JOURNAL OF COMPUTATIONAL PHYSICS 55, 254–267 (1984)

DERPER—An Algorithm for the Continuation of Periodic Solutions in Ordinary Differential Equations

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Received August 5, 1982; revised June 8, 1983

An algorithm for the continuation of periodic solutions of ODE was derived and tested. The algorithm is based on the shooting method and a standard continuation algorithm. Variational variables are used to compute the Jacobi matrix. The starting point on the periodic orbit is adaptively changed in the algorithm by fixing one component of the solution. Stability of periodic solutions along the continuous branch of solutions is determined by computing characteristic multipliers. Without difficulty the algorithm crosses limit points and at bifurcation points, double-period bifurcation points, and points of tori bifurcation it proceeds along the original branch of solutions. The usefulness of the algorithm is demonstrated in two examples. One of them describes two stirred tank reactors with mutual mass exchange, the other one is the Lorenz model of turbulence.

1. INTRODUCTION

When studying mathematical models in physics, engineering, or biology, we are very often interested in how these behave as functions of model parameters, i.e., we try to construct the so-called *solution diagram* [7] (the term *bifurcation diagram* is also often used for this dependence). Simple mapping methods, sequential use of standard algorithms or certain continuation algorithms have been used to illustrate the dependence of periodic solutions on a parameter.

Consider mathematical models in the form of systems of ordinary differential equations. Stationary solutions of the models result from a set of nonlinear (algebraic) equations dependent on a chosen physical parameter. Several methods for automatic generation of stationary solutions depending on a parameter have been developed: methods using the arc-length of the solution locus as the continuation parameter [1–5]. These algorithms are applicable in the study of flight control [6] and in the study of reaction–diffusion systems [7].

Stable periodic solutions of model equations are attractors of the limit cycle type. Three different types of algorithms are designed to compute periodic solutions. One of the easiest approaches is a dynamic simulation of the studied system leading to a stable periodic orbit. In this way only stable periodic solutions are obtained. Unstable periodic solutions in which all characteristic multipliers are located outside the unit circle are similarly obtained by integrating the equations in the reverse time direction.

0021-9991/84 $3.00

The second approach uses difference methods producing a large system of nonlinear algebraic equations having a band Jacobi matrix [8]. The third algorithm is based on a *shooting* method for solving the nonlinear boundary value problem with mixed boundary conditions [9–12]. One grave disadvantage of the shooting metods is that it fails for *strongly* unstable periodic solutions.

Periodic solutions often depend on a parameter as is the case of stationary solutions. Several recently published papers provide a partial solution to this problem. A continuation of periodic solutions [11] is based on the algorithm DERPAR [1]. However, a description of the algorithm is missing. A sequential approach to continuation of periodic solutions is used by Hassard [9], Rinzel and Miller [8], Seydel [12], and Chibnik [13]. When the Newton method is used sequentially, the previously computed point of the solution diagram is used as an initial estimate. To pass through a limit (turning) point the algorithm has to be modified, in that the parameter and one of the variables are interchanged.

The problem of the expansion of the periodic solution in the neighbourhood of Hopf's bifurcation point has been studied by several authors [9, 12, 14]. These expansions can be used as an initial estimate for the continuation algorithm.

This paper describes an algorithm for continuation of periodic solutions based on the shooting method and on the arc-length continuation algorithm DERPAR [1]. This algorithm uses adaptive adjustment of the fixed variable on the periodic orbit and has been successfully applied to a number of practical problems.

2. Development of an Algorithm Based on a Shooting Method and the Continuation Routine DERPAR

Consider an autonomous system of ordinary differential equations

$$\frac{dy_i}{dt} = f_i(y_1,..., y_n, \alpha), \qquad i = 1, 2,..., n. \tag{1}$$

A periodic solution with the period T satisfies

$$y_i(t + T) = y_i(t), \qquad i = 1, 2,..., n. \tag{2}$$

The transformation $t = Tz$ produces

$$\frac{dy_i}{dz} = Tf_i(y_1,..., y_n, \alpha), \qquad i = 1, 2,..., n \tag{3}$$

and mixed boundary conditions (2) appear in the form

$$y_i(1) - y_i(0) = 0, \qquad i = 1, 2,..., n. \tag{4}$$

Choose initial conditions

$$y_i(0) = x_i, \qquad i = 1, 2, \ldots, n \tag{5}$$

and the value of the period T. Integrate system (3) (for fixed α) starting from $z = 0$ to $z = 1$. (The integration can be performed from $z = 0$ to $z = -1$ alternatively, if the solution of the initial value problem is more stable in the negative orientation of z. However, the conclusions on the stability of the periodic solution will change. We shall not discuss this alternative here).

