

The Nonlinear Buckling Problem of a Spherical Shell: Bifurcation Phenomena in a BVP with a Regular Singularity

Martin Hermann, Thomas Ullmann, Klaus Ullrich

Die Arbeit verfolgt das Ziel, den Einsatz moderner und ausgewiesener numerischer Algorithmen beim quantitativen Studium des Beuerverhaltens von Kugelschalen zu demonstrieren, die durch einen gleichmäßigen Außendruck belastet sind. Die zugehörigen Modellgleichungen stellen ein parameterabhängiges nichtlineares Zweipunkt-Randwertproblem dar, das sowohl verschiedene Bifurkationsphänomene als auch eine sogenannte reguläre Singularität aufweist.

Ein Ausschnitt der numerisch erzeugten Lösungsmannigfaltigkeit wird in Form von Bifurkationsdiagrammen angegeben.

The aim of this paper is to demonstrate the use of modern and sophisticated numerical algorithms in the quantitative study of the buckling problem of a spherical shell under a uniform external pressure. The corresponding governing equations are a parametrized nonlinear two-point boundary value problem which exhibits several bifurcation phenomena as well as a regular singularity. A section of the numerically generated solution manifold of this boundary value problem is represented in form of bifurcation diagrams.

1. Introduction

A number of authors have studied the buckling and post-buckling behavior of elastic shells (see, e. g. [1], [4], [7], [8], [12] – [15], [19], [21], [22]). The corresponding governing equations are parametrized nonlinear ordinary differential equations (ODEs) exhibiting several bifurcation phenomena. The first **quantitative** results for the mathematical model of an axisymmetric spherical shell are given in the paper of Bauer et al. (1970) [1], whereas most of the other publications offer only a **qualitative** insight. The date of publication of this remarkable paper is characterized by a first culminating point in the bifurcation theory. This is confirmed by a series of monographs published later [2], [5], [6], [11], [25], [30]. In contrast to the theory respective numerical approaches have been developed in recent years only [16] – [18], [20], [25], [27], [31]. Thus it is not surprising that the numerical techniques used by Bauer et al. (1970) [1] are quite simple and heuristic.

The aim of this paper is to demonstrate the use of modern and sophisticated numerical algorithms for boundary value problems (BVPs) (see the monographs of Wallisch and Hermann (1987, 1985) [31], [32]) in the **quantitative** study of shell equations. By a quantitative study we understand the computational generation of a section of the solution manifold of the parametrized ODEs.

2. Shell equations

We study the buckling problem of a spherical shell under a uniform external static pressure. The investigations are restricted to the case of a linearly elastic, homogeneous and isotropic material. Further only axisymmetric deformations of the shell are allowed. This latter assumption is not as academic as it might appear at the first moment, because the production process of spherical shells frequently favours axisymmetric imperfections which create a preference for axisymmetric buckling patterns. Moreover, we want to give an application of some theoretical and numerical concepts for handling bifurcation problems. Shell equations fulfilling these requirements are given by Bauer et al.

(1970) [1]. The governing equations can be reduced to a BVP for the following system of 4 first order ODEs:

$$y'(t) = f(t, y; \lambda), \quad 0 \leq t \leq \pi(\pi/2). \quad (1)$$

Here $y(t)$ is a four-dimensional vector with components $y_i(t)$, $i = 1(1)4$, and $f(t, y; \lambda)$ is a four-dimensional vector with components f_i , $i = 1(1)4$, defined by

$$\begin{aligned} f_1 &\equiv (\nu - 1)y_1 \cot(t) + y_2 + \{k \cot^2(t) - \lambda\} y_4 + y_2 y_4 \cot(t), \\ f_2 &\equiv y_3, \\ f_3 &\equiv y_2 \{ \cot^2(t) - \nu \} - y_3 \cot(t) - y_4 - 0.5(y_4)^2 \cot(t), \\ f_4 &\equiv (1 - \nu^2)/k y_1 - \nu y_4 \cot(t). \end{aligned} \quad (2)$$

ν is Poisson's ratio (we have used $\nu = 0.32$ [steel]) and k is proportional to the thickness of the shell (we have used $k = 0.001$). We refer to λ as the **load**.

