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On Crank–Nicolson schemes for non-stationary problems with operators reducible to skew-symmetric form

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Abstract – Higher-order accurate Crank–Nicolson schemes are obtained for solving homogeneous and inhomogeneous Cauchy's problems with operators reducible to a skew-symmetric form. The phase error is diminished owing to a special algorithm of choosing time-steps. For homogeneous problems, by using complex time-steps we obtain difference schemes with an accuracy of $\mathcal{O}(\tau^6)$, $\mathcal{O}(\tau^8)$. On the basis of the difference schemes the algorithms for numerical solution of diffraction problems are presented and the results of calculations are given.

The Crank–Nicolson difference schemes are known to retain the solution norm in the problems with skew-symmetric operators (see, for example, [4]). Therefore an error arising in calculations with the use of these schemes is of a phase nature.

In this paper, owing to a special choice of the time-step sequence τ_n, we construct Crank–Nicolson difference schemes with an accuracy of $\mathcal{O}(\tau^4)$, $\mathcal{O}(\tau^6)$, $\mathcal{O}(\tau^8)$ in the phase, where τ is the average size of the time–step. Some of the schemes considered are schemes with complex steps. Difference schemes are suggested for solving a diffraction problem.

1. INCREASING THE ACCURACY OF CRANK–NICOLSON DIFFERENCE SCHEMES BY CHANGING VARIABLE TIME-STEPS

Let A be an operator reducible to a skew-symmetric form with the aid of an invertible operator Z: $ZAZ^{-1} = -(ZAZ^{-1})^* = B$. Consider a Cauchy problem for a differential equation with the time-independent operator A:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Au, \qquad u\big|_{t=0} = u^0, \qquad t \in [0,T]. \tag{1.1}$$

The exact solution of the problem is obtained in the form:

$$u(t) = \exp(At)u^0, \qquad Zu = \exp(Bt)Zu^0 \tag{1.2}$$

where $\exp(At)$ is an operator exponent.

Let $\{\varphi_i\}$, $\{\lambda_i\}$, $i = 1,2,\ldots,$ be a complete set of eigenvectors and eigenvalues for the operator A. Expand the solution into a Fourier series

$$u(t) = \sum_k c_k \exp(t\lambda_k)\varphi_k \tag{1.3}$$

where

$$u^0 = \sum_k c_k \varphi_k .$$

As the operator exponent of a skew-symmetric operator B is a unitary operator, we have

$$\|Zu(t)\| = \|Zu^0\|. \tag{1.4}$$

Consider now the Crank–Nicolson-type difference scheme:

$$\begin{aligned} \tilde{u}_{i+1} &= (I - \tau_i A)^{-1}(I + \tau_i A)\tilde{u}_i, \quad i = 0,1,\ldots \\ u^0 &= u(0) \end{aligned} \tag{1.5}$$

where the steps τ_i will vary with the index i, and assume that $|\tau_i| = \mathcal{O}(t)$ and $t > 0$ is small.

After n steps, the transition operator is of the form $R_n(A)$, where

$$R_n(x) = \prod_{i=1}^{n} (1 - \tau_i x)^{-1}(1 + \tau_i x). \tag{1.6}$$

The operator $ZR_n(A)Z^{-1} = R_n(B)$ will be a unitary operator for every n due to the operator's B being skew-symmetric. Hence

$$\|Z\tilde{u}_n\| = \|Zu^0\|. \tag{1.7}$$

This implies that the property of retaining the norm will also hold for difference scheme (1.5).

Now let us examine an error induced by the scheme itself.