As a result of the integration we obtain the values of the solution at $z = 1$

$$y_i(1) = \varphi_i(x_1, \ldots, x_n, T, \alpha). \tag{6}$$

The relation (4) has to hold for any periodic solution; thus we have to satisfy n equations

$$F_i(x_1, \ldots, x_n, T, \alpha) = \varphi_i(x_1, \ldots, x_n, T, \alpha) - x_i = 0, \qquad i = 1, \ldots, n \tag{7}$$

with $n + 1$ unknowns $x_1, \ldots, x_n, T$ and one parameter α. Here the value of α is fixed. Therefore, choose a fixed value for one unknown, x_k (except T because the solution of (7) exists only for discrete (and a priori unknown) values of T). If the chosen value actually exists on the trajectory of the kth component of the wanted periodic solution $y_k(z)$, $z \in [0, 1)$, i.e., $x_k = y_k(\bar{z})$ for a certain $\bar{z} \in [0, 1)$, we solve (7), applying Newton's method for unknowns $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n, T$ (with the values of x_k and α fixed).

The standard routine DERPAR [1] is described now. It is designed to continue a branch of solutions of n nonlinear equations for $n + 1$ variables (one of them is a parameter) from a solution on the branch already known. The algorithm consists of two steps, predictor and corrector. A detailed description is given in the Appendix. The evaluation of the Jacobi matrix of Eqs. (7) is necessary for the functioning of the DERPAR-continuation.

The Jacobi matrix of (7) with respect to $n + 2$ variables $x_1, \ldots, x_n, T, \alpha$ can be evaluated by means of variational differential equations. For variational variables,

$$p_{ij}(z) = \frac{\partial y_i}{\partial x_j}, \tag{8}$$

the variational equations have the form

$$\frac{dp_{ij}}{dz} = T \sum_{s=1}^{n} \frac{\partial f_i}{\partial y_s} p_{sj}, \qquad i, j = 1, 2, \ldots, n. \tag{9}$$

Relations (9) are obtained by differentiation of (3) with respect to x_j. Differentiating (3) with respect to α we obtain for

$$q_i = \frac{\partial y_i}{\partial \alpha} \tag{10}$$

the equations

$$\frac{dq_i}{dz} = T \sum_{s=1}^{n} \frac{\partial f_i}{\partial y_s} q_s + T \frac{\partial f_i}{\partial \alpha}, \qquad i = 1, 2, \ldots, n. \tag{11}$$

Initial conditions for these equations are

$$p_{ij}(0) = \delta_{ij}, \qquad q_i(0) = 0, \qquad i, j = 1, \ldots, n, \tag{12}$$

where δ_{ij} is the Kronecker delta.

The elements of the Jacobi matrix of the system (7) are

$$\frac{\partial F_i}{\partial x_j} = p_{ij}(1) - \delta_{ij}, \qquad \frac{\partial F_i}{\partial T} = f_i(y(1), \alpha),^{1} \qquad \frac{\partial F_i}{\partial \alpha} = q_i(1). \tag{13}$$

Column $\partial F_i/\partial x_k$ is redundant for the given continuation algorithm. However, to estimate the stability of a particular periodic solution it is necessary to have a full matrix $\{\partial F_i/\partial x_j\}$.

Thus we have all the necessary information required by the continuation routine DERPAR and the continuation of the solution of the system (7) for variables $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n, T, \alpha$ can proceed until the fixed value x_k *disappears* from the course of periodic solution. To prevent the disappearance, we have to change x_k adaptively in the course of the continuation. The principle of algorithm modified in this way (the algorithm is called DERPER) can be summarized as follows:

(a) k is fixed.

