}$:

$$v_i = (E-hD)^{-1}(E+hB_i)\, v_{i-1} + (E-hD)^{-1} q_{i-1}.$$

Rewrite it in the form

$$v_n = v_{i-1} + h\,(E-hD)^{-1}(D+B_i)\, v_{i-1} + (E-hD)^{-1} q_{i-1}. \qquad (3.22)$$

In space R^{2n}, we introduce the ‘uniform’ matrix norm consistent with the ‘uniform’ vector norm in R^{2n}:

$$\|A\| = \max_{1\leqslant i\leqslant 2n} \sum_{j=1}^{2n} \left|a_{i,j}\right|, \qquad A = \begin{pmatrix} a_{1,1} & \dots & a_{1,2n} \\ \dots & \dots & \dots \\ a_{2n,1} & \dots & a_{2n,2n} \end{pmatrix}.$$

Since

$$(E-hD)^{-1} = \begin{pmatrix} E & hE \\ 0 & E \end{pmatrix}$$

then

$$\left\|(E-hD)^{-1}\right\| = 1+h.$$

Assuming h small enough, we obtain the inequalities

$$\left\|(E-hD)^{-1}(D+B_i)\right\| \leqslant 2L, \quad \left\|(E-hD)^{-1} q_{i-1}\right\| \leqslant 2\left\|q_{i-1}\right\|.$$

The application of these inequalities in (3.22) gives the estimate

$$\|v_i\| \leqslant (1+2hL)\,\|v_{i-1}\| + 2\,\|q_i\|. \qquad (3.23)$$

Now prove the inequality

$$\|v_i\| \leqslant \exp(2ihL)\left(\sum_{j=1}^{i-1} \left\|q_j\right\| + \|v_1\|\right), \quad i = 2,\dots,N. \qquad (3.24)$$

Obviously, it is true for $i = 2$. Let us apply the method of induction. Assuming that it holds for some $i \geqslant 2$, we check it for $i+1$ using (3.23):

$$\|v_{i+1}\| \leqslant (1+2hL)\|v_i\| + 2\|q_i\| \leqslant (1+2hL)\exp(2ihL)\left(\sum_{j=1}^{i-1}\|q_j\| + \|v_1\|\right) + 2\|q_i\|$$
$$\leqslant \exp(2(i+1)hL)\left(\sum_{j=1}^{i}\|q_j\| + \|v_1\|\right).$$

To estimate $\|v_1\|$, we take equations (3.10) and (3.17) for $i = 0$. In view of (3.8), they imply the equalities

$$\xi_1^{h,1} + \xi_{-1}^{h,1} = h^2 \tau_0^{h,1}$$
$$\xi_1^{h,1} - \xi_{-1}^{h,1} = 2h\,\varphi_0^{h,1}.$$

Their half-sum and estimates from (3.9) and (3.16) imply the following inequalities:

$$\left\|\xi_1^{h,1}\right\| \leqslant \frac{h^2}{2}\left\|\tau_0^{h,1}\right\| + h\left\|\varphi_0^{h,1}\right\|$$
$$\|z_1\| = \frac{1}{h}\left\|\xi_1^{h,1}\right\| \leqslant \frac{h}{2}\left\|\tau_0^{h,1}\right\| + \left\|\varphi_0^{h,1}\right\|.$$

Therefore, for sufficiently small h we have

$$\|v_1\| \leqslant c.$$

Considering also the definition q_j with the estimate (3.18), the estimate (3.24) comes to (3.18) with the constant $2\exp(2TL)c$.

Thus, the lemma is proved as well as the final estimate (3.4) of the assertion of Theorem 3.1.

The resulting expansion (3.3) is of interest itself, since it is the key to the application of Richardson extrapolation [2, 7]. Recall that this technique consists in solving the difference problem (2.14)–(2.16) with p multiple steps and then linearly combining the obtained solutions to achieve the order of accuracy $O(h^{2p})$.