Assume that $\|Zu(0)\| = 1$, $\|Z^{-1}B^{2r+1}\| \leqslant M_r$. The difference between the exact solution $Zu = \exp(Bt)Zu_0$ and the approximate solution $Z\tilde{u} = R_n(B)Zu_0$ of problem (1.1) is

$$\begin{aligned} u - \tilde{u} &= Z^{-1}(\exp(Bt) - R_n(B))Zu^0 = Z^{-1}(I - \exp(\ln(R_n(B)) - Bt))Zu \\ &= Z^{-1}(I - \exp(\ln(R_n(B)) - Bt))\exp(Bt)Zu^0 \end{aligned}$$

where

$$\ln(R_n(B)) = \sum_i \ln(R_n(\lambda_i))P_i$$

and P_i is a projector onto the subspace, which is a span of the eigenvector $Z\varphi_i$. Using the expansion

$$\ln\frac{1+x}{1-x} = 2\sum_{m=0}^{\infty} \frac{x^{2m+1}}{2m+1}$$

we obtain

$$u - \tilde{u} = Z^{-1}(I - \exp(\mathcal{D}_n(B))Zu = (\exp(-\mathcal{D}_n(B)) - I)Z\tilde{u} \tag{1.8}$$

where

$$\mathcal{D}_n(x) = \sum_{m=0}^{\infty} 2\sum_{i=1}^{n} \frac{(\tau_i x)^{2m+1}}{2m+1} - xt. \tag{1.9}$$

Let for some $r \geqslant 1$ the steps τ_i satisfy the relations:

$$2\sum_{i=1}^{n} \tau_i = t, \quad \sum_{i=1}^{n} \tau_i^3 = 0, \; \dots, \; \sum_{i=1}^{n} \tau_i^{2r-1} = 0. \tag{1.10}$$

Then the first non-zero term in (1.9) will be a function of $\tau_1, \dots, \tau_n$ of order $\mathcal{O}(t^{2r+1})$ or, more precisely,

$$\mathcal{D}_n(x) = B_r(\tau_1, \dots, \tau_n)(x)^{2r+1} + \mathcal{O}(t^{2r+2}) \tag{1.11}$$

where

$$B_r = \frac{2}{2r+1} \sum_{i=1}^{n} \tau_i^{2r+1}. \tag{1.12}$$

Hence we have

$$\|I - \exp(\mathcal{D}_n(B))\| = \|I - I - \mathcal{D}_n(B) - \mathcal{D}_n(B)/2! - \dots\|$$

$$\leqslant \|\mathcal{D}_n(B)\|(1 + \mathcal{O}(t)) \leqslant M_r B_r (1 + \mathcal{O}(t)) = \mathcal{O}(t^{2r+1})$$

and, similarly,

$$\|\exp(-\mathcal{D}_n(B)) - I\| \leqslant M_r B_r (1 + \mathcal{O}(t)) = \mathcal{O}(t^{2r+1}).$$

Hence

$$\|u - \tilde{u}\| \leqslant M_r B_r (1 + \mathcal{O}(t)) = \mathcal{O}(t^{2r+1}). \tag{1.13}$$

For the phase error we have

$$\varphi = 2\arcsin(\|u - \tilde{u}\|/2) = M_r B_r (1 + \mathcal{O}(t)) = \mathcal{O}(t^{2r+1}). \tag{1.14}$$

Consider now some solutions of system (1.10) for different n. These solutions define algorithm (1.5) for solving problem (1.1). In this algorithm the sequence of time-steps is repeated cyclically with period n and by a certain rule. The time-steps are proportional to a small parameter t, which is chosen from the conditions of local approximation.

Consider some examples.

(1) Let $n = 3$, $r = 2$. Choose τ_1, τ_2, τ_3 so that $\tau_1 = \tau_2$. Then conditions (1.10) take the form:

$$2\tau_1 + \tau_3 = \frac{t}{2}, \qquad -2\tau_1^3 = \tau_3^3.$$

Thus, we have

$$\tau_1 = \tau_2 = \frac{t}{2(2 - \sqrt[3]{2})}, \qquad \tau_3 = \frac{-\sqrt[3]{2}\,t}{2(2 - \sqrt[3]{2})} \tag{1.15}$$

i.e.

$$\tau_3 = -\sqrt[3]{2}\,\tau_1.$$

It is seen from (1.15) that the step τ_3 is negative while τ_1 and τ_2 are positive. Thus, for problem (1.1) with a skew-symmetric operator, the scheme has the phase error $\mathcal{O}(\tau^5)$ and is absolutely exact with respect to the norm.

