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Symbolic-Numerical Method for the Stability Analysis of Difference Schemes on the Basis of the Catastrophe Theory

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We propose a symbolic–numerical method for the stability analysis of *difference initial-value problems approximating initial-value problems* for the systems of partial differential equations of hyperbolic or parabolic type. The basis of the method is constituted by the Fourier method. It is proposed to use the catastrophe theory for an analysis of the manifold of characteristic equation zeros. This equation is derived automatically by symbolic computations which also enables us to automatically generate some FORTRAN subroutines needed for the analysis within the framework of the catastrophe theory. Examples of the application of the developed method are presented. In particular, the necessary stability condition has been obtained for the two-cycle MacCormack scheme of 1969. © 1995 Academic Press, Inc.

1. INTRODUCTION

An important criterion affecting the choice of a difference method for solving problems of mathematical physics and computational fluid dynamics is the stability of a corresponding numerical algorithm. One of the practical methods for the stability investigation of numerical approximations is the Fourier method [1]. However, the application of this method to the stability analyses of difference schemes (d.s.) approximating the partial differential equations whose solutions depend on spatial variables $x_1, ..., x_L$, $L \geqslant 1$, and the time t often proves to be laborious or practically impossible because of the complexity of arising analytic computations. The symbolic computations enable one to carry out all the analytic computations which are characteristic of the Fourier method on a computer. The first work in this direction was published by Wirth [2]. He used a system of analytic computations (SAC) MACSYMA to develop a program package FSTAB for the stability analysis of difference initial-value problems by the Fourier method. The characteristic equation of the difference scheme was derived in FSTAB symbolically and then the stability condition was derived manually. However, in many practically important cases the complexity of arising analytic expressions does not enable one to obtain the desired stability conditions in an analytic form. In this connection it is reasonable to combine *the symbolic computations with the numerical ones with the* purpose of a complete automation of the stability investigation of difference initial-value problems. One of the first works in which this goal was achieved was [3]. In this work the Routh–Hurwitz and Lienard–Chipart criteria [4] were used for the analysis of the distribution of the characteristic polynomial zeros in the complex plane. The left-hand sides of the inequalities obtained from these criteria were derived symbolically on a computer, and then a FORTRAN subroutine was generated automatically for the subsequent numerical computation of the values of the left-hand sides of the above inequalities. The coordinates of points of the stability region boundary were then computed numerically to a given accuracy by solving an optimization problem (see also [5, 6]). The Soviet SAC REFAL was used in [3, 5, 6] for the symbolic computations. In [7] the SAC REDUCE [8] was used for the symbolic computation of the Hurwitz determinant inequalities equivalent to the von Neumann stability criterion [1]. In [9] the SAC REDUCE was used only for the symbolic computation of the characteristic equation coefficients. The localization of the zeros of this equation with respect to the unit disc was then performed numerically with the aid of a modified Routh algorithm. This modification of the Routh algorithm [4] was aimed at the reduction of the roundoff errors accumulation by using the machine arithmetic of stored orders [10] and the balancing of certain 2×2 matrices. This modified algorithm enables one to determine the stability regions of difference schemes for complex real-life problems [6].

The symbolic computations were also used for the stability analyses of difference initial- and boundary-value problems. The pioneering result in this direction was the program package IBSTAB [11–13]. This program implements an algorithm for automatic stability investigation according to the theory of Gustafsson, Kreiss, and Sundström [14]. The symbolic–numeric code SPECTR

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using the SAC REDUCE and the FORTRAN language was developed by Mazepa [15–17] also for the automatic stability analysis of difference initial- and boundary-value problems. The algorithm implemented in the program SPECTR mainly follows the theoretical results of Kreiss [18, 14]. The practical application of these results is difficult because it leads to a complex algebraic problem on finding all zeros z, $|z| \geqslant 1$, of a system of polynomial equations. In this connection only relatively simple model difference initial- and boundary-value problems were considered until now with the aid of the programs IBSTAB and SPECTR.

The amount of numerical computations required by the algorithms of [3, 5–7, 9] becomes significant when these algorithms are applied for the stability investigations of difference initial-value problems approximating, for example, the initial-value problems for two- or three-dimensional Euler or Navier–Stokes equations governing the compressible fluid flows.

In this connection it is necessary to seek for other more efficient ways of the symbolic–numerical realization of the spectral stability analysis of difference schemes. By using the Moebius transformation and computing the resultant $R(\kappa, \xi)$ on the basis of the real and imaginary parts of the coefficients of a transformed characteristic equation the problem of the stability analysis was reduced in [19, 20] to a canonical problem of the catastrophe theory [21] on the determination of a manifold of zeros of a family of functions R. This method was used for the stability analyses of two specific d.s., and the results were otained in [19, 20] by analytic calculations by hand. However, in cases of complicated d.s. even the derivation of an explicit expression for the resultant, not to mention the analysis of the singularities of its manifold of zeroes, is a complicated problem and in practice it is impossible to find its solution in an analytic form by hand.

Previously a survey of the applications of the computer algebra for the realization of analyses on the basis of the catastrophe theory was given in [22]. The corresponding developed programs were used in general relativity, construction of smooth coordinate transformations, and computation of oscillatory integrals. A project to build a package "bifurcation and singularity theory" has been presented in [23]. It was proposed in [23] to use the Groebner bases to determine the codimension of a singularity.

A reasonable combination of symbolic and numerical computations in a procedure for the stability analysis enables one to substantially extend the scope of applicability of the general approach proposed in [19], as shown in the present paper. Examples of the stability analyses are presented for a number of difference initial-value problems. For the majority of considered d.s. the results on the stability have been obtained for the first time.

2. THEORETICAL BACKGROUND

In the domain $\tilde{G}$: $|x_j| < \infty$, $j = 1, ..., L$, $0 \leqslant t \leqslant T$, $T < \infty$, consider a system of hyperbolic or parabolic type,

$$\frac{\partial \mathbf{U}}{\partial t} = L(D)\,\mathbf{U}, \tag{2.1}$$

where $\mathbf{U} = \{U_1(\mathbf{x}, t), ..., U_m(\mathbf{x}, t)\}$ is a vector function of $\mathbf{x}$ and t; $m \geqslant 1$, $\mathbf{x} = (x_1, ..., x_L)$,

$$L(D) = \sum_{\alpha=1}^{p} A_\alpha D^\alpha,$$

$$D^\alpha = D_1^{\alpha_1} D_2^{\alpha_2} \cdots D_L^{\alpha_L}, \qquad \alpha_1 + \cdots + \alpha_L = \alpha,$$

$$D_j = \partial/\partial x_j, \qquad j = 1, ..., L,$$

$$A_\alpha = \|a_{ij}^\alpha\|, \qquad i, j = 1, ..., m; \qquad \alpha = 1, ..., p, \qquad p \geqslant 1;$$

a_{ij}^α are constant quantities. Let us set the initial conditions:

$$\mathbf{U}(\mathbf{x}, 0) = \mathbf{U}_0(\mathbf{x}) \tag{2.2}$$

for the system (2.1), where $\mathbf{U}_0(\mathbf{x})$ is a given vector function. Approximate the system (2.1) by a $(q+1)$th-level difference scheme, $q \geqslant 1$. If $q > 1$, then the system of $(q+1)$th-level difference equations may be replaced with the aid of introducing new dependent variables by a system of two-level equations [1],

$$C_1 \mathbf{U}^{n+1} + C_2 \mathbf{U}^n = 0, \tag{2.3}$$

where C_1 and C_2 are some linear difference (generally matrix) operators with constant coefficients which depend on the time step τ and on the steps $h_1, ..., h_L$ of a uniform computing mesh along the axes $x_1, ..., x_L$, respectively; $\mathbf{U}^n = \mathbf{U}(\mathbf{x}, n\tau)$, $n = 1, ..., [T/\tau]$; the symbol $[a]$ denotes the integral part of the number a.

When investigating the stability of the difference schemes (2.3) by the Fourier method the solutions of the form

$$\mathbf{U}(\mathbf{x}, t) = \mathbf{U}_0 \exp\{i(\mathbf{kx} - \omega t)\} \tag{2.4}$$

are substituted into the scheme, where ω is the wave frequency, $\mathbf{U}_0$ is a constant vector, $\mathbf{x} = (x_1, ..., x_L)$, $L \geqslant 1$, $\mathbf{k} = (k_1, ..., k_L)$ is a real wave vector, $i = \sqrt{-1}$.

