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NONLINEAR DYNAMICS SYSTEMS - BIFURCATIONS, CONTINUATION METHODS, PERIODIC SOLUTIONS

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1. INTRODUCTION

Let us consider a system of autonomous nonlinear ordinary differential equations (nonlinear dynamic system)

$$y' = f(y,p) \quad , \tag{1}$$

where $' = d/dt$, $y \in R^n$, $p \in R^m$ are parameters, $f : R^n \times R^m \to R^n$, $f \in C^1$. Steady state solutions of (1) are defined by

$$f(y,p) = 0 \quad . \tag{2}$$

A set $S(f) \in R^n \times R^m$, $S(f) : (y,p)$, $f(y,p) = 0$, is called "solution diagram" [19], sometimes also "bifurcation diagram" [10]. Solution diagram is mostly considered for one parameter, i.e. p_1 only, while values of remaining parameters $p_2, \ldots, p_m$ are fixed. Continuation algorithms have been developed in the last ten years for an automatic computation of such solution diagrams [e.g., 14, 24, 9, 10, 11]. Stability of steady state solutions can be determined on the basis of eigenvalues λ of the Jacobian matrix $J = \{\partial f / \partial y\}$. If an eigenvalue λ crosses the imaginary axis in complex plane (by varying some parameter, e.g., p_1) a bifurcation occurs in generic cases. Several review papers surveying numerical methods for location of bifurcation points appeared recently [22, 20, 19, 9]. Four iterative algorithms for the evaluation of Hopf bifurcation points have been published in [5] .

Main purpose of this paper is to discuss periodic behaviour observed in two typical mathematical models of chemical and engineering systems, review computational methods for continuation and bifurcation of periodic solutions.

The first model is well known Lorenz model [21] of the flow in the layer of liquid heated from below (the Rayleigh - Bénard problem). The system

$$y_1' = -\sigma y_1 + \sigma y_2 \quad , \quad y_2' = -y_1 y_3 + r y_1 - y_2 \quad , \quad y_3' = y_1 y_2 - b y_3 \tag{3}$$

is obtained by a reduction of the system of Navier Stokes equations and the equation describing heat transfer. The dimensionless parameters $p = (r, \sigma, b)$ correspond to : σ - Prandtl number, r - reduced Rayleigh number, b is related to a wave-number of the convective structure . A detailed description of behaviour of the model can be found in the Sparrow's book [27] , a structure of periodic solutions was discussed in [7] .

The second model describes behaviour of two well mixed reaction cells with linear diffusion coupling and the "Brusselator" reaction kinetic scheme. The model is used as a standard model system for the discussion of dissipative structures in nonlinear chemical systems [23] . It can be written in the form

$$\begin{aligned} y_1' &= A - (B+1)y_1 + y_1^2 y_2 + D(y_3 - y_1) \\ y_2' &= By_1 - y_1^2 y_2 + D(y_4 - y_2)/\varrho \\ y_3' &= A - (B+1)y_3 + y_3^2 y_4 + D(y_1 - y_3) \\ y_4' &= By_3 - y_3^2 y_4 + D(y_2 - y_4)/\varrho \end{aligned} \qquad (4)$$

Here $p = (D,B,A,\varrho)$, A and B are constant concentrations, D and D/ϱ define the intensity of mass exchange between the cells, y_1 , y_2 and y_3 , y_4 are dimensionless concentrations of reaction intermediates in the first and second cell, respectivelly.

2. CONTINUATION OF PERIODIC SOLUTIONS

We shall present here a short description of an algorithm for the continuation (and computation) of periodic solutions based on the shooting method together with a continuation along the arclength of the solution locus. Detailed description of the algorithm is presented in [4] .