Check numerically scheme (1.5) with parameters (1.15) for the problem with a 2×2 skew-symmetric matrix:

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \mathbf{u}(t), \qquad \mathbf{u}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

The differences between the exact solution of this problem and the solutions obtained by the method with constant steps $\tau_1 = \tau_2 = \tau_3 = t/6$ and the method with step sequence (1.15) are listed in Table 1 for different t.

For this scheme Figure 1 shows graphs of e^{-z} and $R_3(z)$ for real z: e^{-z} (curve 4) and its approximation $R_3(z)$ (curve 1). Figure 2 shows real and imaginary parts of e^{-z} and $R_3(z)$ for pure imaginary z: $\cos y$ (curve 4) and its approximation $\mathrm{Re}(R_3(z))$ (curve 1), $\sin y$ (curve 8) and its approximation $\mathrm{Im}(R_3(z))$ (curve 5).

In the general case, when $n \geqslant 3$, for finding τ_i we use the following method: let

$$\sigma_1 = \sum_{i=1}^{n} \tau_i, \ldots, \qquad \sigma_n = \tau_1 \tau_2 \cdots \tau_n$$

be elementary symmetric functions of $\tau_1, \tau_2, \ldots, \tau_n$, and

$$S_k = \sum_{i=1}^{n} \tau_i^k.$$

Table 1.

t	Constant-step method	Variable-step method
0.2	7.4×10^{-5}	2.0×10^{-5}
0.1	9.0×10^{-6}	1.0×10^{-6}
0.05	1.157×10^{-6}	2.107×10^{-8}

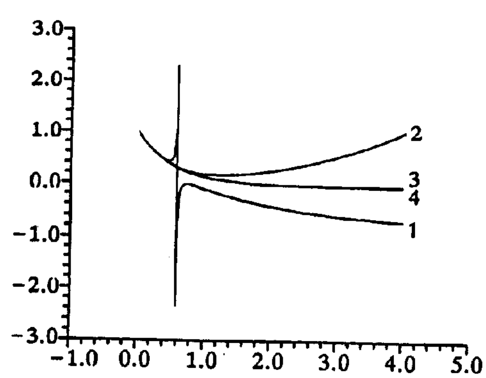

Figure 1.

Consider the system of r equations:

$$S_1 = 1, \quad S_{2k-1} = 0, \quad k = 2,\dots,r. \tag{1.16}$$

For $r < n-1$, some τ_i in (1.16) may be considered as free parameters.

Using Newton's formulae we express the values of S_{2k-1} in terms of σ_i, $i = 1,\dots,n$, to obtain an equivalent system of equations for σ_i, $i = 1,\dots,n$. Having solved this system we find the roots x_i, $i = 1,\dots,n$, of the equation:

$$x^n - x^{n-1} + \sigma_2 x^{n-2} - \dots + (-1)^n \sigma_n = 0. \tag{1.17}$$

Then $\tau_i = x_i t/2$ and the coefficient B_r in the remainder term in (1.11) is explicitly defined in terms of σ_i:

$$B_r = \frac{2S_{2r+1}}{2r+1}\left(\frac{t}{2}\right)^{2r+1} \tag{1.18}$$

(2) Let $n = 3$; then we find from (1.16) that

$$\sigma_2 = \sigma_3 + \tfrac{1}{3}, \quad S_5 = \tfrac{1}{3}(5\sigma_2 - 2). \tag{1.19}$$