Upon substituting (2.4) into a scheme (2.3) one obtains an amplification matrix G. Let

$$f(\lambda, \kappa, \xi) = \sum_{j=0}^{N} a_j(\kappa, \xi)\, \lambda^{N-j}, \qquad N = qm, \tag{2.5}$$

be a characteristic polynomial of the matrix G, $\lambda = e^{i\omega\tau}$, $\kappa = (\kappa_1, ..., \kappa_M)$; the nondimensional complexes $\kappa_1, ..., \kappa_M$,

($M \geqslant 1$) usually appear in the process of obtaining the characteristic polynomial of the matrix G and depend on the steps $h_1, ..., h_L, \tau$ (for example, the Courant number), on dimensional quantities entering the coefficients of scheme (2.3) and on nondimensional physical similarity criteria (for example, the Reynolds number); $\xi = (\xi_1, ..., \xi_L)$, $\xi_j = k_j h_j$, $j = 1, ..., L$. The quantities $\xi_1, ..., \xi_L$ will be called spectral parameters in the following. Let $\lambda_1, ..., \lambda_N$ be the eigenvalues of G. Then a von Neumann necessary stability condition has the form [1]

$$|\lambda_j| \leqslant 1 + O(\tau), \qquad j = 1, ..., N. \tag{2.6}$$

In view of (2.4) the coefficients $a_j(\kappa, \xi)$ of the polynomial (2.5) are periodic functions of the spectral parameters $\xi_1, ..., \xi_L$ with the periods $T_1, ..., T_L$, respectively.

Consider in an L-dimensional Euclidean space E^L of the ξ points a parallelepiped

$$\Pi: \{0 \leqslant \xi_l \leqslant T_l, l = 1, ..., L\}. \tag{2.7}$$

Denote by E^M an M-dimensional Euclidean space of the points $\kappa = (\kappa_1, ..., \kappa_M)$. Let the parallelepiped

$$P: \{\kappa_p^{\min} \leqslant \kappa_p \leqslant \kappa_p^{\max}, p = 1, ..., M\} \tag{2.8}$$

be given in E^M, where $\kappa_p^{\min}$, $\kappa_p^{\max}$ are given quantities and it is assumed that the stability domain D is to be determined in P. Let us make as in [20] the Moebius transformation $\lambda = (w+1)/(w-1)$ in the polynomial (2.5). Introduce the notation

$$g(w, \kappa, \xi) = (w-1)^N f((w+1)/(w-1), \kappa, \xi). \tag{2.9}$$

Then the condition $\operatorname{Re} w_j \leqslant 0$, $j = 1, ..., N$, corresponds to the condition $|\lambda_j| \leqslant 1$, $j = 1, ..., N$, where w_j are the zeroes of the polynomial $g(w, \kappa, \xi)$. On the boundary Γ of the domain D the polynomial (2.9) should have at least one purely imaginary zero. Let us set $w = i\sigma$ and consider the polynomial

$$\phi(\sigma, \kappa, \xi) = g(i\sigma, \kappa, \xi). \tag{2.10}$$

As was shown in [19, 20], on the boundary Γ the resultant $R(\kappa, \xi)$ determined by the polynomials $\operatorname{Re}\phi$ and $\operatorname{Im}\phi$ as

$$R(\kappa, \xi) = \operatorname{res}(\operatorname{Re}\phi, \operatorname{Im}\phi) \tag{2.11}$$

should vanish. As is known, the resultant of the polynomials $a_0\sigma^n + a_1\sigma^{n-1} + \cdots + a_n$ and $b_0\sigma^m + b_1\sigma^{m-1} + \cdots + b_m$ is a determinant of the form

$$R = \begin{vmatrix} a_0 & a_1 & \cdots & a_n & 0 & \cdots & 0 \\ 0 & a_0 & a_1 & \cdots & a_n & 0 & \cdots & 0 \\ \vdots & & & & \vdots & & & \\ 0 & 0 & \cdots & 0 & a_0 & \cdots & a_n \\ b_0 & & \cdots & b_m & 0 & \cdots & 0 \\ 0 & b_0 & \cdots & & b_m & 0 & \cdots & 0 \\ \vdots & & & & & & & \\ 0 & & \cdots & & 0 & b_0 & \cdots & b_m \end{vmatrix} \begin{matrix} \\ \\ \\ \\ \\ \\ \\ \\ \end{matrix} \begin{matrix} \\ \\ \\ \} m \text{ rows} \\ \\ \\ \\ \} n \text{ rows} \\ \\ \end{matrix}$$

Thus the problem on the determination of the boundary Γ may be considered as a problem on studying the zeroes of the equation

$$R(\kappa, \xi) = 0, \tag{2.12}$$

where the family of functions R depends on M variables $\kappa_1, ..., \kappa_M$ and on L parameters $\xi_1, ..., \xi_L$. Just these problems are solved in the catastrophe theory.

We propose the following procedure to determine the solutions of Eq. (2.12). Let (κ_0, ξ_0) be some solution of (2.12), where $\kappa_0 \in \Gamma$. Set $\kappa = \kappa_0 + \mathbf{u}$ and introduce the notation

$$\Phi(\mathbf{u}, \xi) = R(\kappa_0 + \mathbf{u}, \xi). \tag{2.13}$$

We shall consider Φ as a family of functions of one variable u_{i_0} depending on $M - 1 + L$ parameters:

$$(u_1, ..., u_{i_0-1}, u_{i_0+1}, ..., u_M, \xi_1, ..., \xi_L) \equiv (\mathbf{u}', \xi).$$

Consider the derivatives

$$\partial^l \Phi / \partial u_i^l |_{\mathbf{u}=0, i=1,...,M, l=1,2,...} \qquad \forall \xi \in \Pi \tag{2.14}$$

in order to determine the inner variable u_{i_0}.

Let $l = k$ be the last order of a derivative at which at least one derivative (2.14) is different from zero, that is,

$$\begin{gathered} \partial^k \Phi / \partial u_{i_s}^k |_{\mathbf{u}=0, \xi=\xi_0} \neq 0, \\ s = 1, 2, ..., S; \qquad S \geqslant 1, \qquad \forall \xi \in \Pi. \end{gathered} \tag{2.15}$$

Then it is possible to take for u_{i_0} any of the coordinates u_{i_s} and to consider Φ as an $(L - 1 + M)$-dimensional unfolding of a k-determined function $F(x; 0)$ [21], where

$$F(x; \mathbf{u}', \xi) = \Phi(\mathbf{u}, \xi), \qquad x \equiv u_{i_0}. \tag{2.16}$$

It follows from the catastrophe theory [21] that there exists

such a smooth transform $x = X(t; \mathbf{u}', \xi)$ (it is even analytical, since the resultant R is an analytic function [24]) that

$$F(X(t; \mathbf{u}', \xi); \mathbf{u}', \xi) = \pm t^k + b_{k-2}(\mathbf{u}', \xi)\, t^{k-2} + \cdots + b_0(\mathbf{u}', \xi) \qquad (2.17)$$

(at even k the sign of t^k is uniquely determined by the sign of the derivative (2.15) for u_{i_0}). Note that a family $\tilde{F}$ such that $F = d\tilde{F}/dx$ may be found to correspond to the family F. Therefore, in accordance with the classical catastrophe theory, we shall say that the family $F(x, \mathbf{u}', \xi)$ (2.17) has a singularity of the type A_k [24, 25]. Since the resultant $R(\boldsymbol{\kappa}, \xi)$ is a polynomial of a finite degree N in the variables κ_i, $\Phi(\mathbf{u}, \xi)$ in (2.16) has the form

$$\Phi(\mathbf{u}, \xi) = \sum_{p=0}^{N} \alpha_p(\xi)\, u^p, \qquad (2.18)$$

where $p = (p_1, \ldots, p_M)$ is a multiindex and $u^p = u_1^{p_1} \cdots u_M^{p_M}$.

Let us set

$$X(t; \mathbf{u}', \xi) = \sum_{s=1}^{\infty} c_s(\mathbf{u}', \xi)\, t^s. \qquad (2.19)$$

As was shown in [24], the series (2.19) has a nonzero radius of convergence.