The components of y are defined in terms of physical quantities by $y_1 = m(t)$, $y_2 = q(t)$, $y_3 = s(t)$, where m , q , s are proportional, respectively, to the radial bending moment, the transversal shear, and the circumferential membrane stress. y_4 is proportional to the angle of rotation of a tangent to a meridian.

Finally we consider the **hemisphere** only. The corresponding boundary conditions are

$$y_2 = y_4 = 0, \quad t = 0, \pi/2 \quad (\text{Hemisphere}). \quad (3)$$

3. The bifurcation problem

The equations (1) – (3) represent a bifurcation problem which can be written in the form of an operator equation

$$T(y, \lambda) = 0, \quad T: Z \equiv X \times \mathbf{R} \rightarrow Y, \quad (4)$$

where $T(y, \lambda) \equiv y' - f(\cdot, y; \lambda)$ and X , Y are appropriate Banach spaces [31].

It can be easily seen that the trivial solution $y(t) \equiv 0$ is a solution for all values of the parameter λ , i. e.

$$T(0, \lambda) = 0 \quad \forall \lambda \in \mathbf{R}. \quad (5)$$

The aim of our contribution is to present a section of the solution field of (4). To do this we have to handle the following numerical problems:

- (i) determination of the primary bifurcation points,
- (ii) determination of nontrivial solutions in the neighbourhood of these singular points,
- (iii) after some solutions have been determined on a nontrivial branch, tracing this curve (and detecting other singular points: turning points or secondary bifurcation points).

Our approach to problems (i)–(iii) consists in the use of the sophisticated multiple shooting code **RWPM** (see the appendix in the book of Wallisch and Hermann (1985) [32]). Singularities are removed by embedding the original equations in extended systems or by the application of indirect methods.

Apart from the bifurcation phenomena, problem (4) exhibits one further difficulty: the right-hand side (2) has a **singularity** at $t = 0$. Thus, in the shooting method the initial value problem- (IVP-) codes fail.

De Hoog and Weiss (1985) [10] study IVPs of the form

$$z' = (1/t)Mz + g(t, z) \equiv G(t, z), \quad 0 \leq t \leq 1, \\ z \in C^1([0, 1], \mathbb{R}^n), z(0) = \eta, \quad (6)$$

where z and g are n -vectors and M is a constant $n \times n$ matrix. The authors prove the following result.

Theorem 1: Assume that

- (i) M has no eigenvalues which are purely imaginary or have a positive real part,
- (ii) the initial vector satisfies $\eta \in N(M)$, and
- (iii) $g(t, z)$ is continuous w.r.t. t and uniformly Lipschitz continuous w.r.t. z for $0 \leq t \leq 1$ and all z .

Then (6) has a unique continuously differentiable solution $z(t)$. Furthermore, if g is p times continuously differentiable, then $z \in C^{p+1}([0, 1], \mathbb{R}^n)$. ■

Let

$$y_1 = z_1, \quad y_2 = tz_2, \quad y_3 = z_3, \quad y_4 = tz_4. \quad (7)$$

Then (1), (2) can be written in form (6) with

$$\text{cot}(t) = 1/t - c\dot{\text{ot}}(t) \quad [c\dot{\text{ot}}(0) = 0], \quad z \equiv (z_1, z_2, z_3, z_4)^T,$$

$$M \equiv \begin{pmatrix} \nu - 1 & 0 & 0 & k \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ \frac{(1-\nu^2)}{k} & 0 & 0 & -(1+\nu) \end{pmatrix}$$

$$g_1 = (1-\nu)z_1 c\dot{\text{ot}}(t) + tz_2 + [k(t \cdot c\dot{\text{ot}}^2(t) - 2c\dot{\text{ot}}(t)) - t\lambda]z_4 \\ + (t - t^2 c\dot{\text{ot}}(t))z_2 z_4,$$

$$g_2 = 0,$$

$$g_3 = z_2(t \cdot c\dot{\text{ot}}^2(t) - 2c\dot{\text{ot}}(t) - \nu t) + z_3 c\dot{\text{ot}}(t) \\ - tz_4 - 0.5(t - t^2 c\dot{\text{ot}}(t))(z_4)^2, \quad (8)$$

$$g_4 = \nu z_4 c\dot{\text{ot}}(t).$$

Obviously the eigenvalues of M are $\{-2, 0, 0, -2\}$, and the assumptions of **Theorem 1** are fulfilled. When the shooting method is used, the relevant initial conditions are

$$z_2(0) - z_3(0) = 0, \quad kz_4(0) + (\nu - 1)z_1(0) = 0 \Leftrightarrow z(0) \in N(M) \quad (9)$$