Thus, equation (1.17) has the form:

$$x^3 - x^2 + (\sigma_3 + \tfrac{1}{3})x - \sigma_3 = 0. \tag{1.20}$$

Imposing the requirement that two roots of equation (1.20) be identical, we obtain solution (1.15). Now let $r = 3$ then according to (1.19), $S_5 = 0$, i.e. $\sigma_2 = 2/5$ and $\sigma_3 = 1/15$. Subject to these conditions, the roots of equation (1.19) are

$$\begin{aligned} x_1 &= -0.1236886881517035 \\ x_{2,3} &= 0.5618443440758517 \pm 0.472565881923747\,\mathrm{i}. \end{aligned} \tag{1.21}$$

In addition, we have $S_7 = 1/15^2$, i.e. according to (1.7), $B_3 = t^7/(7 \times 120^2)$.

For this scheme Figure 1 gives a graph of $R_3(z)$ for real z: $R_3(x)$ (curve 2). Figure 2 gives real and imaginary parts of $R_3(z)$ for pure imaginary z: $\mathrm{Re}(R_3(z))$ (curve 2) and $\mathrm{Im}(R_3(z))$ (curve 6).

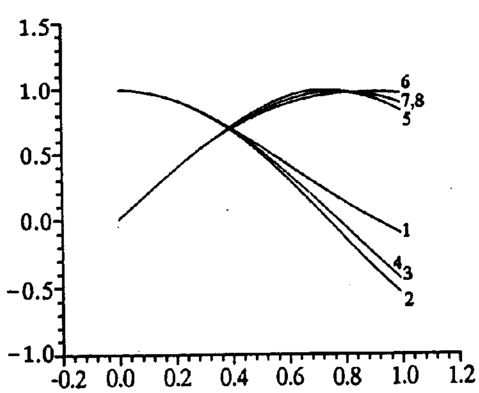

Figure 2.

(3) Let $n = 4$. We find from (1.16) that

$$\sigma_2 = \tfrac{2}{5} + 3\sigma_4, \quad \sigma_3 = \tfrac{1}{15} + 3\sigma_4, \quad S_7 = \tfrac{1}{15}(\tfrac{1}{15} - 7\sigma_4).$$

Thus, equation (1.17) takes the form:

$$x^4 - x^3 + (\tfrac{2}{5} + 3\sigma_4)x^2 - (\tfrac{1}{15} + 3\sigma_4)x + \sigma_4 = 0. \tag{1.22}$$

Let $r = 4$, then $S_7 = 0$, hence $\sigma_2 = 3/7$, $\sigma_3 = 2/21$, $\sigma_4 = 1/105$. For these values the roots of equation (1.22) will be complex conjugate:

$$\begin{aligned} x_{1,2} &= 0.3168675194685621 \pm 0.0948820251422306\,\mathrm{i} \\ x_{3,4} &= 0.183132480531438 \pm 0.2313252260262510\,\mathrm{i} \end{aligned} \tag{1.23}$$

and $S_9 = -1/11025$, i.e. $B_4 = -t^9/1260^2$.

For this scheme Figure 1 illustrates a graph of $R_4(z)$ for real z: $R_4(x)$ (curve 3). Figure 2 illustrates real and imaginary parts of $R_4(z)$ for pure imaginary z: $\mathrm{Re}(R_4(z))$ (curve 3) and $\mathrm{Im}(R_3(z))$ (curve 7).

The following theorem is known (see, for example, [1]).