Substituting the expressions (2.16), (2.18), (2.19) into Eq. (2.17) and equalling the terms having the same degrees in t, we obtain a recurrence equation system which uniquely determines the functions $c_s(\mathbf{u}', \xi)$ and, consequently, the function $X(t; \mathbf{u}', \xi)$.

Denote by $t_i(\mathbf{u}', \xi)$, $i = 1, \ldots, k$, the solutions of

$$\mp t^k + b_{k-2}(\mathbf{u}', \xi)\, t^{k-2} + \cdots + b_0(\mathbf{u}', \xi) = 0. \qquad (2.20)$$

Then the set of smooth functions $u_{i_0}^{(l)} = X(t_l(\mathbf{u}', \xi); \mathbf{u}', \xi)$ gives a complete description of a manifold of the solutions of Eq. (2.12) in some neighborhood of the initial point $(\mathbf{k}_0, \xi_0)$ (in the language of the catastrophe theory the functions $u_{i_0}^{(l)}(\mathbf{u}', \xi)$ describe the manifold of a catastrophe of the type A_k). The boundary Γ of the stability domain of a difference scheme is an envelope of the family of the solutions of Eq. (2.12) with the parameters ξ of the family. Therefore, the values of the parameters $\xi_i = \xi_i^{(l)}(\mathbf{u}')$ $(l = 1, \ldots, k)$ at which the functions $u_{i_0} = u_{i_0}^{(l)}(\mathbf{u}', \xi^{(l)}(\mathbf{u}'))$ $(l = 1, \ldots, k)$ describe the boundary Γ are determined by the equations of the form

$$\partial F(u_{i_0}^{(l)}(\mathbf{u}', \xi); \mathbf{u}', \xi)/\partial \xi_i = 0, \qquad i = 1, \ldots, L. \qquad (2.21)$$

The condition (2.21) is necessary, but it is not sufficient to ensure that the values of the parameters ξ_i correspond to the boundary Γ. Therefore, in the numerical realization of the proposed algorithm the condition (2.21) should be completed by some refinement procedure (see steps 6 and 7 in the next section). Thus the functions $u_{i_0} = u_{i_0}^l(\mathbf{u}', \xi^{(l)}(\mathbf{u}'))$ describe the boundary Γ of the d.s. stability domain in some neighborhood of the point $\boldsymbol{\kappa}_0$. Taking some value $\mathbf{u}' = \mathbf{u}_0'$ which belongs to this neighborhood, we can take the point $\boldsymbol{\kappa}_0 + \mathbf{u}_0^{(l)}$ $(\mathbf{u}^{(l)} = (u_{i_0}^{(l)}(\mathbf{u}_0'), \mathbf{u}_0'))$ as an initial point and repeat the overall procedure. As a result of this we obtain one more piece of the boundary Γ. Sequential repetition of this process will yield a description of the overall boundary Γ. An essential merit of the proposed method is that it gives a correct description of all the singularities of a d.s. stability domain boundary.

3. AUTOMATIC GENERATION OF FORTRAN SUBROUTINES

On the basis of the above presented method we have developed a symbolic–numerical algorithm for studying the d.s. stability at $1 \leqslant L \leqslant 2$, $M = 2$. Since the stability domain of a difference scheme with $M = 2$ is located in the (κ_1, κ_2) plane, the boundary Γ of the stability domain may have the singularities only at some points of this plane. Therefore, almost all the boundary is a regular curve and at the first stage one can restrict oneself to a consideration of the transform (2.17) with $k = 1$. In this case the family Φ (2.18) has the form

$$\Phi(u_1, u_2, \xi_1, \xi_2) = R(\kappa_1^0, \kappa_2^0, \xi_1, \xi_2) + \sum_{l=1}^{N} \left(\sum_{j=0}^{l} \alpha_{l-j,j} (u_1(t))^{l-j} u_2^j \right) = t + b, \qquad (3.1)$$

where $b = \text{const}$.

As it follows from the foregoing section, the first step of the determination of the Γ boundary is the determination of an initial point $(\boldsymbol{\kappa}_0, \xi_0)$. We used a FORTRAN subroutine ROUTH [9] for finding a point $\boldsymbol{\kappa}_0 \in \Gamma$. In its turn, ROUTH calls a subroutine COEF which enables us to compute the values of the coefficients of the polynomial (2.9) at a given point $(\boldsymbol{\kappa}, \xi)$. The subroutine COEF was automatically generated as in [7] by means of the REDUCE package [8], departing from a specific form of a difference scheme. The subroutine ROUTH implements a variant of the Routh algorithm for studying the Hurwitz property of a polynomial; see a more detailed description in [9]. The module RESULTANT available in the REDUCE library enables us to calculate the resultant (2.11) in an analytical form. The overall length of the expression for the resultant obtained on a computer usually can be substantially reduced by applying the trigonometric substitutions

$$\cos^2 \xi_j = 1 - \sin^2 \xi_j, \qquad j = 1, \ldots, L.$$

The FORTRAN function RESULT, the output of which is the value of the resultant at a given point (κ, ξ), was automatically generated by means of the REDUCE system. And, finally, REDUCE was used to determine the analytic expressions for the coefficients $\alpha_{l-j,j}$ in (3.1) and to generate a FORTRAN subroutine CATAS at the output of which the elements $FF(i, j)$ of the two-dimensional array of numbers FF were obtained which contained the numerical values of the coefficients α_{ij} in (3.1) computed at a given point (κ_0, ξ_0).

4. ALGORITHM FOR THE NUMERICAL DETERMINATION OF THE STABILITY REGION BOUNDARY

In the practical computations we used the inequalities

$$|\alpha_{10}| = |\partial\Phi/\partial u_1|_{u=0,\xi=\xi_0} > \varepsilon,$$
$$|\alpha_{01}| = |\partial\Phi/\partial u_2|_{u=0,\xi=\xi_0} > \varepsilon$$

to check the conditions (2.15) at $k=1$ (ε is a small positive number, for example, $\varepsilon = 10^{-6}$). The function $u_1(t; u_2, \xi)$ entering (3.1) was approximated by a finite truncation of the series (2.19):

$$u_1(t; u_2, \xi) = \sum_{i=1}^{m} c_i(u_2, \xi)\, t^i. \tag{4.1}$$

This formula was employed in the case when the coefficients α_{10} and α_{01} entering (3.1) satisfied the relationship

$$|\alpha_{10}(\kappa_1^0, \kappa_2^0, \xi_0)| \geqslant |\alpha_{01}(\kappa_1^0, \kappa_2^0, \xi_0)|. \tag{4.2}$$

The computations for specific difference schemes showed that at sufficiently small increments u_2 one can take $m=2$ in (4.1). Let us write down the necessary recurrence formulas for the calculation of the values c_1, c_2, and b for the case $m=2$. Substituting the right-hand side of formula (4.1) into (3.1) instead of u_1 and neglecting the terms of the order $O(t^k)$, $k \geqslant 3$, we obtain the formulas for c_1, c_2, and b,

$$\begin{aligned} c_1 &= 1/(\alpha_{13}u_2^3 + \alpha_{12}u_2^2 + \alpha_{11}u_2 + \alpha_{10}), \\ c_2 &= -c_1^3(\alpha_{22}u_2^2 + \alpha_{21}u_2 + \alpha_{20}), \\ b &= R_0 + \alpha_{04}u_2^4 + \alpha_{03}u_2^3 + \alpha_{02}u_2^2 + \alpha_{01}u_2, \end{aligned} \tag{4.3}$$

where we have introduced the notation

$$R_0 = R(\kappa_1^0, \kappa_2^0, \xi_1^0, \xi_2^0).$$

It follows from Eq. (2.20) that $t=-b$. Thus, in the case when the inequality (4.2) is satisfied the solution of Eq. (2.12) in the neighborhood of a regular point (κ_0, ξ_0) has the form

$$u_1(u_2, \xi_1, \xi_2) = \sum_{i=1}^{2} c_i(u_2, \xi_1, \xi_2)[-b(u_2, \xi_1, \xi_2)]^i. \tag{4.4}$$