Since $z(0) \in N(M)$, we have $z' = (1/t)M\{z(t) - z(0)\} + g(t, z)$. Then the relation

$$\lim_{t \rightarrow 0} z'(t) = \lim_{t \rightarrow 0} M\{z(t) - z(0)\}/t + \lim_{t \rightarrow 0} g(t, z(t)) \text{ implies} \\ z'(0) = (I - M)^{-1}g(0, z(0)), \text{ i.e. } G(0, z(0)) = (0, 0, 0, 0)^T. \quad (10)$$

Thus, before applying the multiple shooting code to (1)–(3), we have transformed these equations into the form (6) using the change of variables (7). The resulting BVP

$$z'(t) = \begin{cases} G(t, z(t)), & t \neq 0 \\ (0, 0, 0, 0)^T, & t = 0 \end{cases} \quad (11)$$

$$kz_4(0) + (\nu - 1)z_1(0) = z_2(0) - z_3(0) = 0,$$

$$z_2(\pi/2) = z_4(\pi/2) = 0$$

is well-defined at $t = 0$. Our experience is that the Bulirsch/Stoer/Gragg extrapolation method (1980) [29] works very reliably in combination with our multiple shooting code **RWPM** applied to (11). Moreover, in comparison with other numerical techniques for BVPs with a regular singularity (e.g. Taylor expansion methods [23, 29]) our approach requires much less amount of computational work and/or cumbersome analytical evaluations to achieve a prescribed accuracy. But the main advantage is that standard codes (multiple shooting, extrapolation) can be used immediately.

4. Numerical determination of the primary simple bifurcation points

In order to compute the bifurcation points $z_0 \equiv (0, \lambda_0) \in X \times \mathbb{R}$ with standard codes, we used the following determining system

$$\hat{T}(\hat{z}) = 0 \quad (12)$$

where

$$\hat{T}: \begin{cases} \hat{Z} \equiv \mathbb{R} \times X \rightarrow Y \times \mathbb{R} \\ \hat{z} \equiv (\lambda, \phi) \rightarrow \begin{cases} T_Y(0, \lambda)\phi \\ \phi_0^* \phi - 1 \end{cases} \end{cases}$$

and

$$\phi_0 \in X: T_Y(0, \lambda_0)\phi_0 = 0, \quad \|\phi_0\| = 1; \quad \phi_0^* \in X^*: \phi_0^* \phi_0 = 1.$$

There is a one-to-one correspondence between the bifurcation points of problem (4) and the isolated solutions of (12) (see e.g. [31]).

If we use the functional

$$\phi_o^* v \equiv \int_0^{\pi/2} \phi_o(t)^T v(t) dt$$

and express the conditions $\phi_o^* \phi_o = 1$ and $\lambda = \text{const.}$ in form of ODEs

$$\xi'(t) = \phi_o(t)^T \phi_o(t), \quad \xi(0) = 0, \quad \xi(\pi/2) = 1; \quad \lambda'(t) = 0,$$

then the determining system for (1) – (3) is a BVP of order 6 ($= n + 2$). This BVP exhibits the same regular singularity as the original problem (1) – (3). The singularity can be eliminated with the transformation (7), i. e.