Theorem 1.1. The only rational function with the power of the numerator equal to k and the power of the denominator equal to m that approximates the exponent e^{-z} with an accuracy of $\mathcal{O}(m + k)$ is the (k,m) Pade approximation of the exponent:

$$Q_{k,m} = \frac{\sum_{i=0}^{k} \frac{k!}{(k-i)!} \frac{(m+k-i)!}{(m+k)!} \frac{(-z)^i}{i!}}{\sum_{i=0}^{k} \frac{m!}{(m-i)!} \frac{(m+k-i)!}{(m+k)!} \frac{(z)^i}{i!}}. \tag{1.24}$$

Therefore, when $n = r$, transition operator (1.6) approximates the exponent with an accuracy of $2n$, i.e. it is identical with the (n,n) Pade approximation; hence the parameters x_i, $i = 1,\ldots,n$, are the roots of the equation:

$$\sum_{i=0}^{k} \frac{k!}{(k-i)!} \frac{(2k-i)!}{(2k)!} \frac{(-2x)^{k-i}}{i!} = 0. \tag{1.25}$$

For $n = 3$ and $n = 4$ the parameters x_i are given in (1.21) and (1.23), respectively.

The schemes with parameters (1.21) and (1.23) lead to complex time-steps. Therefore while implementing the transition operator $R_n(A)$ (1.6), different approaches are possible. For example, one can perform calculations in complex numbers or, taking into account the fact that the factors in (1.6) commute with one another, one can combine complex conjugate operators into a single operator and implement it in a real space.

2. CONSTRUCTING FOURTH-ORDER ACCURATE METHOD FOR A SYSTEM OF NON-LINEAR ORDINARY DIFFERENTIAL EQUATIONS

Let us consider an s-stage Runge–Kutta method for a system of ordinary differential equations with a sufficiently smooth right side:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y,t) \tag{2.1}$$

$$\begin{aligned} Y^i &= y_n + h\sum_{j=1}^{s} a_{ij} f(Y^j, t_n + c_j h), \qquad j = 1,\dots,s \\ y_{n+1} &= y_n + h\sum_{j=1}^{s} b_i f(Y^i, t_n + c_i h). \end{aligned} \tag{2.2}$$

Method (2.2) can be represented schematically as a Butcher table:

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \qquad \text{or} \qquad \begin{array}{c|c} \mathbf{c} & M \\ \hline & \mathbf{b}^{\mathrm{T}} \end{array} \tag{2.3}$$

where $\mathbf{b} = (b_1, b_2, \dots, b_s)^{\mathrm{T}}$, $\mathbf{c} = (c_1, c_2, \dots, c_s)^{\mathrm{T}}$, and M is the matrix with elements a_{ij}.

Harrier and Wanner [2] showed that for the order of accuracy of method (2.2) to be p it is necessary and sufficient that the parameters of the method satisfy the relations:

$$\begin{aligned} p = 1 \quad & (1)\ (a)\ \sum b_i = 1, \quad (b)\ c_i = \sum_j a_{ij} \\ p = 2 \quad & (2)\ \sum b_i a_{ij} = \sum b_i c_i = \tfrac{1}{2} \\ p = 3 \quad & (3)\ \sum b_i c_i^2 = \tfrac{1}{3}, \quad (4)\ \sum b_i a_{ij} a_{ik} = \tfrac{1}{6} \\ p = 4 \quad & (5)\ \sum b_i c_i^3 = \tfrac{1}{4}, \quad (6)\ \sum b_i c_i a_{ij} c_i = \tfrac{1}{8} \\ & (7)\ \sum b_i a_{ij} c_j^2 = \tfrac{1}{12}, \quad (8)\ \sum b_i a_{ij} a_{jk} a_{kl} = \tfrac{1}{24}. \end{aligned} \tag{2.4}$$

In Section 1 we constructed a series of methods, which, having been combined, yield a phase error of order $\mathcal{O}(h^{q+1})$, where $q = 4,6,8$, and retain the norm of solution for problem (1.1). For linear homogeneous problems the order of accuracy of these methods is $p = q$. However, for problems of the form of (2.1), due to their being inhomogeneous and non-linear, the order of accuracy of the methods is 2. We will construct a fourth-order accurate Runge–Kutta method that retains the norm of solution for problems of the type of (1.1), the so-called P-stable method [6].