In the case when the inequalities

$$|\alpha_{01}(\kappa_1^0, \kappa_2^0, \xi_0| > |\alpha_{10}(\kappa_1^0, \kappa_2^0, \xi_0)| \tag{4.5}$$

are satisfied at the point (κ_0, ξ_0), we set the increment u_1 and seek the function $u_2(t; u_1, \xi)$ as

$$u_2(t; u_1, \xi) = \sum_{i=1}^{m} \tilde{c}_i(u_1, \xi)\, t^i. \tag{4.6}$$

In the case $m=2$ the formulas for $\tilde{c}_1$, $\tilde{c}_2$, and $\tilde{b}$ have the form

$$\begin{aligned} \tilde{c}_1 &= 1/(\alpha_{31}u_1^3 + \alpha_{21}u_1^2 + \alpha_{11}u_1 + \alpha_{01}), \\ \tilde{c}_2 &= -\tilde{c}_1^3(\alpha_{22}u_1^2 + \alpha_{12}u_1 + \alpha_{02}), \\ \tilde{b} &= R_0 + \alpha_{40}u_1^4 + \alpha_{30}u_1^3 + \alpha_{20}u_1^2 + \alpha_{10}u_1. \end{aligned} \tag{4.7}$$

As a result we find the function $u_2(u_1, \xi_1, \xi_2)$ in the form

$$u_2(u_1, \xi_1, \xi_2) = \sum_{i=1}^{2} \tilde{c}_i(u_1, \xi_1, \xi_2)[-\tilde{b}(u_1, \xi_1, \xi_2)]^i. \tag{4.8}$$

Note that the inequalities (4.2) and (4.5) determine the form of the description of a piece of the stability region boundary which is under consideration. As it follows from the formulas (4.1) and (4.6), the boundary is described more accurately, if $|c_i|$ or $|\tilde{c}_i|$ are small. It may be seen from (4.3) and (4.7) that c_i are inversely proportional to α_{10} and $\tilde{c}_i$ are inversely proportional to α_{01}. Therefore, in the case of the satisfaction of the inequality (4.2) it is reasonable to use the description (4.1), and in the case of the satisfaction of the inequality (4.5) it is reasonable to use the description (4.6).

If $|\alpha_{01}(\kappa_1^0, \kappa_2^0, \xi_0)| < \varepsilon$ and $|\alpha_{10}(\kappa_1^0, \kappa_2^0, \xi_0)| < \varepsilon$, then the corresponding point κ_0 in the (κ_1, κ_2) plane is assumed to be a critical point of the family (2.12), and then it is necessary to apply at this point an analysis procedure presented above in Section 2.

Let us describe the technique for the computation of the coordinates of the vector ξ_0 entering the formulas (4.3) and (4.7), which was applied by us. In accordance with Section 2, the vector ξ_0 should satisfy the necessary envelope condition (2.21). Let $\kappa_0 \in \Gamma$ and assume that (κ_0, ξ_0) is a regular point of the family (2.12). Then at fixed κ_0 the conditions (2.21) coincide with the necessary conditions for the extremum of $|R(\kappa_0, \xi)|$. Since the relationship $R(\kappa_0, \xi_0) = 0$

should be satisfied on the boundary Γ, the point ξ_0 should be the point of the minimum of the quantity $|R(\kappa_0, \xi)|$ over $\xi \in \Pi$, where the domain Π is determined in accordance with (2.7).

In practical computations the coordinates of the vector ξ_0 were calculated with regard for the above considerations in the following way. The domain Π was discretized by a rectangular uniform grid G_ξ having J_l nodes along the coordinate ξ_l, $l = 1, ..., L$. After that, ξ_0 was determined with the aid of a uniform search for the minimum of the quantity $|R(\kappa_0, \xi)|$ over all the nodes $\xi \in G_\xi$:

$$\xi_0 = \operatorname{Arg} \min_{\xi \in G_\xi} |R(\kappa_0, \xi)|. \tag{4.9}$$

The quantities $J_1, ..., J_L$ involved in the construction of the grid G_ξ were calculated automatically at the stage of computing the coordinates of the starting point $(\kappa_1^0, \kappa_2^0) \in \Gamma$. Let ε be a desired magnitude of the absolute error in determining the coordinates (κ_1^0, κ_2^0). Suppose that $J_1 = \cdots = J_L = J$. Denote by $\kappa_J^{(k)}$ the point of the boundary Γ found along some fixed curve $L^{(k)}$ intersecting Γ. In the present work the curves $L^{(k)}$ were chosen to be the polar beams in the (κ_1, κ_2) plane. We have taken a small number of such curves $L^{(k)}$, $k = 1, ..., K$ (in the range $4 \leqslant K \leqslant 12$). Beginning from some starting value $J = J_0$ (for example, $J_0 = 8$) we increased its value by 2. If at some J the inequality

$$\max_{1 \leqslant m \leqslant M, 1 \leqslant k \leqslant K} |(\kappa_m^{(k)})_J - (\kappa_m^{(k)})_{J+2}| \leqslant \varepsilon \tag{4.10}$$

was satisfied, we assumed that $J_1 = \cdots = J_L = J + 2$. In (4.10) $(\kappa_m^{(k)})_J$ denotes the value of the mth coordinate κ_m, $1 \leqslant m \leqslant M$, calculated at the point of intersection of the curve $L^{(k)}$, $k = 1, ..., K$, with the boundary Γ.

Since the point $(\kappa_1^0, \kappa_2^0) \in \Gamma$, the quantity $|R_0|$ should be small. But if the quantity $|u_2|$ is too big, the quantity $|b|$, where b is computed in accordance with (4.3), may already be not small. The size of the quantity u_2 was controlled in the following way: at first the quantities c_1, c_2, and b were calculated at fixed u_2 (say, $u_2 = 0.04$), in accordance with (4.3). Then the inequality

$$|0.5c_1| > |c_2 b| \tag{4.11}$$

was checked. If it was not satisfied, we specified a new value of the increment u_2 by the formula $(u_2)_{\text{new}} = 0.8(u_2)_{\text{old}}$ and repeatedly computed the quantities c_1, c_2, and b by formulas (4.3). A similar control of the quantity u_1 was applied while using the representation (4.6).

Since the formulas (4.3), (4.4) and (4.7), (4.8) are approximate, the coordinates of a new point $(\kappa_1, \kappa_2) \in \Gamma$ computed by the formulas

$$\kappa_1 = \kappa_1^0 + u_1, \qquad \kappa_2 = \kappa_2^0 + u_2 \tag{4.12}$$

are approximate. Since the quantity R_0 enters directly in the computational formulas (4.3) and (4.7), it is very important to ensure the smallness of $|R_0|$ in order that the application of the formulas (4.3) and (4.7) be justified. In this connection we applied an algorithm for the refinement of the values κ_1 and κ_2 found by (4.12). For this purpose we introduced a new local Cartesian rectangular coordinate system $(O'\tilde{\kappa}_1\tilde{\kappa}_2)$ whose origin was placed at the point (κ_1, κ_2) determined by (4.12); the $O'\tilde{\kappa}_1$ axis was directed along the tangent to the boundary Γ at the (κ_1, κ_2) point, and the $O'\tilde{\kappa}_2$ axis was directed along a normal to Γ. If (κ_1, κ_2) is a regular point of the curve Γ and if the increment $(u_1^2 + u_2^2)^{0.5}$ is not large, then it is reasonable to suppose that the $O'\tilde{\kappa}_2$ axis will intersect Γ at some point $(\tilde{\kappa}_1^*, \tilde{\kappa}_2^*)$. For the calculation of the coordinate $\tilde{\kappa}_2^*$ we applied the bisection process. For this purpose we constructed the function

$$H(\tilde{\kappa}_2) = \begin{cases} 1, & \operatorname{sign} R(\tilde{\kappa}_1, \tilde{\kappa}_2, \xi) = \text{const}, \quad \forall \xi \in \Pi, \\ -1, & \text{otherwise}, \end{cases} \tag{4.13}$$

where R is the resultant and the value $\tilde{\kappa}_1$ is assumed to be fixed (it is computed on the basis of the values κ_1 and κ_2 by the transformations of coordinate rotation and translation). The construction (4.13) is based on the fact that the stability region boundary is an envelope of the family (2.12) and, hence, there are no curves of the family (2.12) inside the stability region. Let $u_{\max} = \max(|u_1|, |u_2|)$. A search for the zero $\tilde{\kappa}_2^*$ of the function (4.13) was performed in the intervals

$$-0.25u_{\max}k \leqslant \tilde{\kappa}_2 \leqslant 0.25u_{\max}k, \qquad k = 1, ..., 16. \tag{4.14}$$

At first the value $k = 1$ was taken. If it turned out that $\operatorname{sign} H(-0.25u_{\max}) = \operatorname{sign} H(0.25u_{\max})$, then the value $k = 2$ was taken and H was again computed at the ends of an extended interval, etc. As a rule, the different signs of the function H were observed already at the ends of the first of the intervals (4.14). The bisection process was continued until a given accuracy of computing the zero $\tilde{\kappa}_2^*$ was achieved. Let the length of an interval on the $\tilde{\kappa}_2$ axis in which $\tilde{\kappa}_2^*$ is to be determined be equal to $0.5u_{\max}$. Then it is easy to find that there are required

$$O\left(\log_2(0.5u_{\max}/\varepsilon) \prod_{l=1}^{L} J_l\right) \tag{4.15}$$

computations of the resultant R for obtaining the value $\tilde{\kappa}_2^*$ with the accuracy ε.