A periodic solution with the period T fulfils

$$y(T) - y(0) = 0 \quad . \qquad (5)$$

Considering shooting method we choose initial conditions

$$y(0) = x \quad , \qquad (6)$$

$x \in R^n$, and the value of the period T . Then the system (1) can be numerically integrated for fixed p from $t = 0$ to $t = T$, the results of integration

$$y(T) = \Psi(x,T,p) \qquad (7)$$

are dependent on the choice of x , T and p . Inserting (7) into (5) we obtain a system of n nonlinear equations

$$F(x,T,p) = \Psi(x,T,p) - x = 0 \qquad (8)$$

with $n + 1$ unknowns x , T and m parameters p . We have to fix one variable except T (or add some "normalization" equation). Let us fix x_k for some k , in such a way that x_k actually exists on the trajectory of the k-th component of the wanted periodic solution $y_k(t)$, $t \in [0,T]$. To continue periodic solutions in dependence on one parameter, say p_1 , we can use standard continuation algorithm DERPAR [14, 19] for continuation of solutions of n equations (8) for n unknowns $x_1,\ldots,$ x_{k-1}, $x_{k+1},\ldots,$ x_n, T and one parameter p_1 . This continuation algorithm requires an evaluation of the functions F in (8) and of the Jacobi matrix $\partial F/\partial x$, $\partial F/\partial T$, $\partial F/\partial p_1$. Elements of the Jacobi matrix can be determined on the basis of variational differential equations for variational variables

$$V(t) = \partial y/\partial x \quad , \quad q(t) = \partial y/\partial p_1 \quad , \qquad (9)$$

V is n by n matrix and q is n by 1 , i.e.,

$$V' = JV \quad , \quad V(0) = I \quad , \quad q' = Jq + \partial f/\partial p_1 \quad , \quad q(0) = 0 \quad . \tag{10}$$

The elements of the Jacobi matrix of the system (8) are then defined as

$$\partial F/\partial x = V(T) - I \quad , \quad \partial F/\partial T = f(y(T),p) \quad , \quad \partial F/\partial p_1 = q(T) \quad . \tag{11}$$

The continuation routine can proceed until the fixed value of x_k "disappears" from the course of the periodic solution. To avoid this disappearance, the algorithm exchanges x_k adaptively.

Several solution diagrams obtained by the continuation algorithm are presented in Figs 1 - 3 .

The stability of the computed periodic solution can be determined on the basis of characteristic multipliers, i.e., of eigenvalues μ of the monodromy matrix

$$M = \partial\psi/\partial x = V(T) \quad . \tag{12}$$

One multiplier is always equal to 1 because (1) is autonomous. If all remaining multipliers lie inside the unit circle, the periodic solution is stable, if at least one of them lies outside, then the periodic solution is unstable.

The use of the above described continuation algorithm is limited by the applicability of the shooting method. If the initial value problems are unstable, i.e., there are multipliers of the order 10^5 or higher, the integration and thus the simple shooting method usually fails. In such cases the multiple shooting method can be successfully used as, e.g., for the Hodgkin - Huxley model of the conduction of the nervous impulse, where $\mu \sim 10^9$ [6].

3. BIFURCATIONS OF PERIODIC SOLUTIONS

Bifurcation of periodic solutions occurs when a multiplier crosses the unit circle when varying a parameter. It can happen in three qualitatively different ways, i.e., when $\mu = 1$; $\mu = -1$; $|\mu| = 1$, $\mu^s \neq 1$, s = 1, 2, 3, 4. The cases $\mu^3 = 1$ and $\mu^4 = 1$ are of special interest [e.g., 8] .

3.1 LIMIT POINTS AND SYMMETRY BREAKING BIFURCATION POINTS ($\mu = 1$)

The monodromy matrix M has $\mu = 1$ as an eigenvalue (of multiplicity two) and, therefore, the Jacobi matrix $\partial F/\partial x$ has two zero eigenvalues. It means that no unique dependence of the periodic solutions on a parameter exists in the neighbourhood of this point. The bifurcation point can be either limit (turning) point (cf., e.g., point denoted L.P. in the Fig. 1) or symmetry breaking bifurcation point when there exists an inherent symmetry in the system (cf. point denoted SB in the fig. 1). Both bifurcation points can be determined by using shooting (or multiple shooting) method and methods for steady-state bifurcations. Either methods which use evaluation of the determinant of a matrix [13, 18, 19] or method without evaluation of the determinant [e.g., 1, 26] can be used.