(b) Choose an initial approximation of $x_1, \ldots, x_n, T, \alpha$ and give all necessary control parameters for DERPAR-routine. The value of x_k is to remain fixed during continuation.

(c) Call DERPAR for the variables $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n, T, \alpha$. DERPAR proceeds in a standard way in $n+1$ variables $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n, T, \alpha$. In each step the following inequalities are tested:

$$x_k^- < x_k < x_k^+, \tag{14}$$

$$y_k^+ - y_k^- > (1 - \omega_2) H_{\max}, \tag{15}$$

where

$$\begin{aligned} x_k^- &= \tfrac{1}{2}[(1 + \omega_1) y_k^- + (1 - \omega_1) y_k^+], \\ x_k^+ &= \tfrac{1}{2}[(1 - \omega_1) y_k^- + (1 + \omega_1) y_k^+]. \end{aligned} \tag{16}$$

The values of y_k^- and y_k^+ are the minimum and the maximum of $y_k(z)$, respectively,

[1] Variational equations similar to (11) can be derived for $r_i = \partial y_i/\partial T$, too. However, the relation used in (13) is simpler and does not require any integration.

on the (maximum) interval $z \in [0, z_1] \cup [z_2, 1]$, where $y_k(z)$ is monotonous. $H_{\max}$ is maximum difference between maximum and minimum of the monotonic part of $y_k(z)$ on the entire interval $z \in [0, 1]$, i.e., $H_{\max} = y_k(z^+) - y_k(z^-)$. The extrema are schematically shown in Fig. 1. The values of ω_1, $\omega_2 \in (0, 1]$ are usually chosen from the interval 0.5-0.8.

If both inequalities (14) and (15) are satisfied, the value of x_k is not changed and DERPAR utilizes a multistep (Adams-Bashforth) predictor formula.

(d) If the inequality (14) or (15) is not satisfied, then x_k is changed according to the formula

$$x_k^{\text{new}} \approx \tfrac{1}{2}[y_k(z^+) + y_k(z^-)]. \tag{17}$$

The remaining components $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n$ must be reevaluated using known (stored) profiles $y_1(z), \ldots, y_n(z)$ calculated last. This is done by finding coordinate z^* between z^- and z^+, where the relation

$$y_k(z^*) \approx x_k^{\text{new}} \tag{18}$$

is approximately valid. Then $x_i^{\text{new}} = y_i(z^*)$. The multistep predictor in DERPAR is then restarted beginning from the first order (Euler method). At the same time some control parameters in DERPAR are reorganized. This is necessary particularly for direction parameters used to keep direction along the solution locus curve.

Denote $N_1, \ldots, N_{n+1}$ the direction parameters corresponding to the variables $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n$, T, α. The values of N_i are either $+1$ (corresponding variable increases along the solution locus curve with increasing arc-length parameter) or -1 (corresponding variable decreases with increasing arc-length parameter). Reevaluating (17) does not cause any change in N_n and N_{n+1} because it does not

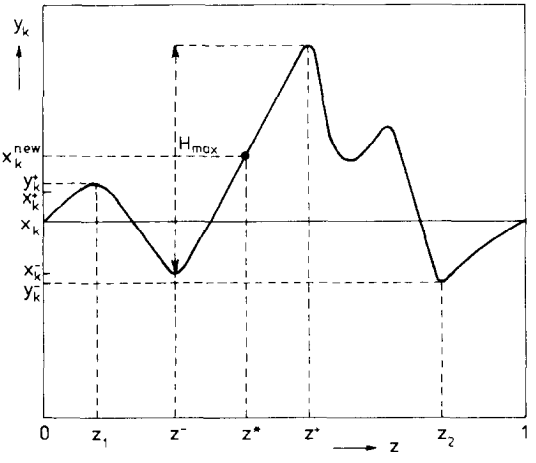

FIG. 1. Schematic picture of a periodic solution.