In the present paper, we offer to use the obtained expansion as the initial one to justify the successive increase in the accuracy order of the problems (2.20)–(2.22) solved on the same difference grid.

Meanwhile, the justification of expansions in the form (3.3) for solutions of intermediate problems (2.20)–(2.22) with numbers $k = 2,\ldots,p-1$ is associated with a huge amount of complex formulae, far beyond the scope of this article. Therefore, further on the theoretical level, we restrict ourselves for the first acquaintance with this approach to a relatively simple theoretical substantiation of the convergence for the fourth-order scheme (2.17)–(2.19).

Thus, let the following expansion be proved for the problem (2.14)–(2.16):

$$x_i^{h,1} = x_i + h^2 z(t_i) + h^4 \xi_i^h, \quad i = 0,\dots,N \tag{3.25}$$

where $z(t)$ is a vector function independent of h; ξ_i^h are values of the grid vector function depending on the choice of h but uniformly bounded in h:

$$\max_{0 \leqslant i \leqslant N} \left\| \xi_i^h \right\| \leqslant c. \tag{3.26}$$

Theorem 3.2. *Let problem* (1.1) *satisfy smoothness conditions* (3.1)*,* (3.2) *with* $p = 2$*. Then for the solution* $x_i^{h,2}$ *of the difference scheme* (2.17)–(2.19)*, the expansion is valid*

$$x_i^{h,2} = x_i + h^4 \zeta_i^h, \quad i = 0,\dots,N \tag{3.27}$$

with the uniform estimate

$$\max_{0 \leqslant i \leqslant N} \left\| \zeta_i^h \right\| \leqslant c. \tag{3.28}$$

Proof. Since $x_i^{h,2}$ and x_i are uniquely determined in the expansion (3.27), ζ_i^h it is also uniquely determined from it. Thus, it remains to prove estimate (3.28). We use the initial conditions (1.1) and (2.17) in expansion (3.27) for $i = 0$:

$$\zeta_0^h = 0. \tag{3.29}$$

Now substitute (3.27) into the left side of (2.18). Using the Taylor formula at the point $t = 0$, we arrive at the expansion

$$\frac{x_1^{h,2} - x_{-1}^{h,2}}{2h} = \sum_{r=0}^{1} \frac{h^{2r}}{(2r+1)!} x_0^{(2r+1)} + h^4 \varphi_0^{h,1} + h^4 \frac{\zeta_1^h - \zeta_{-1}^h}{2h}, \quad \left\| \varphi_0^{h,1} \right\| \leqslant c. \tag{3.30}$$

When substituting (3.27) into the right-hand side of (2.18), we first use the increment formula with respect to the second argument with the estimate of the remainder term:

$$x_0' + \frac{h}{12}\left(f(t_1, x_1^{h,1}) - f(t_{-1}, x_{-1}^{h,1}) \right) = x_0' + \frac{h}{12}\left(f(t_1, y_1^h) - f(t_{-1}, y_{-1}^h) \right) + h^4 \zeta_i^{h,1} \tag{3.31}$$

$$\left\| \zeta_i^{h,1} \right\| \leqslant c$$

where $y^h(t) = x(t) + h^2 z(t)$. After that, we use the Taylor formula for time at the point $t = 0$:

$$\frac{h}{12}\left(f(t_j, y_j^h) - f(t_{-j}, y_{-j}^h) \right) = \frac{jh^2}{6} f'(0, y^h(0)) + h^4 \zeta_0^{h,j}, \quad \left\| \zeta_0^{h,j} \right\| \leqslant c. \tag{3.32}$$

Now we use the Taylor formula for the second argument for the function $f_0' = \mathrm{d}f\big/\mathrm{d}t(0, y^h(0))$:

$$f'\left(0,\, x_0 + h^2 z(0)\right) = f'(0, x_0) + h^2 \sigma_0^{h,2}, \quad \left\|\sigma_0^{h,2}\right\| \leqslant c. \tag{3.33}$$