The stability function of an s-stage method is a rational function in which the numerator and denominator are polynomials of degree no greater than s. The stability function can be expressed in terms of the parameters of method (2.3) by the formula [1]:

$$R(z) = 1 + \mathbf{b}^{\mathrm{T}}(I - zM)^{-1}\mathbf{e} = \frac{\det(1 - zM + z\mathbf{e}\mathbf{b}^{\mathrm{T}})}{\det(1 - zM)} \tag{2.5}$$

where $\mathbf{e} = (1,1,\ldots,1)^{\mathrm{T}}$ is the s-dimensional vector. It is seen from (2.5) that for small z

$$R(z) = 1 + \sum_{j=0}^{\infty} \mathbf{b}^{\mathrm{T}} M^{j} \mathbf{e} z^{j+1}. \tag{2.6}$$

For the method to be P-stable it is necessary that for $z = \mathrm{i}\lambda$, $\lambda \in (-\infty, \infty)$,

$$|R(z)| = 1. \tag{2.7}$$

While constructing method (2.2) we consider $R(z)$ to be of the form:

$$R(z) = \frac{1 + \sum_{i=1}^{s} d_i z^i}{1 + \sum_{i=1}^{s} d_i(-z)^i} = \frac{\prod_{i=1}^{s}(1 + \alpha_i z)}{\prod_{i=1}^{s}(1 - \alpha_i z)} \tag{2.8}$$

where $\alpha_i = a_{ii}$, $i = 1,\ldots,s$, then d_i will be symmetric functions of α_i.

It is seen from (2.5) that the roots of the denominator $R(z)$ are eigenvalues of the matrix M. In the sequel, we will construct Runge–Kutta methods for which $a_{ij} = 0$ at $i < j$, i.e. the matrix M is lower triangular. Hence for (2.8) to hold it is necessary that $\alpha_i = a_{ii}$, $i = 1,\ldots,s$.

The product $R(z)\prod_{i=1}^{s}(1 - a_{ii}z)$ is a polynomial of the third degree. The conditions to be imposed on the method parameters for the stability function to have the form of (2.8) can be found by using the equality

$$R(z)\prod_{i=1}^{s}(1 - a_{ii}z) - \prod_{i=1}^{s}(1 - a_{ii}z) = 0.$$

Substituting expansion (2.6) in the equality and equating the sum of factors in the equal-degree terms to zero, we obtain the relations

$$\begin{aligned}
&\sum b_i - 2d_1 = 0\\
&\sum b_i a_{ij} - \sum b_i d_1 = 0\\
&\sum b_i a_{ij} a_{jk} - \sum b_i a_{ij} d_1 + \sum b_i d_2 - 2d_3 = 0\\
&\sum b_i a_{ij} a_{jk} a_{km} - \sum b_i a_{ij} a_{jk} d_1 + \sum b_i a_{ij} d_2 - \sum b_i d_3 = 0.
\end{aligned} \tag{2.9}$$

It follows from relations (2.9) that for the stability function to approximate the exponent with the fourth-order accuracy and to be of the form of (2.8) it is necessary that conditions (1), (2), (4) in (2.4) and

$$d_1 = \sum_{i=1}^{s} a_{ii} = \frac{1}{2}, \quad 2d_3 - d_2 = 2\sum_{i<j<k}^{s} a_{ii}a_{jj}a_{kk} - \sum_{i<j}^{s} a_{ii}a_{jj} = -\frac{1}{12} \tag{2.10}$$

be fulfilled. Note also that equations (2.10) give a monoparametric family of solutions of system (2.9) and a unique solution exists, which coincides with the (s,s) Pade approximation, for which the stability function approximates the exponent with order $2s$. However, in this case we obtain complex-valued parameters a_{ii} and to avoid calculations with complex numbers we choose the parameters d_i so that a_{ii} be real. If we put $a_{ii} = \tau_i$, $i = 1,\ldots,s$, $s = 3$, where τ_i are taken from (1.15) then relations (2.10) will hold. Moreover, if relations (1), (2), (4) in (2.4) hold then (8) in (2.4) will also hold. The remaining parameters of the method will be found from conditions (2.4). In this case there are nine equations in eight unknowns. Nevertheless, in the case under consideration there exists a solution for which all relations (2.4) are satisfied.