change the period T or the parameter α. The remaining N_i can be changed, because the variables $x_1,\ldots,x_{k-1}$, $x_{k+1},\ldots,x_n$ have been changed. For the reevaluation of N_i the following transformations are used

$$\begin{aligned} N_i^{\text{new}} &= N_i \operatorname{sign} p_{ii}(z^*), & i < k, \\ N_i^{\text{new}} &= N_i \operatorname{sign} p_{i+1,i+1}(z^*), & i \geqslant k. \end{aligned} \tag{19}$$

The profiles $p_{ii}(z)$ are stored together with the profiles $y_i(z)$, $i = 1, 2,\ldots, n$. A schematic flow diagram of the algorithm is shown in Fig. 2. The stability of the computed periodic solution is determined on the basis of characteristic multipliers (e.g., [16]), i.e., eigenvalues λ of the monodromy matrix

$$B = \{\partial\varphi_i/\partial x_j\} = \{p_{ij}(1)\}, \qquad i,j = 1,\ldots, n, \tag{20}$$

where the p_{ij} are evaluated after corrector, cf. Fig. 2. The eigenvalues are computed by using standard algorithms, see, e.g., [15]. For small n they could be evaluated as the roots of the characteristic polynomial

$$P(\lambda) = \det(B - \lambda I). \tag{21}$$

If all multipliers are located inside the unit circle (one of them always equals the unity), the periodic solution is stable. The presence of at least one multiplier outside the unit circle in the complex plane indicates instability of the periodic solution.

The continuation procedure DERPER described above *travels* on the branch of the periodic solutins in question. Problems with the continuation method could arise when the so-called bifurcation points, i.e., those where some multiplier goes through the unit circle, are encountered. (All such cases can be detected if the development of multipliers along the branch is followed.) The algorithm continues on the original branch of periodic solutions in the three following cases:

(a) $\lambda = -1$ (double period bifurcation point),

(b) $\lambda_{12} = \xi_1 \pm i\xi_2$, $\xi_1^2 + \xi_2^2 = 1$ (bifurcation to invariant torus),

(c) $\lambda = 1$ (bifurcation point in the solution diagram).

The bifurcated branch of periodic or quasiperiodic solutions is not followed. However, we can start the algorithm at a chosen periodic solution located on such new branch. This solution is found, e.g., by trial and error technique or some expansion algorithm can be used [2-5, 7, 19, 22]. The case

(d) $\lambda = 1$ (limit point in solution diagram),

where two branches of periodic solutions coincide and the number of periodic solutions is changed by two, causes no trouble. DERPER continues on the second branch of the solutions. The disappearance of periodic solutions at the point of Hopf bifurcation can also be detected by the algorithm (cf. Fig. 2). The more complicated cases should be analyzed by the user.