$$\phi_1 = y_1, \quad \phi_2 = ty_2, \quad \phi_3 = y_3, \quad \phi_4 = ty_4; \quad \xi = y_5, \quad \lambda = y_6,$$

which results in a well-posed BVP

$$y' = (1/t) \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} y + g(t, y), \quad y \equiv (y_1, y_2, \dots, y_6)^T \quad (13)$$

$$y_2(0) - y_3(0) = ky_4(0) + (\nu - 1)y_1(0) = 0, \quad y_5(\pi/2) = 1, \\ y_5(0) = y_2(\pi/2) = y_4(\pi/2) = 0; \text{ see formula (8) for the definition of } M \in \mathbf{R}^{4 \times 4}.$$

g satisfies $g(0, y(0)) = [0, 0, 0, 0, y_1(0)^2 + y_3(0)^2, 0]^T$. We used a homotopy strategy for evaluating as much as possible bifurcation points from (13). For this purpose we computed a solution of (13) with the code RWPM (starting from a small value of the load parameter $y_6 = \lambda$). Then we increased the load successively and used the result of the preceding step as a starting trajectory for the actual call of RWPM. Approximations of the first 7 bifurcation points $z_i \equiv (0, \lambda_i)$ are given in Table I.

Table I
Bifurcation Points of Problem (1) – (3)

i	Bifurcation Point Computed with RWPM (Formula (13))	Bifurcation Point Approximated with a Linear Buckling Theory [1]	a_2
1	7.061 597 232 D-2	7.061 60 E-2	8.5 D-2
2	7.505 725 485 D-2	7.505 73 E-2	-1.6 D-1
3	9.360 460 190 D-2	9.360 46 E-2	5.3 D-2
4	1.309 927 688 D-1	1.309 93 E-1	3.6 D-2
5	1.795 041 756 D-1	1.759 04 E-1	2.7 D-2
6	2.196 021 300 D-1	2.196 02 E-1	-4.4 D-1
7	2.379 916 695 D-1	2.379 92 E-1	2.1 D-2

The intrinsic quality of the bifurcation points (e. g. **symmetric** or **nonsymmetric** points) is reflected by the second bifurcation coefficient [9]

$$a_2 \equiv \psi_o^* T_{yy}^o \phi_o^2 \quad (T_{yy}^o \equiv T_{yy}(0, \lambda_o) \text{ etc.}) \quad (14)$$

where $\psi_o^* \in Y^*$: $\mathbf{N}(T_{yy}^o) = \text{span}(\psi_o^*)$, $\|\psi_o^*\| = 1$.

In order to compute and to check a_2 , we have combined the BVP (12) for ϕ_o and the corresponding **adjoint** BVP for ψ_o .

If we define

$$\psi_o^* v \equiv \int_0^{\pi/2} \psi_o(t)^T v(t) dt \text{ and transform } a_2 = -\psi_o^* f_{yy}^o \phi_o^2$$

into DE form $\xi'(t) = -\psi_o(t)^T f_{yy}^o \phi_o(t)^2$, $\xi(0) = 0$, then the second bifurcation coefficient is $\xi(\pi/2) = a_2$. Therefore we have added this scalar DE to the determining system for ϕ and ψ resulting in a BVP of order 13 ($= 2n + 5$):

$$\phi' = f_y(t, 0; \lambda) \phi \quad \phi_2(0) = \phi_4(0) = 0, \quad \phi_2(\pi/2) = \phi_4(\pi/2) = 0 \\ \lambda' = 0, \quad \xi' = \phi^T \phi \quad \psi_1(0) = \psi_3(0) = 0, \quad \psi_1(\pi/2) = \psi_3(\pi/2) = 0$$

$$\psi' = -f_y(t, 0; \mu)^T \psi \quad \xi_1(0) = \xi_2(0) = \xi_3(0) = 0 \\ \mu' = 0, \quad \xi_2' = \psi^T \psi \quad \xi_1(\pi/2) = \xi_2(\pi/2) = 1 \\ \xi_3' = -\psi^T f_{yy}(t, 0; \lambda) \phi^2. \quad (15)$$