3.2 PERIOD - DOUBLING BIFURCATIONS

When the monodromy matrix has $\mu = -1$ as an eigenvalue, then the so called

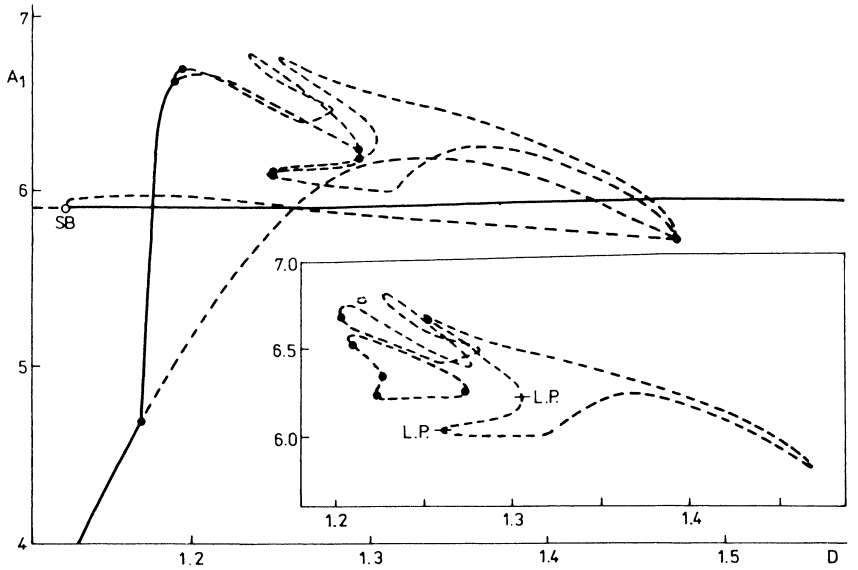

FIG. 1 : Solution diagram of periodic solutions of (4), A = 2, B = 5.9, ϱ = 0.1 [25]. A_1 - amplitude of y_1 . ● - period-doubling bifurcation point, o - symmetry breaking bifurcation point. —— stable, ---- unstable.

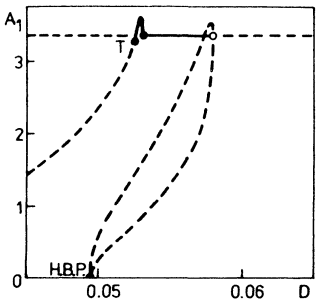

FIG. 2 : Solution diagram of periodic solutions of (4), A = 2, B = 5.5, ϱ = 0.1 [25]. T - tori bifurcation point, H.B.P. - two mutually symmetric Hopf bifurcation points. Further see legende to Fig. 1.

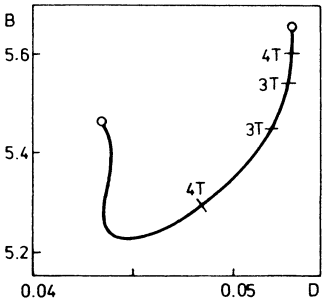

FIG. 4 : Bifurcation diagram of periodic solutions of (4), tori bifurcation points. A = 2, ϱ = 0.1. o - point of higher degeneration.

period-doubling bifurcation occurs, i.e., a branch of periodic solutions with approximately double period (asymptotically) branches off the original branch of periodic solutions (cf. points denoted ● in the Figs 1 - 3).

DETERMINATION OF PERIOD - DOUBLING BIFURCATION POINTS (μ = -1). Four iteration algorithms for computation of period-doubling bifurcation points have been publi-

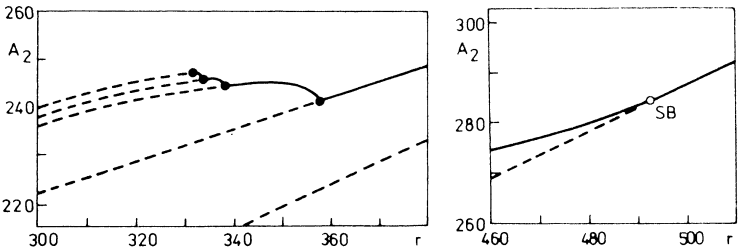

FIG. 3 : Solution diagram of periodic solutions of (3), $\sigma = 4$, $b = 16$ [7]. A_2 - amplitude of y_2 . ● - period doubling bifurcation point, o - symmetry breaking bifurcation point, —— stable, ---- unstable.

shed and are compared in [3]. We shall summarize very briefly two of them.