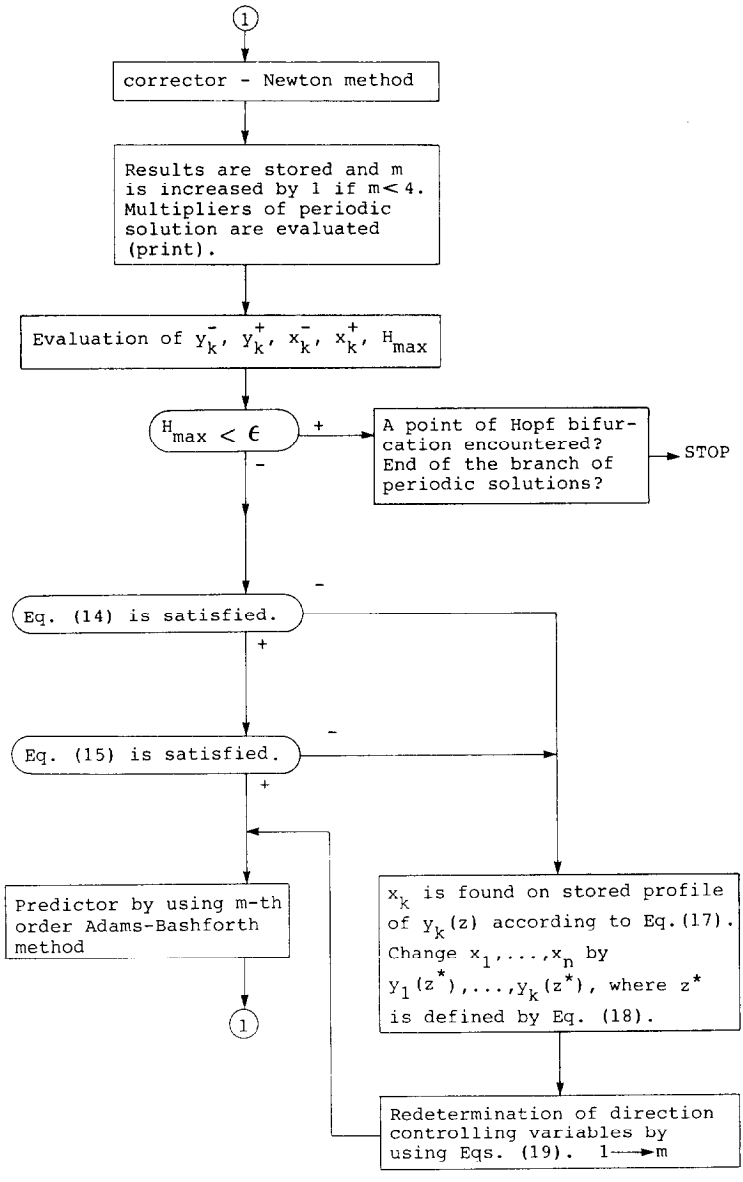

FIG. 2. Schematic flow-diagram of DERPER continuation algorithm.

3. Application

The algorithm DERPER has been successfully applied to a number of practical problems. To illustrate, consider the problem of two interconnected well mixed cells where chemical reaction takes place. As a model chemical reaction the so-called Brusselator [17] scheme is chosen. The governing equations appear in the following form ($n = 4$ in relation (1)):

$$\begin{aligned}
\frac{dy_1}{dt} &= a - (b+1)y_1 + y_1^2 y_2 + \alpha(y_3 - y_1), \\
\frac{dy_2}{dt} &= by_1 - y_1^2 y_2 + \frac{\alpha}{\rho}(y_4 - y_2), \\
\frac{dy_3}{dt} &= a - (b+1)y_3 + y_3^2 y_4 + \alpha(y_1 - y_3), \\
\frac{dy_4}{dt} &= by_3 - y_3^2 y_4 + \frac{\alpha}{\rho}(y_2 - y_4).
\end{aligned} \tag{22}$$

Computed results are presented in Fig. 3. Here $k = 1$. The step length Δs (of the independent variable of continuation, i.e., of the arc length of the solution locus) is 0.05 and the points on the obtained curve of the solutions are numbered. The relation

$$(\Delta x_2)^2 + (\Delta x_3)^2 + (\Delta x_4)^2 + (\Delta T)^2 + (\Delta \alpha)^2 \approx 0.05^2$$

is approximately satisfied for the neighbouring points in the figure in accordance with the Euclidean arc-length definition. The last relation is not valid between points no. 40 and 41, where the algorithm changed the value of x_k from 2.07664 to 3.79427. As a result, the dependences $x_i(s)$ are discontinuous between these two points. The values of the variables from the dependences in Fig. 3 for several points are presented in Table I.

The leading characteristic multiplier λ_2 of the periodic solutions in question (in dependence on α) is presented in the upper part of the Fig. 3. Multiplier λ_1 is always equal to unity and the remaining two multipliers are always located in a close neighbourhood of the origin. Dependence $\lambda_2(s)$ crosses the constant line $\lambda_2 = 1$ four times. All these intersection points correspond to the limit points on the dependences of the solution on the parameter α, i.e., to the extrema on the curve $\alpha(s)$; these points are denoted L.P. in Fig. 3. More complete results are shown in Fig. 4, where the dependence of the amplitude of the periodic solutions on the parameter α (obtained by using DERPER), is presented [18]. Note that there are four narrow intervals of the parameter α, where the periodic solutions in question are stable, i.e., the parts of the curves where $\lambda_2 \in (-1, 1)$. Four points of intersections of the dependence $\lambda_2(s)$