Summing up the above material of this section, we enumerate the numerical stages of the proposed symbolic–numerical method as the following sequence of steps.

Step 1. Compute coordinates (κ_1^0, κ_2^0) and the integers $J_1, ..., J_L$ by the Routh algorithm [4].

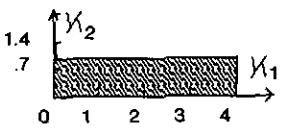

FIGURE 1

Step 2. Compute ξ_0 as a solution of the optimization problem (4.9).

Step 3. Compute the increments u_1 and u_2 either by formulas (4.3), (4.4) or by formulas (4.7), (4.8) depending on the inequality (4.2) or (4.5), respectively.

Step 4. Check the satisfaction of the inequality (4.11). If it is violated, reduce the increment u_2 and return to Step 3.

Step 5. Compute the coordinates κ_1, κ_2 by formulas (4.12) and go over to the coordinate system $O'\tilde{\kappa}_1\tilde{\kappa}_2$.

Step 6. Find the zero $\tilde{\kappa}_2^*$ of the equation $H(\tilde{\kappa}_2)=0$ by the bisection process, where H is determined by (4.13).

Step 7. Compute the final coordinates (κ_1, κ_2) of the next point of the Γ boundary on the basis of found values $(\tilde{\kappa}_1, \tilde{\kappa}_2^*)$.

Step 8. If the found point (κ_1, κ_2) is outside the quadrant of the (κ_2, κ_2) plane under consideration, return to the starting point (κ_1^0, κ_2^0) found at the Step 1, change the sign of the increment u_2 while using formulas (4.3), (4.4) or the sign of the increment u_1 while using formulas (4.7), (4.8), and go over to Step 2.

Step 9. If the found point (κ_1, κ_2) remains within the quadrant under consideration, then this point is taken as an initial point; that is, it is assumed that $\kappa_1^0=\kappa_1$, $\kappa_2^0=\kappa_2$, and then one returns to Step 2.

The pieces of the Γ boundary are determined by the above algorithm independently in each of the four quadrants of the (κ_1, κ_2) plane. This is done for the purpose of the economy of CPU time, because one of the $O\kappa_1$ or $O\kappa_2$ axes often proves to be a part of the Γ boundary, see Figs. 1 and 2.

In the cases when it is not known a priori how the stability region D is located with respect to the found boundary Γ, one can efficiently use the function (4.13). Indeed, let the function H be positive at one of the ends of the interval (4.14) obtained at some k. Then the (κ_1, κ_2) coordinates corresponding to this end can be stored in two one-dimensional number arrays. It is obvious that such points will be located on a stable side of the line Γ. Therefore, they can subsequently be used for the dashing of the subregions in the (κ_1, κ_2) plane which correspond to the stability region of the difference scheme under consideration.

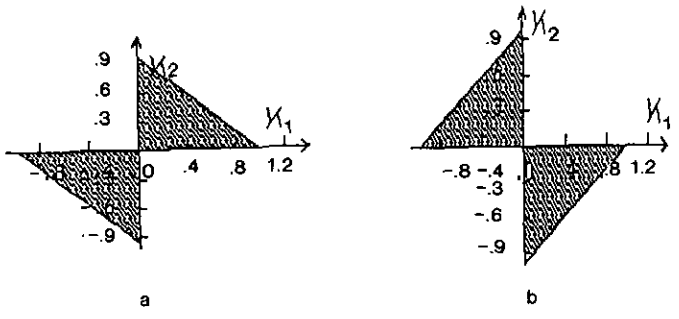

FIGURE 2

5. EXAMPLES OF PRACTICAL APPLICATION

Let us demonstrate the efficiency of the above proposed symbolic–numerical method at the examples of three different schemes approximating scalar equations of the hyperbolic type.

5.1. *The Family of Schemes for One-Dimensional Advection Equation*

Consider the advection equation

$$\partial u/\partial t + c\,\partial u/\partial x_1 = 0, \tag{5.1}$$

where $c=\text{const}>0$. Then one of the schemes employing the MUSCL-type differencing may be written as [26–28]

$$\begin{aligned}(u_j^{n+1}-u_j^n)/\tau + (1-\alpha)\,c(u_j^n-u_{j-1}^n)/h_1 \\ + \alpha c(u_j^{n+1}-u_{j-1}^{n+1})/h_1 + c((1+\beta)/(4h_1)) \\ \times (u_{j+1}^n - 2u_j^n + u_{j-1}^n) + c((1-\beta)/(4h_1)) \\ \times (u_j^n - 2u_{j-1}^n + u_{j-2}^n) = 0.\end{aligned} \tag{5.2}$$

Here α, β are nondimensional weight parameters, $0\leqslant\alpha\leqslant 1$, $-1\leqslant\beta\leqslant 1$. At $\beta=\frac{1}{3}$ the scheme (5.2) has an order of approximation $O(h_1^3)$ in x_1; at $\beta\neq\frac{1}{3}$ the approximation order in x_1 is $O(h_1^2)$. It follows from (5.2) that the stability domain D may be determined in the case under consideration in the plane of nondimensional quantities κ_1 and κ_2 where $\kappa_1=c\tau/h_1$, $\kappa_2=\beta$. In Fig. 1 we show the stability region of the scheme (5.2) at $\alpha=0.5$, which was obtained by the proposed symbolic–numerical method in a rectangular domain P of the form (2.8) with $\kappa_1^{\min}=0$, $\kappa_1^{\max}=4$, $\kappa_2^{\min}=0$, $\kappa_2^{\max}=2$. To check the correctness of the obtained results we carried out an analytic investigation of the characteristic polynomial of this scheme which has the form

$$\lambda(a_1+ia_2)+(b_1+ib_2)=0, \tag{5.3}$$

where

$$a_1 = 1 + \alpha\kappa_1(1-\cos\xi_1),$$
$$a_2 = \alpha\kappa_1 \sin\xi_1, \qquad i=\sqrt{-1},$$
$$b_1 = (1-\cos\xi_1)\,\kappa_1\left[\frac{(1-\beta)}{2}(1-\cos\xi_1)-\alpha\right]-1, \tag{5.4}$$
$$b_2 = (1-\alpha)\,\kappa_1\sin\xi_1 + \kappa_1\left(\frac{1-\beta}{2}\right)\sin\xi_1(1-\cos\xi_1).$$

Then the resultant R is expressed by the formula

$$R = b_1^2 + b_2^2 - a_1^2 - a_2^2. \tag{5.5}$$

At small $|\kappa_1|$ we obtain from (5.4) and (5.5) at $\alpha=\frac{1}{2}$ the following formula for R:

$$R = \kappa_1(1-\cos\xi_1)^2\,(\beta-1) + O(\kappa_1^2). \tag{5.6}$$

Let λ_1 be the root of Eq. (5.3). The the formula (5.5) may be rewritten in the form

$$R = (a_1^2 + a_2^2)(|\lambda_1|^2 - 1) \tag{5.7}$$

We obtain from the von Neumann conditions (2.6) and from (5.7) that the inequality $R \leqslant 0$ should be satisfied in the stability region of scheme (5.2). According to (5.6), this inequality is satisfied at $\beta \leqslant 1$ in the case of small $|\kappa_1|$. At $\kappa_1 \to +\infty$ and $\alpha = 0.5$ we obtain from (5.4) at $\beta = -\varepsilon$, where ε is a small positive number,

$$R \simeq \kappa_1^2(a/4)(1+\varepsilon)[a^3(1+\varepsilon) - 2a^2 + 2\sin^2\xi_1 + a(1+\varepsilon)\sin^2\xi_1],$$

where $a = 1-\cos\xi_1$. At $\xi_1 = \pi$ we obtain from this expression that $R = 4\kappa_1^2(1+\varepsilon)$, $\varepsilon > 0$; that is, we have instability with regard to (5.7). Thus it follows from the above numerical and analytic studies that at $\alpha = 0.5$ the stability region of scheme (5.2) is represented by a half-strip,

$$0 \leqslant \kappa_1 < \infty, \qquad 0 \leqslant \beta \leqslant 1, \tag{5.8}$$

in the (κ_1, β) plane. The difference scheme (5.2) is a scalar one-step scheme. Therefore, the stability condition (5.8) is also a sufficient condition in accordance with the stability theory presented in [1].