Let the characteristic polynomial of the monodromy matrix M be

$$P(\mu) = (-1)^n \det(M - \mu I) = \mu^n + a_1\mu^{n-1} + \ldots + a_{n-1}\mu + a_n \quad . \tag{13}$$

The coefficients a_j can be computed by using standard software. $\mu = -1$ is the root of (13) if

$$F_{n+1}(x,T,p) = 1 + \sum_{i=1}^{n} (-1)^i a_i = 0 \quad . \tag{14}$$

As a result we obtain $n + 1$ nonlinear equations (8) (14) for $n + 1$ unknowns $x_1,\ldots, x_{k-1}, x_{k+1},\ldots, x_n, T, p_1$. Newton method is used to solve this system.

$P(\mu)$ must have one root equal to unity, therefore, it can be decomposed into the form

$$P(\mu) = (\mu + 1)(\mu - 1)(\mu^{n-2} + b_1\mu^{n-3} + \ldots + b_{n-2}) + C\mu + D \quad . \tag{15}$$

The coefficients $b_1, \ldots, b_{n-2}, C, D$ can be evaluated recurrently. If we determine the periodic solution where $C = 0$ and $D = 0$, we have a period doubling bifurcation point. We can use

$$F_{n+1}(x,T,p) = D = 0 \tag{16}$$

instead of (14) and solve the system (8) (16) again by Newton method ($C = 0$ automatically for the solution).

A number of period-doubling bifurcation points has been successfully computed in this way. Some of them are reported in Figs 1 - 3 .

CASCADE OF PERIOD - DOUBLING BIFURCATIONS. FEIGENBAUM SEQUENCE. High accuracy of computed period-doubling bifurcation points enables to test the validity of Feigenbaum´s results also for more complicated and continuous dynamic systems. Several period-doubling bifurcation points of the Lorenz model (3) are presented in the Table 1. Results in the Table correspond to a cascade of period-doubling bifurcations, cf. Fig. 3. The values of the parameter r ($= p_1$) at the individual bifurcation points form a Feigenbaum sequence $\{r_j\}$ [2] . The values

TABLE 1 : A cascade of period-doubling bifurcation points in the Lorenz model (3), $\sigma = 16$, $b = 4$, $k = 1$, $x_k = 3.82038$.

j	x_2	x_3	T_j	r_j	δ_j
1	20.90946	273.34849	0.30618	356.93391	
2	16.85987	246.64055	0.63009	338.06197	4.9740
3	21.19530	259.36006	1.26750	334.26789	4.7313
4	17.29002	244.99724	2.53818	333.46599	4.6824
5	17.24223	244.70901	5.07771	333.29472	4.6707
6	17.25889	244.74356	10.15599	333.25806	

$$\delta_j = (r_{j+1} - r_j)/(r_j - r_{j-1}) \qquad (17)$$

are presented in the table, too. We can observe a very good convergence to a limit, which is approximately $\delta^* \sim 4.6692$ [2] .

DIRECTION OF EMANATING BRANCHES. Let us have a period-doubling bifurcation point (x^*,T^*,p^*) , determined, e.g., by the algorithms described above. Let us seek periodic solutions with the period approximately equal to $2T^*$ in the neighbourhood of (x^*,T^*,p^*) . Therefore, we define a nonlinear system

$$G(x,T,p) = \psi[\psi(x,T,p),\ T,\ p] - x = 0 \qquad (18)$$

for the unknowns $x_1,\ldots,\ x_{k-1},\ x_k,\ldots,\ x_n,\ T$, and the parameters p . The system (18) has a bifurcation (crossection) point at (x^*,T^*,p^*) . There are two branches which intersect at this point. One branch is a branch of "composed" periodic solutions obtained by a composition of two original periodic solutions on a known branch. The second branch is the bifurcated branch of solutions with a double period. Directions of the branches can be evaluated by the algorithm described in [17] . Let us note that we need second derivatives of G (computed,e.g., by finite differences). Directions of branches resulting for the first period-doubling bifurcation point from the Table 1 are presented in the Table 2 together with starting points used for the continuation of the bifurcated branch. More detailed description will be presented in [16] .

TABLE 2 : Directions of branches emanating from the first bifurcation point in the Table 1.