Let $a_{11} = a_{22} = \tau_1$, $a_{33} = \tau_3$, where τ_i are taken from (1.15). Then

$$c_1 = a_{11} \tag{2.11}$$

b_1 will be a parameter, and the remaining b_i and c_i, $i = 2,3$, will be found from relations (1), (2), (3), (5) in (2.4):

$$b_2 + b_3 = 1 - b_1 = f_1$$

$$b_2c_2 + b_3c_3 = 1 - b_1c_1 = f_2$$

$$b_2c_2^2 + b_3c_3^2 = 1 - b_1c_1^2 = f_3$$

$$b_2c_2^3 + b_3c_3^3 = 1 - b_1c_1^3 = f_4 .$$

The solution of the system has the form:

$$c_{3,2} = \frac{-l_1 \pm \sqrt{l_1 - 4l_0}}{2} \tag{2.12}$$

where

$$l_0 = \frac{-f_3^2 + f_2f_4}{f_1f_3 - f_2^2}, \quad l_1 = \frac{-f_1f_4 + f_2f_4}{f_1f_3 - f_2^2}, \quad b_2 = \frac{f_1c_3 - f_2}{c_3 - c_2}, \quad b_3 = \frac{f_2 - f_1c_2}{c_3 - c_2}.$$

Parameters a_{31} and a_{32} are found from the linear system of equations:

$$b_3c_1a_{31} + b_3c_2a_{32} = \frac{1}{6} - b_3c_3a_{33} - \sum_{i<3} b_ic_ja_{ij} = \xi_1$$

$$a_{31} + a_{32} = c_3 - a_{33} = \xi_2 \tag{2.13}$$

$$a_{31} = \frac{\xi_1 b_3c_2 - \xi_2}{b_3(c_2 - c_1)}, \quad a_{32} = \frac{\xi_2 - c_1b_3c_1}{b_3(c_2 - c_1)}.$$

Parameters (2.12) and (2.13) define a family of the schemes that depends on the parameter b_1. Let us consider some of these schemes.

For $b_1 = 0$ the order of accuracy of the method is 3, however, its parameters satisfy relations (5), (8) in (2.4). Hence for some classes of problems the order of accuracy of such a method is 4, for example, for problem (1.1):

(2.14)

0.67560359597982	0.67560359597982	0	0
0.21132486540518	−0.46427873057464	0.67560359597982	0
0.78867513459481	1.78558235476376	−0.14570002820929	−0.8512071919596
	0	0.5	0.5

For $b_1 = 0.67296857785705738$ all relations (2.4) hold and the order of accuracy of the method is 4:

(2.15)

0.67560359597982	0.67560359597982	0	0
0.10314973700795	−0.57245385897187	0.67560359597982	0
1.85120719195965	−7.97339753367139	10.6758119206332	−0.8512071919596
	0.672968577785705	0.3203915925434	0.00663982959946

In conclusion, let us write down convenient design formulae for problems of the form:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Au + f(t). \tag{2.16}$$