In the case $\alpha = 0$ in (5.2) (an explicit scheme) both numerical computations by the above proposed method and the analytic studies show that the scheme is unstable.

5.2. *Monocyclic MacCormack Schemes*

The MacCormack scheme [29–31] was used especially widely in the 1970s [31]. At present it is also used in computations of applied problems, see, for example, [32, 33] among the recent works. However, MacCormack scheme may be unstable in some flow directions; some of works where this instability was observed are enumerated in [31]. In the present paper we present the results of the application of the above proposed symbolic–numerical method for the stability investigation of several variants of the MacCormack scheme as applied to the two-dimensional advection equation

$$\partial u/\partial t + A\,\partial u/\partial x_1 + B\,\partial u/\partial x_2 = 0, \tag{5.9}$$

where A and B are scalar constants. The most frequently used variant of the MacCormack scheme is

$$\tilde{u}_{ij} = u_{ij}^n - \tau\,\Delta_{x_1}^+(Au_{ij}^n) - \tau\,\Delta_{x_2}^+(Bu_{ij}^n),$$
$$u_{ij}^{n+1} = \tfrac{1}{2}(u_{ij}^n + \tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_1}^-(A\tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_2}^-(B\tilde{u}_{ij}), \tag{5.10}$$

where the differencing operators in x_1 and x_2 are determined by the formulas

$$\Delta_{x_1}^+ u_{ij} = (u_{i+1,j} - u_{ij})/h_1;$$
$$\Delta_{x_1}^- u_{ij} = (u_{ij} - u_{i-1,j})/h_1,$$
$$\Delta_{x_2}^+ u_{ij} = (u_{i,j+1} - u_{ij})/h_2; \tag{5.11}$$
$$\Delta_{x_2}^- u_{ij} = (u_{ij} - u_{i,j-1})/h_2.$$

It was pointed out in [29] that (5.10) is only one of four methods of second-order accuracy. Three other variants of the MacCormack method are obtained, if instead of first using two forward spatial differences and the two backward differences, the reverse procedure could be followed, or one forward and one backward difference could be followed by the corresponding backward and forward difference, see also [30]. Below we present these three remaining variants of the MacCormack scheme by using the operator notations (5.11):

$$\tilde{u}_{ij} = u_{ij}^n - \tau\Delta_{x_1}^+(Au_{ij}^n) - \tau\,\Delta_{x_2}^-(Bu_{ij}^n),$$
$$u_{ij}^{n+1} = \tfrac{1}{2}(u_{ij}^n + \tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_1}^-(A\tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_2}^+(B\tilde{u}_{ij}), \tag{5.12}$$
$$\tilde{u}_{ij} = u_{ij}^n - \tau\,\Delta_{x_1}^-(Au_{ij}^n) - \tau\,\Delta_{x_2}^-(Bu_{ij}^n),$$
$$u_{ij}^{n+1} = \tfrac{1}{2}(u_{ij}^n + \tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_1}^+(A\tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_2}^+(B\tilde{u}_{ij}), \tag{5.13}$$
$$\tilde{u}_{ij} = u_{ij}^n - \tau\,\Delta_{x_1}^-(Au_{ij}^n) - \tau\,\Delta_{x_2}^+(Bu_{ij}^n),$$
$$u_{ij}^{n+1} = \tfrac{1}{2}(u_{ij}^n + \tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_1}^+(A\tilde{u}_{ij}) - \tfrac{1}{2}\tau\,\Delta_{x_2}^-(B\tilde{u}_{ij}). \tag{5.14}$$

It is convenient to obtain the stability regions of schemes (5.10)–(5.14) in the plane of nondimensional complexes κ_1 and κ_2 defined by formulas

$$\kappa_1 = A\tau/h_1, \qquad \kappa_2 = B\tau/h_2. \tag{5.15}$$

The characteristic polynomial of d.s. (5.10) has the form (2.5) with $N=1$, where

$$a_0(\kappa, \xi)=1, \qquad a_1(\kappa, \xi)=b_1(\kappa, \xi)+ib_2(\kappa, \xi),$$

and

$$\begin{aligned} b_1(\kappa, \xi) &= -1+\kappa_1^2(1-\cos\xi_1)+\kappa_2^2(1-\cos\xi_2) \\ &\quad +\kappa_1\kappa_2[(1-\cos\xi_1)(1-\cos\xi_2)+\sin\xi_1\sin\xi_2]; \\ b_2(\kappa, \xi) &= \kappa_1\sin\xi_1+\kappa_2\sin\xi_2. \end{aligned} \tag{5.16}$$

It was shown in [20] with the aid of the catastrophe theory and with the use of the expressions (5.16) that the stability region of scheme (5.10) is determined by the inequalities

$$|\kappa_1|+|\kappa_2|\leqslant 1, \qquad \kappa_1\kappa_2\geqslant 0. \tag{5.17}$$

Now consider the characteristic polynomial of scheme (5.12) in order to analyze the stability of this scheme. In this case $N=1$ in (2.5) and

$$a_0(\kappa, \xi)=1, \qquad a_1(\kappa, \xi)=b_1(\kappa, \xi)+ib_2(\kappa, \xi),$$

where

$$\begin{aligned} b_1(\kappa, \xi) &= -1+\kappa_1^2(1-\cos\xi_1)+\kappa_2^2(1-\cos\xi_2) \\ &\quad +\kappa_1\kappa_2[\sin\xi_1\sin\xi_2-(1-\cos\xi_1)(1-\cos\xi_2)], \\ b_2(\kappa, \xi) &= \kappa_1\sin\xi_1+\kappa_2\sin\xi_2. \end{aligned} \tag{5.18}$$

To complete the analysis it is sufficient to compare the formulas (5.18) and (5.16). Indeed, it is easy to see that after a change of variables,

$$\begin{aligned} &\kappa_1'=-\kappa_1, \qquad \xi_1'=2\pi-\xi_1, \\ &\qquad \xi_1\in[0, 2\pi], \qquad \xi_1'\in[0, 2\pi], \\ &\kappa_2'=\kappa_2, \qquad \xi_2'=\xi_2, \end{aligned}$$

the resultant of scheme (5.12) expressed by the formula $R=b_1^2+b_2^2-1$ completely coincides with the resultant for scheme (5.10). Consequently the stability region of this scheme has in the (κ_1', κ_2') plane the same form as in the case of scheme (5.10). Returning to the original variables κ_1 and κ_2, we obtain the stability region of scheme (5.12):

$$|\kappa_1|+|\kappa_2|\leqslant 1, \qquad \kappa_1\kappa_2\leqslant 0. \tag{5.19}$$

In Fig. 2 we show the stability regions of schemes (5.10) and (5.12) obtained by the above symbolic–numerical method. In formulas (4.3) and (4.4) we have taken the value $|u_2|=0.03$, and in formulas (4.7), (4.8), the value $|u_1|=0.03$. It follows from Fig. 2 that the numerically determined stability regions coincide with the regions obtained with the aid of an analytic study in [20] and described by mathematical inequalities (5.17) and (5.19).