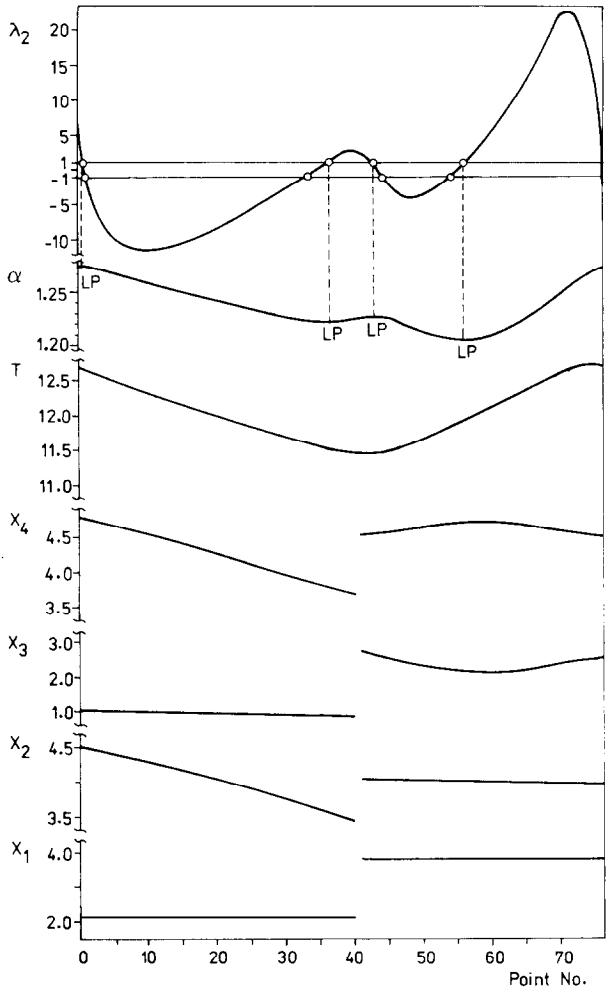

FIG. 3. A closed (isolated) dependence of periodic solutions on the arc-length parameter s. Results of the continuation algorithm ($a = 2$, $b = 5.9$, $\rho = 0.1$).

with the line $\lambda_2 = -1$ correspond to the so-called double period bifurcation points (or Brunovsky bifurcation) where a new branch of periodic solutions bifurcates from the original one and the period is doubled [19]. These branches are also included in Fig. 4 (dashed lines). There are lots of other branches of periodic solutions for the Brusselator model (22). Some of them (obtained by the DERPER algorithm) are shown in Fig. 5. More detailed discussion of the steady state and periodic behaviour of the model (22) will be published in [18].

TABLE I

Coordinates of Several Points in Fig. 3[a]

Point Number	$y_1(0)$	$y_2(0)$	$y_3(0)$	$y_4(0)$	T	α	λ_2
0	2.07664	4.52951	1.03402	4.79073	12.67268	1.274178	5.6
20	2.07664	4.02883	0.93175	4.26953	12.00893	1.242149	−9.0
40	2.07664	3.47374	0.88418	3.66905	11.44121	1.224062	2.5
41	3.79427	4.05095	2.71528	4.52935	11.42782	1.225034	2.6
50	3.79427	4.02935	2.37206	4.64518	11.66778	1.213523	−3.9
65	3.79427	3.98939	2.20792	4.65871	12.35977	1.225408	11.3

[a] $a = 2$, $b = 5.9$, $\rho = 0.1$.

A model exhibiting the rich structure of periodic solutions is the Lorenz model of convection [21]

$$\begin{aligned} \frac{dy_1}{dt} &= -\sigma y_1 + \sigma y_2, \\ \frac{dy_2}{dt} &= -y_1 y_3 + \alpha y_1 - y_2, \\ \frac{dy_3}{dt} &= y_1 y_2 - b y_3. \end{aligned} \tag{23}$$

For this model, too, the DERPER algorithm has proved its effectiveness. More than twenty branches of periodic solutions have been successfully continued [23]. An example of such continuation is shown in Fig. 6. The starting points characterized by (P) for continuation on individual branches,