Introduce expansions (3.30)–(3.33) into equality (2.18):

$$\sum_{r=0}^{1} \frac{h^{2r}}{(2r+1)!} x_0^{(2r+1)} = h^4 \frac{\zeta_1^h - \zeta_{-1}^h}{2h} + x_0' + \frac{h^2}{6} f_0' + h^4 \rho_0^{h,3}, \quad \left\|\rho_0^{h,3}\right\| \leqslant c.$$

Since the first sum cancels out with two terms of order $O(1)$ and $O(h^2)$, after dividing by h^4 we arrive at the initial condition

$$\frac{\zeta_1^h - \zeta_{-1}^h}{2h} = \rho_0^{h,3}. \tag{3.34}$$

Now we substitute (3.27) into the left side of (2.19). Using the Taylor formula at the point $t = 0$, we get the expansion

$$\begin{aligned} \frac{x_{i+1}^{h,2} - 2x_i^{h,2} + x_{i-1}^{h,2}}{h^2} =& 2\sum_{r=0}^{1} \frac{h^{2r}}{(2r+2)!} x_i^{(2r+2)} + h^4 \eta_i^{h,1} + h^4 \frac{\zeta_{i+1}^h - 2\zeta_i^h + \zeta_{i-1}^h}{h^2} \\ & \left\|\eta_i^{h,1}\right\| \leqslant c. \end{aligned} \tag{3.35}$$

When substituting (3.27) and (3.25) into the right side of (2.19), we first use the increment formula for the second argument:

$$\begin{aligned} & f(t_i, x_i^{h,2}) + \frac{1}{12}\left(f(t_{i-1}, x_{i-1}^{h,1}) - 2f(t_i, x_i^{h,1}) + f(t_{i+1}, x_{i+1}^{h,1})\right) \\ & \quad = f(t_i, x_i) + h^4 J(t_i, \rho_i^{h,2})\, \zeta_i^h \\ & \qquad + \frac{1}{12}\left(f(t_{i-1}, y_{i-1}^h) - 2f(t_i, y_i^h) + f(t_{i+1}, y_{i+1}^h)\right) + h^4 \zeta_i^{h,1}, \quad \left\|\zeta_i^{h,1}\right\| \leqslant c \end{aligned} \tag{3.36}$$

where components of the vector $\rho_i^{h,2}$ belong to the intervals with ends determined by components of the vectors $x_i^{h,2}$ and x_i. After that, we use the Taylor formula for time at the point $t = 0$:

$$f(t_{i-1}, y_{i-1}^h) - 2f(t_i, y_i^h) + f(t_{i+1}, y_{i+1}^h) = h^2 f''(t_i, y_i^h) + h^4 \zeta_i^{h,2}, \quad \left\|\zeta_i^{h,2}\right\| \leqslant c. \tag{3.37}$$

Now we use the Taylor formula for the second argument for the function $f''(t_i, y_i^h) = \mathrm{d}^2 f\big/\mathrm{d}t^2(t_i, y_i^h)$:

$$f''\left(t_i,\, x_i + h^2 z_i\right) = f''\left(t_i,\, x_i\right) + h^2 \sigma_i^{h,2}, \quad \left\|\sigma_i^{h,2}\right\| \leqslant c. \tag{3.38}$$

We introduce expansions (3.35)–(3.38) into equality (2.19):

$$2\sum_{r=0}^{1}\frac{h^{2r}}{(2r+2)!}x_i^{(2r+2)}+h^4\,\frac{\zeta_{i+1}^h-2\zeta_i^h+\zeta_{i-1}^h}{h^2}$$
$$=f(t_i,x_i)+h^4J(t_i,\rho_i^{h,2})\,\zeta_i^h+\frac{h^2}{12}f''\,(t_i,\,x_i)+h^4\rho_i^{h,4},\quad \left\|\rho_i^{h,4}\right\|\leqslant c.$$