Direction on original branch	Direction on bifurcated branch	Starting point ($\Delta x_2 = 0.1$)
$\frac{dx_2}{dr} = 0.1262$	$\frac{dx_3}{dx_2} = 2.9431$	$x_2 = 21.0095$ (+) * $x_3 = 273.643$ (+)
$\frac{dx_3}{dr} = 1.0042$	$\frac{dT}{dx_2} = 0.56E\text{-}7$	$T = 0.30617$ (+) (period = 2T)
$\frac{dT}{dr} = -0.43E\text{-}3$	$\frac{dr}{dx_2} = -0.17E\text{-}3$	$r = 356.93$ (-)

* sign of the change of individual variables for starting continuation (direction parameters).

3.3 TORI BIFURCATIONS

The monodromy matrix M has the eigenvalues

$$\mu_{1,2} = a \pm ib \quad , \quad a^2 + b^2 = 1 \quad , \quad \mu_{1,2}^s \neq 1 \quad , \quad s = 1, 2, 3, 4 \quad . \tag{19}$$

Decomposition of the characteristic polynomial (13) gives

$$P(\mu) = (\mu^2 - \omega\mu + 1)(\mu^{n-2} + b_1\mu^{n-3} + \ldots + b_{n-2}) + C\mu + D \quad , \tag{20}$$

where $\omega = 2a$ and $(\mu^2 - \omega\mu + 1) = (\mu - \mu_1)(\mu - \mu_2)$. The coefficients $b_1, \ldots, b_{n-2}$, C, D can be again evaluated recurrently similarly as above. Two additional equations

$$F_{n+1}(x,T,p,\omega) = C = 0 \quad , \quad F_{n+2}(x,T,p,\omega) = D = 0 \tag{21}$$

have to be fulfilled at the tori bifurcation point. As a result we have $n + 2$ equations (7) (21) for $n + 2$ unknowns $x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n, T, p, \omega$. The Newton method can be used to solve this nonlinear system.

A modified method makes use of the fact that $\mu = 1$ is an eigenvalue of M , i.e., the decomposition of $P(\mu)$ is in the form

$$P(\mu) = (\mu^3 - (2a + 1)\mu^2 + (2a + 1)\mu - 1)(\mu^{n-3} + b_1\mu^{n-4} + \ldots + b_{n-3}) + C\mu^2 + D\mu + E \quad . \tag{22}$$

Coefficients $b_1, \ldots, b_{n-3}$, C, D, E can be evaluated recurrently and the Newton method is used for the solution of the $n + 2$ by $n + 2$ nonlinear system (8) (21). $E = 0$ automatically at the resulting tori bifurcation point.

Resulting tori bifurcation points for the model (4) are shown in the Table 3, cf. Fig. 2 for $B = 5.5$. The parameter D ($= p_1$) has been considered as a bifurcation parameter. If we continue tori bifurcation points in dependence on another parameter of the problem, here, e.g., B ($= p_2$) , we obtain so called bifurcation diagram [19] . Results of one such continuation are presented in Fig. 4 . The points where $\mu^3 = 1$ or $\mu^4 = 1$ are denoted 3T or 4T , respectively. The curve ends at the point where $\mu_1 = \mu_2 = \mu_3 = 1$.

4. DISCUSSION AND REMARKS

The algorithm for the continuation of periodic solutions can be used also for parabolic partial differential equations when these are transformed into a set of ordinary differential equations by using a semidiscretization (method of lines) [12] .

TABLE 3 : Resulting tori bifurcation points for (4), $A = 2$, $\rho = 0.1$, $k = 1$, $x_1 = 2$.

B	x_2	x_3	x_4	T	a	D
5.3	2.43727	1.90236	2.49646	7.15820	- 0.01694	0.048626
5.4	2.45219	1.92098	2.50011	7.62984	- 0.36244	0.051152
5.5	2.47887	1.92659	2.52457	8.32408	- 0.54139	0.052495
5.6	2.51478	1.92259	2.56374	9.19639	- 0.12304	0.053030

An algorithm for evaluation of Hopf bifurcation points in parabolic equations has been published recently [15] . The algorithms for evaluation of period-doubling and tori bifurcation points can be easily used for most autonomous dynamic systems of lower order, say $n < 20$. Of course, the use of the algorithms is limited by the applicability of the shooting method (stability). Simple modifications of the algorithms can be used also for a nonautonomous system with a time-periodic right hand side.

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