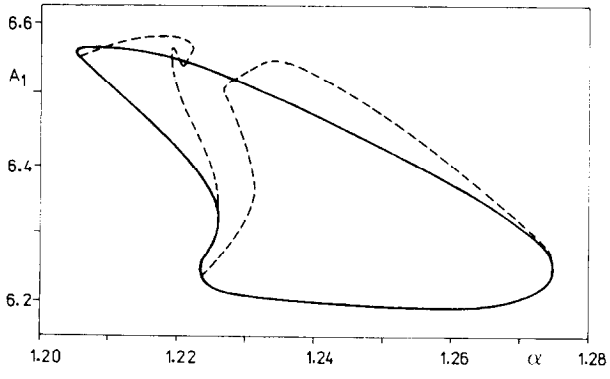

FIG. 4. Dependence of the amplitude of y_1 of the periodic solutions on the parameter α ($a = 2$, $b = 5.9$, $\rho = 0.1$).

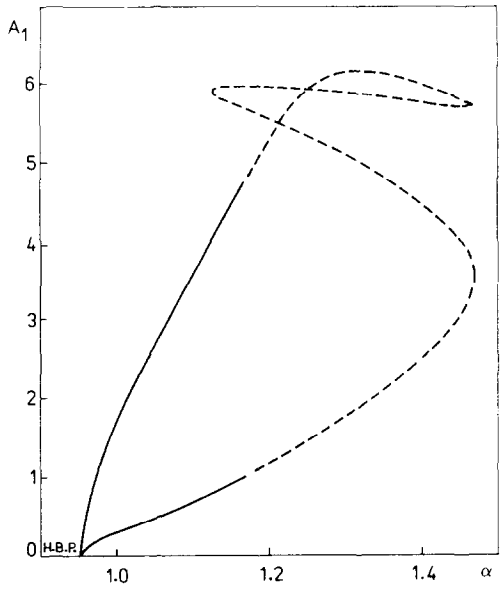

FIG. 5. Dependence of the amplitude of y_1 of periodic solutions of Eqs. (22) on the parameter α ($a = 2$, $b = 5.9$, $\rho = 0.1$, (—) stable, (– – –) unstable, H.B.P.-Hopf bifurcation points).

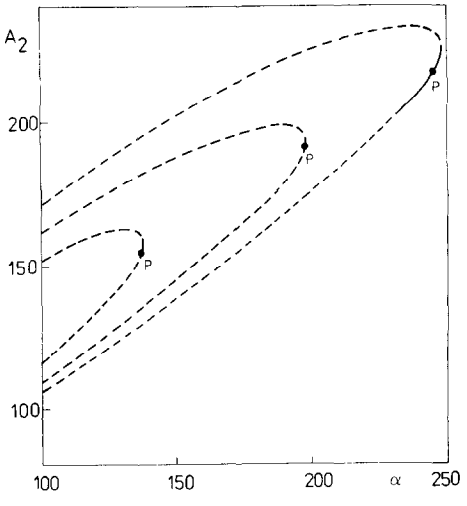

FIG. 6. Dependence of the amplitude of y_2 of periodic solutions of the Lorenz system (23) on the parameter α ($\sigma = 16$, $b = 4$, (—) stable, (– – –) unstable).

y_1	y_2	y_3	T	α	A_2
−0.067550	−56.4816	228.439	0.73934	245	217
−0.001030	−9.75909	154.598	1.65427	198	191
−0.026240	−36.5315	135.279	1.48629	137	154

are stable periodic solutions obtained by transient simulation of Eqs. (23) for a sufficiently long time interval.

4. Conclusions

The DERPER algorithm is effective as a tool for continuation of the dependence of periodic solutions on a parameter in a number of studied cases. It has also been applied to problems in neurophysiology [20] and various reaction–diffusion models. The algorithm is applicable in situations where the characteristic multipliers are not too large. When the multipliers are of 10^5 order, the shooting method used for numerical integration of the initial value problems usually fails as in the case of the Hodgkin–Huxley model [20] where some parts of the dependence of periodic solutions can not be obtained by the DERPER algorithm. Sometimes we can reverse the direction of integration from $z = 0$ to $z = -1$, but usually a new large multiplier appears here again. In such situations a multiple shooting or finite-difference method can be used instead of the simple shooting method. Modified versions of the algorithm are under development.