Since (15) also contains the adjoint equations, the elimination technique for the regular singularity (in these equations) has to be modified. In fact, the following change of variables transforms (15) into a BVP of the form (6):

$$\phi_1 = y_1, \quad \phi_2 = ty_2, \quad \phi_3 = y_3, \quad \phi_4 = ty_4, \quad \xi_1 = y_5, \quad \lambda = y_6 \\ \text{(see (13)),}$$

$$\psi_1 = t^2 y_7, \quad \psi_2 = ty_8, \quad \psi_3 = t^2 y_9, \quad \psi_4 = ty_{10}, \quad \xi_2 = y_{11}, \\ \mu = y_{12}, \quad \xi_3 = y_{13}. \quad (16)$$

The resulting well-posed problem is ($y \equiv (y_1, y_2, \dots, y_{13})^T$):

$$y' = \frac{1}{t} \begin{bmatrix} M & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \bar{M} & 0 \\ 0 & 0 & 0 \end{bmatrix} y + g(t, y)$$

$$y_2(0) - y_3(0) = 0, \quad y_2(\pi/2) = y_4(\pi/2) = 0, \\ ky_4(0) - (1 - \nu)y_1(0) = 0, \quad y_5(0) = 0, \quad y_5(\pi/2) = 1, \\ y_8(0) + y_9(0) = 0, \quad y_7(\pi/2) = y_9(\pi/2) = 0, \\ ky_7(0) + (1 - \nu)y_{10}(0) = 0, \quad y_{11}(0) = 0 \\ y_{11}(\pi/2) = 1, \quad y_{13}(0) = 0; \text{ where}$$

$$\bar{M} \equiv \begin{bmatrix} -(1 + \nu) & 0 & 0 & \frac{1 - \nu^2}{k} \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -k & 0 & 0 & -(1 - \nu) \end{bmatrix} \quad (17)$$

and g satisfies $g(0, y(0)) = [0, \dots, 0, y_1(0)^2 + y_3(0)^2, 0, \dots, 0]^T$. The second bifurcation coefficients given in Table I have been obtained by applying the code RWPM to the transformed problem (17).

5. Numerical determination of solutions in the neighbourhood of the bifurcation points

Assume that the (primary simple) bifurcation points $z_o \equiv (0, \lambda_o)$ and the corresponding vector functions ϕ_o have been computed. Hermann (1986) [9] proposed a transformation technique which enables to determine nontrivial solutions of (4) – (5) in dependence on the problem parameter λ . We adapted this technique for the model equations (1) – (3). As can be seen in Table I all bifurcation points are non-symmetric ones, i. e. $a_2 \neq 0$. The suitable ansatz for nontrivial branching solutions is

$$y(\lambda) = -2(a_1/a_2)(\lambda - \lambda_o)\phi_o + (\lambda - \lambda_o)^2[u + (\rho + q)\phi_o] \\ + (\lambda - \lambda_o)^3 v, \quad |\lambda - \lambda_o| \leq \varepsilon; \quad (18)$$

where $a_1 \equiv \Psi_0^* T_{y\lambda}^0 \phi_0$ (first bifurcation coefficient), $p, q \in \mathbf{R}$ and $u, v \in \mathbf{N}(T_y^0)$. The unknown vector functions u, v and constants p, q are the solutions of the following BVP:

$$\begin{aligned} u' &= f_y^0 u + \Phi(\phi_0), \quad \xi_1' = \phi_0^T(u + p\phi_0), \\ v' &= f_y^0 v + F(u, v, p, q, \phi_0, \lambda - \lambda_0), \quad \xi_2' = \phi_0^T v, \\ p' &= 0, \quad q' = 0, \\ u_2(0) &= u_4(0) = u_2(\pi/2) = u_4(\pi/2) = 0, \\ v_2(0) &= v_4(0) = v_2(\pi/2) = v_4(\pi/2) = 0, \\ \xi_1(0) &= \xi_1(\pi/2) = 0, \quad \xi_2(0) = \xi_2(\pi/2) = 0. \end{aligned} \quad (19)$$

Φ and F are vector functions which are defined by f and its derivatives w.r.t. y up to the 3rd order at $y \equiv 0, \lambda = \lambda_0$.