We have also compared the computational efficiency of the proposed symbolic–numerical method with the symbolic–numerical method of the work [9] which was based on the modified Routh algorithm. In this comparison we did not take into account the machine time needed in both of the methods for an automatic generation of the necessary FORTRAN subroutines with the aid of the REDUCE system. This is related to the fact that this machine time is usually small in comparison with the machine time spent at the numerical stages of the compared methods. This comparison showed that the above proposed approach requires, for the numerical determination of the coordinates (κ_1, κ_2) of one point of the boundary Γ, the machine time which is about a factor of 2.2 smaller than in the case of the application of the Routh algorithm variant from [9].

It is convenient for the following to use the operator notations for schemes (5.10), (5.12)–(5.14):

$u^{n+1}=L_1u^n$, scheme (5.10)
$u^{n+1}=L_2u^n$, scheme (5.12)
$u^{n+1}=L_3u^n$, scheme (5.13)
$u^{n+1}=L_4u^n$, scheme (5.14).

It is easy to show that at constant coefficients A and B, $L_1=L_3$ and $L_2=L_4$. Consequently, the above presented results of the analyses of schemes (5.10) and (5.12) are applicable to schemes (5.13) and (5.14), respectively.

The stencil of the first equation of scheme (5.10) consists of three points at the nth level and of one point at the $(n+1)$th level. Since all the MacCormack schemes considered here are explicit, they are characterized by the presence of only one point in the stencil at the $(n+1)$th level. This point is always located over the node (i, j, n) in the (x_1, x_2, t) space. As we will see in the following, the disposition of the points of stencils for the schemes (5.10) and (5.12) at the nth level is different. In this connection the set of the stencil points lying in the plane $t=n\tau$ will be called the stencil of the nth level. Imposing the (i, j) point of the stencil of Fig. 3a on the points of the stencil of Fig. 3b, it is easy to obtain the stencil of the nth level for the scheme (5.10). We proceed in a similar way in the case of scheme (5.12). In Fig. 4 we present the stencils of the nth level for

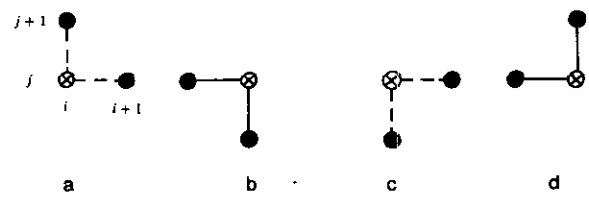

FIGURE 3

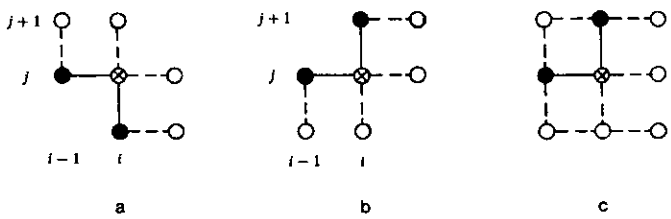

FIGURE 4

schemes (5.10) and (5.12). We can see that these stencils include seven points and are nonsymmetric with respect to the point (i, j).

It follows from inequalities (5.17) and (5.19) that in the case of using the composite difference scheme of the form

$$u^{n+1} = \begin{cases} L_1 u^n, & \kappa_1 \kappa_2 \geqslant 0, \\ L_2 u^n, & \kappa_1 \kappa_2 < 0, \end{cases} \tag{5.20}$$

the computations should be stable, provided that

$$|\kappa_1| + |\kappa_2| \leqslant 1. \tag{5.21}$$

If the coefficients A and B in (5.9) are variable and can change their sign at some (x_1, x_2, t) points with increasing t, then the stencil of the nth level, being symmetric with respect to the node (i, j), is obtained in the case of the application of the composite scheme (5.20) (see Fig. 4c).

Note that the difference schemes considered in this section are scalar two-level difference schemes. Therefore, the stability conditions obtained above for these schemes are not only necessary, but also they are the sufficient stability conditions [1].

5.3. *Two-Cycle MacCormack Scheme*

It was proposed in [29] to apply the four methods (5.10), (5.12)–(5.14) in sequence cyclically with the purpose of reducing the amplification error of the scheme when going from one time level to the next time level. Thus it was proposed in [29] to obtain the solution u^{n+4} as a result of the execution of the operator sequence

$$\begin{aligned} &u^{n+1} = L_1 u^n, \qquad u^{n+2} = L_2 u^{n+1}, \\ &u^{n+3} = L_3 u^{n+2}, \qquad u^{n+4} = L_4 u^{n+3}. \end{aligned} \tag{5.22}$$

We obtain the following formula from (5.22):

$$u^{n+4} = L_4 L_3 L_2 L_1 u^n. \tag{5.23}$$

As was pointed out above, $L_1 = L_3$ and $L_2 = L_4$ in the case of constant coefficients A and B. Therefore, in this case the application of the sequence (5.21) is equivalent to two sequential applications of the two-cycle scheme

$$u^{n+2} = L_2 L_1 u^n. \tag{5.24}$$

Obtaining an explicit expression for the right-hand side of Eq. (5.24) by hand proves to be rather a laborious task. We have solved this problem with the aid of a small program written in the REDUCE system. In Fig. 5 we show the stencil of the nth level of scheme (5.24). This stencil includes 21 points and is easily constructed by a superposition of the stencil of Fig. 4a on the points of the stencil of Fig. 4b. It may be seen that the stencil of the nth level of scheme (5.24) is symmetric with respect to the (i, j) node.

It turned out in the result of the calculation of the resultant by the formula (2.11) in a symbolic form that $N = 8$ for formula (3.1). Since a small personal computer was used by us for symbolic computations, we faced the problem of memory shortage while calculating the symbolic expressions $\alpha_{l-j,j}$ entering (3.1). In this connection we had to modify the algorithm. We used instead of (3.1) the formulas

$$R(\kappa_1^0 + u_1, \kappa_2, \xi) = \sum_{i=0}^{v} d_i^{(1)}(\kappa_1^0, \kappa_2, \xi)\, u_1^i, \tag{5.25}$$

$$R(\kappa_1, \kappa_2^0 + u_2, \xi) = \sum_{i=0}^{v} d_i^{(2)}(\kappa_1, \kappa_2^0, \xi)\, u_2^i. \tag{5.26}$$

Further, we considered by analogy with (4.2) and (4.5) the cases

$$|d_1^{(1)}(\kappa_1^0, \kappa_2^0, \xi_0)| \gtrless |d_1^{(2)}(\kappa_1^0, \kappa_2^0, \xi_0)|. \tag{5.27}$$

If $|d_1^{(1)}| \geqslant |d_1^{(2)}|$, we substituted the right-hand side of formula (4.1) instead of u_1 into the right-hand side of (5.24). Neglecting then in (5.24) the terms $O(u_1^k)$, $k \geqslant 3$, we obtain the following equation for determining c_1, c_2, b:

$$\begin{aligned} &d_0^{(1)}(\kappa_1^0, \kappa_2^0 + u_2, \xi_0) + d_1^{(1)}(\kappa_1^0, \kappa_2^0 + u_2, \xi_0)(c_1 t + c_2 t^2) \\ &\quad + d_2^{(1)}(\kappa_1^0, \kappa_2^0 + u_2, \xi_0)(c_1 t + c_2 t^2)^2 = b + t. \end{aligned}$$

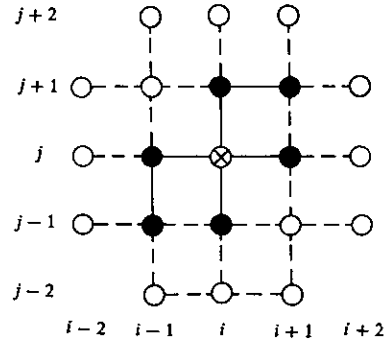

FIGURE 5

From this we find with an error $O(t^3)$ the following expressions for the constants c_1, c_2, b:

$$b = d_0^{(1)}, \qquad c_1 = 1/d_1^{(1)}, \qquad c_2 = -c_1^3 d_2^{(1)}. \quad (5.28)$$

From the requirement that $b + t = 0$, we find $t = -b$, and then $u_1(u_2; \xi_1, \xi_2)$ is computed by formula (4.4). The case $|d_1^{(1)}| < |d_1^{(2)}|$ is considered in a similar way.