Since the first sum cancels out with two terms of order $O(1)$ and $O(h^2)$, after dividing by h^4 we arrive at the grid equation

$$\frac{\zeta_{i+1}^h-2\zeta_i^h+\zeta_{i-1}^h}{h^2}+J(t_i,\rho_i^{h,2})\,\zeta_i^h=\rho_i^{h,4},\quad i=1,\ldots,N-1. \tag{3.39}$$

As a result, we have obtained the difference problem (3.29), (3.34), (3.39) for determining the grid function ζ_i^h. To estimate this grid function, we use Lemma 3.1 that gives estimate (3.28). □

Expansion (3.27) indeed exhibits fourth-order convergence, since

$$\max_{0\leqslant i\leqslant N}\left\|x_i^{h,2}-x_i\right\|\leqslant h^4\left\|\zeta_i^h\right\|\leqslant ch^4.$$

4. Computational illustration

To illustrate the successive increase in the order of accuracy of the schemes used, consider the one-dimensional problem

$$x''(t)=-36x,\quad t\in[0,2]$$
$$x(0)=1,\quad x'(0)=0$$

with the exact solution $x(t)=\cos(6t)$. The results of the successive application of difference schemes (2.14)–(2.16), (2.17)–(2.19), and (2.20)–(2.22) for $k=3$ are given in Table 3 and indeed give a successive increase in the order of convergence by two units. Note that the scheme (2.17)–(2.19) really serves as a corrector for the previous scheme and a predictor for the next one. Here $e^{h,k}=\max_{0\leqslant i\leqslant N}\left\|x_i^{h,k}-x_i\right\|$ is the maximum error of the difference solution $x^{h,k}(t)$ on a grid with a step h, and $s^{h,k}=\log_2\left(e^{2h,k}/e^{h,k}\right)$ is the order of convergence of the difference solution with the number k.

5. Conclusion

So, we presented an approach for constructing a sequence of difference schemes with the properties of a predictor and a corrector with an increasing order of convergence based on the application of the Störmer method with additional corrective terms calculated using the previous predictor solutions. The approach is essentially

Table 3. Convergence order of difference schemes.

	Difference scheme (2.14)–(2.16), $k = 1$		Difference scheme (2.17)–(2.19), $k = 2$		Difference scheme (2.20)–(2.22), $k = 3$	
Step h	$e^{h,1}$	$s^{h,1} \approx 2$	$e^{h,2}$	$s^{h,2} \approx 4$	$e^{h,3}$	$s^{h,3} \approx 6$
0.1	0.1677		0.01937		0.0009193	
0.05	0.04172	2.01	0.001141	4.08	1.355e-5	6.08
0.025	0.01037	2.01	6.377e-5	4.16	2.103e-7	6.01
0.0125	0.002589	2.00	3.635e-6	4.13	3.373e-9	5.96
0.00625	0.0001617	2.00	2.149e-7	4.08	5.597e-11	5.91

within the framework of Defect Correction Methods [2], but instead of a polynomial approximation of the residual, an approximation of the approximation error is used, which is explicitly expressed through the right-hand side, in this case, the second derivative of the solution. The approach of correction by higher order differences [9, 16] is similar in idea. But in our approach, the correcting differences are taken not for approximate solutions, but for the right-hand sides, which lowers the order of the differences by 2.

A good difference from explicit multistep symmetric difference schemes [4, 6–8, 11, 14] is the unconditional stability (periodicity) of the Störmer difference scheme used with different right-hand sides. The point is that explicit multistep high-order symmetric difference schemes have a smaller stability (periodicity) interval with an increase in the order of approximation [6, 7, 11]. Moreover, these intervals can be isolated from zero. This can lead to an unexpected loss of periodicity as the grid step decreases [7].

Subsequently, we will compare the results of applying the presented approach to solving orbital tasks.

As a perspective of using this approach, we note that the use of Numerov implicit difference scheme with corrective additions promises an increase in the order of convergence by 4 for each subsequent scheme, and not by 2 as for the Störmer scheme with corrections.

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