In order to make use of IVP-codes with automatic step-size control, we constructed an enlarged BVP. It consists of the determining system for λ_0, ϕ_0 and (19). Unfortunately, this BVP has a regular singularity, too. However, the change of variables

$$\begin{aligned} \phi_i &= \hat{\phi}_i, \quad u_i = \hat{u}_i, \quad v_i = \hat{v}_i, \quad i = 1, 3; \quad \phi_j = t\hat{\phi}_j, \\ u_j &= t\hat{u}_j, \quad v_j = t\hat{v}_j, \quad j = 2, 4, \end{aligned}$$

leads to a well-posed BVP in the transformed variables. We solved this BVP with the standard shooting code RWPM and a continuation strategy for increasing values of $|\lambda - \lambda_0|$.

6. Path following, detection and computation of singular points

After determining some solutions of problem (1) – (3) in the neighbourhood of a bifurcation point (using the methods explained in Section 5), we applied path following techniques in order to compute further points on the corresponding solution branch. The basic tool was our curve tracing code **RWPKV** [31] which will be described in the following. It is an implementation of Seydel's algorithm (1982) [28] and is based on the multiple shooting code **RWPM**. Thus all BVPs have to be formulated in standard form, i.e. as a system of m (nonlinear) ODEs subjected to m (nonlinear) boundary conditions:

$$z' = H(t, z), \quad R(z(a), z(b)) = 0. \quad (20)$$

The adequate (augmented) representation of the BVP (1) – (3) suitable for path following is:

$$T^0(y, \lambda) \equiv \begin{bmatrix} y' - f(y, \cdot; \lambda) \\ \lambda' \\ r(y(a), y(b)) \\ r_{n+1} \equiv y_k(a) - \eta \text{ [or } \equiv \lambda - \eta] \end{bmatrix} = 0, \quad (21)$$

where $r = 0$ is the operator form of the boundary conditions (3) and η is a fixed boundary value. k is referred to as **homotopy index**. It has to be updated at each homotopy step. It can be easily seen that (21) is a BVP tractable by RWPM. Namely, if we set

$$\begin{aligned} z_j &\equiv y_j, \quad j = 1(1)n; \quad z_{n+1} \equiv \lambda; \quad H \equiv (f, 0)^T, \\ R &\equiv (r, r_{n+1})^T \text{ and } m \equiv n + 1, \end{aligned}$$

then (21) takes on the standard form (20).

The following choice of the homotopy index k is crucial for path following along **simple solution branches** (i.e. curves consisting of regular points and simple turning points only):

$$k = l_{\max}, \quad \Delta l_{\max} = \max_l |(z^{l-1}(a) - z^{l-2}(a)) / z^{l-1}(a)|, \quad (22)$$

$$1 \leq l \leq n + 1,$$

where l denotes the actual number of the homotopy step. With choice (22), it can be proved that the Frechet-derivative of the operator T^0 [see formula (21)] is regular at points on a simple solution branch. In order to detect **simple turning points** $z^u \equiv (y^u, \lambda^u)$, the step size in λ -direction has only to be examined at each homotopy step. A change in the sign of

$$d \equiv (\lambda^l - \lambda^{l-1}) \cdot (\lambda^{l-1} - \lambda^{l-2})$$

indicates that a simple turning point has been run over. In that case an approximation $\hat{\lambda}^u$ of the critical parameter value λ^u is determined by the interpolation of the last three points on the branch (which have been computed during the homotopy process) using the quadratic polynomial

$$\lambda = c_1(z_k(a) - c_2)^2 + c_3. \quad (23)$$

In formula (23), k is the actual homotopy index. If $z^l, j = i-2, i-1, i$, are the corresponding points in the neighbourhood of z^u , (22) guaranties $k \neq n + 1$. Thus we obtain

$$\hat{\lambda}^u = c_3 \quad \text{and} \quad \hat{y}_k^u = c_2, \quad (24)$$

where $\hat{y}_k^u(a)$ is an approximation of $y_k^u(a)$ which corresponds with $\hat{\lambda}^u$. In RWPKV the rough approximation $\hat{y}_k^u(a)$ is used as a starting point (see **Step 2** in **Algorithm 1**) for the computation of the simple turning point by the following indirect method.