Note that the two-cycle MacCormack scheme (5.24) is a three-level difference scheme. Therefore, the stability condition for this scheme which can be obtained with the aid of the von Neumann stability analysis will be also a sufficient stability condition if the amplification matrix G is normal [1], that is

$$GG^* = G^*G. \quad (5.29)$$

It is easy to show that the condition (5.29) is not satisfied in the case of scheme (5.24). Let us indeed introduce an auxiliary dependent variable $v^n = u^{n+1}$. Then we can rewrite scheme (5.24) in the form of the two-level scheme,

$$U^{n+1} = SU^n,$$

where

$$U^n = \begin{pmatrix} u^n \\ v^n \end{pmatrix}, \qquad S = \begin{pmatrix} 0 & 1 \\ L_2 L_1 & 0 \end{pmatrix}.$$

Performing the Fourier transform we obtain that the amplification matrix G has the form

$$G = \begin{pmatrix} 0 & 1 \\ a + ib & 0 \end{pmatrix},$$

where $a + ib$ is the Fourier symbol of the operator $L_2 L_1$, and a and b are real-valued functions of κ and ξ. It is easy to find that

$$GG^* = \begin{pmatrix} 1 & 0 \\ 0 & a^2 + b^2 \end{pmatrix}, \qquad G^*G = \begin{pmatrix} a^2 + b^2 & 0 \\ 0 & 1 \end{pmatrix}.$$

It may be seen from here that condition (5.29) is not satisfied inside the stability region. In this connection we will call the region in which the von Neumann necessary stability conditions (2.6) are satisfied, the NSC region (necessary stability condition region).

In Fig. 6 we present the NSC region of scheme (5.24) obtained by the above-described modified symbolic–numerical method: $|u_2| = 0.04$ in formula (5.26), $\varepsilon = 0.01$ in the bisection process described in Section 4 and employing the function (4.13). It may be seen that the NSC region has no symmetry properties, although the stencil of the nth level (see Fig. 5) is symmetric with respect to the (i, j) point. It appears that the asymmetry of the NSC region is related to a possible asymmetry of the expressions for coefficients affecting 21 grid values u_{kl}^n entering the difference equation (5.24).

Although the NSC region of the scheme under consideration is asymmetric, its boundary Γ cuts equal segments on the κ_1 and κ_2 axes. The length of these segments may easily be found analytically by using the expressions for the coefficients of the characteristic polynomial (2.5) which have been obtained with the aid of the REDUCE system. We do not present them here because of their bulky form and consider a particular case when $\kappa_2 = 0$, $\kappa_1 \neq 0$ in these coefficients; that is we seek the coordinate κ_1 of the point of intersection of the boundary Γ with the $O\kappa_1$ axis.

It was found from the numerical computations by the proposed symbolic–numerical method that the condition for an envelope (2.21) is satisfied near the $O\kappa_1$ axis at $\xi_1 = \xi_2 = \pi$. Substituting these values into the characteristic polynomial coefficients and assuming also that $\kappa_2 = 0$, we arrive at the following characteristic equation:

$$4\lambda^2 - 16\kappa_1^4 + 4\kappa_1^2 - 2 = 0.$$

From the requirement that $|\lambda| \leqslant 1$ we obtain the inequality

$$4y^2 - y - \tfrac{1}{2} \leqslant 0,$$

where $y = \kappa_1^2$. This inequality is easily solved and it is found that the inequality $y \leqslant \frac{1}{2}$ should be satisfied. Thus the boundary Γ intersects the $O\kappa_1$ axis at points with the abscissas $\kappa_1 = \pm 1/\sqrt{2} = \pm 0.70710678\cdots$. In computations to a given accuracy $\varepsilon = 10^{-2}$ we obtained the following values of the abscissa κ_1 by the proposed symbolic–numerical method at the points of intersection of the line Γ with the

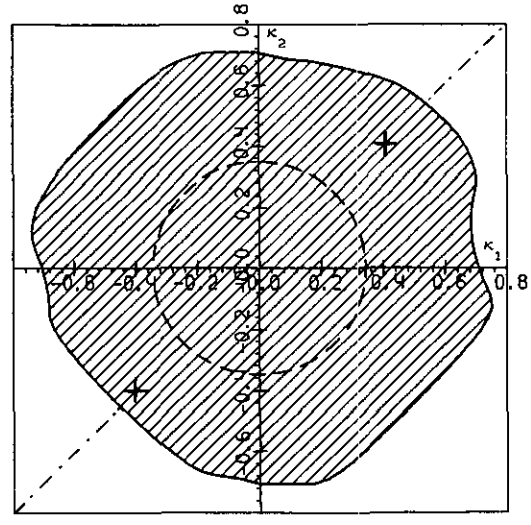

FIGURE 6

$O\kappa_1$ axis: $\kappa_1 = -0.7070193$; $\kappa_1 = 0.7075254$. It can also be seen in Fig. 6 that the slope of the curve Γ changes continuously when passing from one quadrant to another quadrant, although the computations on the determination of Γ in each quadrant were performed independently. This can also serve as evidence of the correctness of the result obtained.

An approximate von Neumann analysis of scheme (5.24) was carried out in [34], see also [35]. The following condition for satisfaction of the von Neumann criterion was obtained in [34, 35] by making a few estimates of the amplification factor of the scheme (in particular, with the aid of Schwarz's inequality):

$$\kappa_1^2 + \kappa_2^2 \leqslant 2(1 + \tfrac{1}{8})^{1/2} - 2 = 3/\sqrt{2} - 2 \approx 0.12132034. \quad (5.30)$$

Thus the Γ boundary is in accordance with (5.30) a circle of the radius $r = (3/\sqrt{2} - 2)^{1/2} \approx 0.3483107$. In Fig. 6 this circle is plotted by a dashed line. It was stressed in [34, 35] that the bound (5.30) is far from optimal, because at $\kappa_1 = \kappa_2$ the estimate

$$\kappa_1^2 + \kappa_2^2 \leqslant 0.3266$$

works. In Fig. 6 the two points lying on the bisector $\kappa_1 = \kappa_2$ and having the polar radius $r = \sqrt{0.3266}$ are marked by the crosses. It can be seen that these two points already lie rather close to the boundary computed by our symbolic–numerical method.

It follows from Fig. 6 that the NSC region of scheme (5.24) can be fitted analytically by the inequality

$$(\kappa_1^2 + \kappa_2^2)^{0.5} \leqslant \theta/\sqrt{2}. \quad (5.31)$$

It is easy to choose the safety factor θ in (5.31) in the way that all the points of the region (5.31) lie inside the NSC region of scheme (5.24). For example, the value $\theta = 0.905$ meets this requirement.

In view of the fact that the amplification matrix G of the difference scheme (5.24) does not meet the normality requirement (5.29) further investigations are needed for determination of the sufficient stability conditions of scheme (5.24). This difficult problem goes beyond the scope of the present paper, because we would like to show here a possibility of automation of the von Neumann stability analysis of difference initial-value problems with the aid of the algebra of the resultants, the catastrophe theory, and symbolic computations.

When numerically solving a specific problem with the aid of the two-cycle MacCormack scheme (5.24) one can use the trial-and-error procedure to find the actual stability region. For this purpose one can try the values of θ in (5.31) in the range $0 < \theta \leqslant 0.905$. For the given value of θ the step τ can be computed with regard to (5.15) by the formula

$$\tau = \theta/\{2[(A/h_1)^2 + (B/h_2)^2]\}^{0.5}.$$

CONCLUSION

The above-presented results show that the proposed symbolic–numerical method is an efficient means for determining the necessary (and, in some cases, sufficient) stability conditions of difference schemes. Although we have presented in this work a symbolic–numerical realization of the method only for determining the regular points of the boundary Γ as obtained on the basis of the von Neumann analysis, nevertheless this method gives an opportunity to correctly describe all the singularities of this boundary Γ. It is easy to see that a symbolic–numeric realization of the transformation (2.17) may be constructed in a similar way for the case $k > 1$. This will enable us to carry out a numerical computation of singular points of a boundary and to automate completely a procedure for determining at least the necessary stability conditions of a difference scheme.

As regards a similar computer-aided automation of obtaining the sufficient stability conditions of difference initial-value problems and difference initial- and boundary-value problems, the available GKS theory [18, 14] mentioned in the Introduction strongly resists such automation in the case of several spatial dimensions. Therefore, the development of alternative well-formalizable mathematical procedures for such analyses is of present interest. This work is now in progress (see, in particular, our recent paper [36]).

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