The starting of the continuation algorithm poses another problem: the choice of index k and the value x_k. Sometimes, we can use a priori knowledge of some periodic solution on the branch under study. If no a priori information is available the k, x_k, and x_1, x_2,..., x_{k-1}, x_{k+1},..., x_n, T, α values can be generated at random as a guess for initial Newton iteration. When we have managed to obtain the starting point successfully, the algorithm continues the branch of periodic solutions and controls the choice of x_k, while the value of the index k remains fixed. An improved algorithm could include an adaptive change of k depending on the structure of the sensitivity matrix B.

The concept suggested can be also applied to nonautonomous systems. There T is fixed and the iteration proceeds in the variables x_1,..., x_n and the parameter α. Thus, the algorithm is simpler because there is no need to fix k and x_k.

The algorithm suggested can also be used for partial differential equations. If the method of lines is used for the discretization of the original parabolic equations a large system of ordinary differential equations is obtained. Periodic solutions of these equations can be obtained using DERPER. However, computer time consumption is relatively high.

APPENDIX: CONTINUATION OF SOLUTION OF NONLINEAR EQUATIONS DEPENDING ON A PARAMETER ALONG AN ARC-LENGTH OF THE SOLUTION LOCUS-DERPAR [1]

Let us consider a system of nonlinear equations

$$g_i(u_1,..., u_n, \alpha) = 0, \qquad i = 1, 2,..., n \tag{A1}$$

depending on the parameter α. Let us denote $u_{n+1} = \alpha$. Differentiation of Eq. (A1) with respect to s gives

$$\frac{dg_i}{ds} = \sum_{j=1}^{n+1} \frac{\partial g_i}{\partial u_j} \frac{du_j}{ds} = 0, \qquad i = 1, 2,..., n. \tag{A2}$$

An additional equation

$$\left(\frac{du_1}{ds}\right)^2 + \left(\frac{du_2}{ds}\right)^2 + \cdots + \left(\frac{du_{n+1}}{ds}\right)^2 = 1 \tag{A3}$$

determines the parameter s as the arc-length of the curve $u(\alpha)$ in the space $(u - \alpha)$. Equations (A2) can be presolved with respect to the unknowns $du_1/ds,..., du_{m-1}/ds$, $du_{m+1}/ds,..., du_{n+1}/ds$ depending on dx_m/ds in the form

$$\frac{du_i}{ds} = \beta_i \frac{du_m}{ds}, \qquad i = 1, 2,..., m-1, m+1,..., n+1. \tag{A4}$$

On substituting (A4) into (A3) we obtain

$$\left(\frac{du_m}{ds}\right)^2 = \left(1 + \sum_{\substack{i=1 \\ i \neq k}}^{n+1} \beta_i^2\right)^{-1}. \tag{A5}$$

The sign of du_m/ds is given by the orientation of the parameter s along the curve, sign $(du_m/ds) = N_m$. All derivatives du_i/ds are then determined by Eq. (A4). The Adams–Bashforth explicit multi-step method with an automatic change in the order of approximation is used for the integration of differential equations (A4) and (A5). This step is called predictor. Initial conditions are in the form

$$s = 0: \qquad u_i = u_i^0, \qquad \alpha = \alpha^0, \quad i = 1,..., n, \tag{A6}$$

where

$$g_i(u_1^0,..., u_n^0, \alpha^0) = 0, \qquad i = 1,..., n. \tag{A7}$$

In the course of integration the truncation (approximation) error causes a deviation between the calculated solutions $u(s)$ and the correct profiles $u(s)$. The Newton method for variables $u_1,..., u_{m-1}, u_{m+1},..., u_{n+1}$ is then used as the corrector to

improve the calculated profiles. The value of u_m remains unchanged during these corrector iterations.

More detailed explanation can be found in [1].

ACKNOWLEDGMENTS

The authors would like to acknowledge their debt to Professor Miloš Marek for his kind encouragement and assistance, as well as to Mr. Jiří Prančl for his help with English.

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