To obtain a solution of problem (2.16) by formulae (2.14) or (2.15), we solve s ($s = 3$) equations of the form:

$$(I - ha_{ii}A)Y^i = F_i, \qquad i = 1,\dots,s, \qquad s = 3$$

where

$$F_i = y_n + h\sum_{j=1}^{s-1} a_{ij}(AY^j + f(t_n + c_jh)) + a_{ii}hf(t_n + c_ih)$$

$$y_{n+1} = y_n + h\sum_{j=1}^{s} b_i(AY^i + f(t_n + c_jh)).$$

3. NUMERICAL SOLUTION OF DIFFRACTION PROBLEM

Consider the following problem:

$$\frac{\partial F}{\partial z} = \mathrm{i}K\frac{\partial^2 F}{\partial x^2}, \qquad z \in (0,Z], \qquad x \in (-1,1) \tag{3.1}$$

$$F\big|_{z=0} = F_0(x) \tag{3.2}$$

$$F\big|_{x=-1} = F\big|_{x=1} = 0. \tag{3.3}$$

Equation (3.1) occurs in studying the diffraction of a plane electromagnetic wave on a slit. In this case $F_0(x)$ is the amplitude of the wave incident on the screen, $F(x,z)$ is the amplitude of the diffracted wave at a point (x,z) behind the screen, k is the wave number ($k = 2\pi\lambda$, where λ is a wavelength). It is assumed that the slit $(-d,d)$, where $0 < d < 1$, is at the centre of the screen $[-1,1]$, the wave is incident normally to the screen, the screen and the slit are infinitely long; the slit is allowed for in the initial condition, namely in the function $F_0(x)$.

The solution of problem (3.1)–(3.3) will be sought by using the finite difference method. To this end, we first of all construct a second-order accurate approximation to this problem with respect to x. Let x_i, $i = 0,\dots,N$, be a uniform grid with step h on the segment $-1 \leqslant x \leqslant 1$: $x_i = -1 + ih$, $h = 2/N$. Then, taking into account boundary conditions (3.3), we arrive at the following difference-differential problem:

$$\frac{\partial \hat{F}}{\partial z} = \mathrm{i}A\hat{F} \tag{3.4}$$

$$\hat{F}\Big|_{z=0} = \hat{F}_0 \tag{3.5}$$

where A is the tridiagonal matrix, while $\hat{F}(z)$ is the vector function defined at the nodes of the grid x_i:

$$A = \frac{K}{h^2}\begin{bmatrix} -2 & 1 & & \text{O} \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ \text{O} & & 1 & -2 \end{bmatrix}, \quad \hat{F}(z) = \begin{bmatrix} \hat{F}_1(z) \\ \vdots \\ \hat{F}_{N-1}(z) \end{bmatrix}, \quad \hat{F}_i(z) = F(x_i,z). \tag{3.6}$$

To solve problem (3.4), (3.5) we apply the Crank–Nicolson-type difference scheme:

$$\frac{F^{j+1} - F^j}{\tau_j} = \frac{1}{2}\mathrm{i}A(F^{j+1} + F^j), \qquad F^0 = \hat{F}^0 \tag{3.7}$$

where $F^j = \hat{F}(z_i)$ is an $(N-1)$-dimensional vector, while τ_j are variable steps over z, which will be considered complex: $\tau_j = \tau_{1j} + i\tau_{2j}$.

Then, to find F^{j+1} we obtain a linear system of algebraic equations with the tridiagonal matrix

$$\Lambda F^{j+1} = \bar{\Lambda} F^j \tag{3.8}$$

where $\Lambda = I - \frac{1}{2}\mathrm{i}\tau A$ (I is the $(N-1)\times(N-1)$ identity matrix) and the overscribed bar denotes a complex conjugate.

Let $F(x,z) = u(x,z) + \mathrm{i}v(x,z)$ and $F^j = u^j + \mathrm{i}v^j$, where u^j and v^j are the vectors of dimension $N-1$. We will solve system (3.8) by using only real numbers. In this case at each step, a solution is sought by the formulae:

$$D_j u^{j+1} = B_j u^j + C_j v^j \tag{3.9}$$

$$v^{j+1} = v^j + \frac{1}{\tau_{1j}}(\tau_{2j}(u^{j+1} - u^j) + \tfrac{1}{2}(\tau_{1j}^2 + \tau_{2j}^2)A(u^{j+1} + u^j)) \tag{3.10}$$

[redacted]