Algorithm 1

Step 1:

Set $z^{(1)} := z^{l-2}, z^{(2)} := z^{l-1}, z^{(3)} := z^l, z^{(4)} := z^{(2)}$;

Choose $\varepsilon_{\text{rel}} > 0, itmax > 0, j := 0$;

Step 2:

$j := j + 1; \eta := \hat{z}_k^u(a)$ {see (24)};

Compute $z^{(0)}$ as the solution of (21);

Step 3:

IF $|z_k^{(0)}(a) - z_k^{(4)}(a)| / |z_k^{(0)}(a)| < \varepsilon_{\text{rel}}$

THEN $z^u := z^{(0)}$ and **Stop**.

IF $|\lambda^{(0)} - \lambda^{(4)}| / |\lambda^{(0)}| < \varepsilon_{\text{rel}}$

THEN $z^u := z^{(0)}$ and **Stop**.

IF $j > itmax$

THEN **Stop**.

Step 4:

IF $(z_k^{(1)}(a) - z_k^{(2)}(a)) \cdot (z_k^{(0)}(a) - z_k^{(2)}(a)) > 0$

THEN

$$\text{IF } (\lambda^{(1)} - \lambda^{(2)}) \cdot (\lambda^{(0)} - \lambda^{(2)}) > 0$$

$$\text{THEN } z^{(1)} := z^{(0)}$$

$$\text{ELSE } z^{(3)} := z^{(2)}; z^{(2)} := z^{(0)}$$

END IF.

ELSE

$$\text{IF } (\lambda^{(3)} - \lambda^{(2)}) \cdot (\lambda^{(0)} - \lambda^{(2)}) > 0$$

$$\text{THEN } z^{(3)} := z^{(0)}$$

$$\text{ELSE } z^{(1)} := z^{(2)}; z^{(2)} := z^{(0)}$$

END IF

END IF

$$z^{(4)} := z^{(2)};$$

Step 5:

With $z^{(1)}$, $z^{(2)}$ and $z^{(3)}$ interpolate according to (23), (24) and go to **Step 2**.

Our code RWPKV is also designed to detect **bifurcation points** during the path following process. Here we will give a short description of the fundamentals of the underlying strategy.

Definition:

Let z^b be a simple bifurcation point of the original problem (1) – (3).

Then $\tau(z)$ is called a **testfunction** for (21) \leftrightarrow

(a) $\tau(z)$ is a continuous function, and

(b) z^b is a zero of $\tau(z)$ with multiplicity one.

There are many possibilities to define special test functions [3], [13], [27]. In our algorithm the test function is related to the system of nonlinear **algebraic** equations $F(s) = 0$ which has to be solved in the multiple shooting method. The reason for using the associated shooting equations is that the following implications are valid:

$$(T^0)'(z) \text{ is singular} \leftrightarrow \det(F'(s)) = 0,$$

where $s \equiv (s^1, \dots, s^M)^T$, $s^l \equiv (s_{1,l}^1, \dots, s_{n+1,l}^1)^T$, $s_j^l \equiv z_j(t_l)$, $j = 1(1)n+1$, $l = 1(1)M$, M – total number of shooting points.

For a solution z^l of (21) we define the value

$$\tau^l \equiv (-1)^w \prod_{j=1}^{(n+1)M} u_{jl}, \quad (25)$$

where $F' = LU$ is the LU-factorization of the Jacobian F' and w counts the row interchanges during the Gaussian elimination.

If we have computed the three values τ^l , τ^{l-1} and τ^{l-2} in the last three homotopy steps and it holds

$$\tau^{l-2} \cdot \tau^{l-1} > 0 \text{ and } \tau^{l-1} \cdot \tau^l < 0, \quad (26)$$

then the passing of a bifurcation point $z^b \equiv (y^b, \lambda^b)$ is indicated. A first approximation of the critical parameter value λ^b is computed by interpolation. Inserting the last three homotopy points z^l , $j = i-2, i-1, i$, as well as the associated values of the test function τ into the ansatz

$$\tau = f_1 z_k(a)^2 + f_2 z_k(a) + f_3, \quad (27)$$

we determine the unknown coefficients f_i , $i = 1, 2, 3$. Then an approximation $\hat{z}_k^b(a)$ of the critical value $z_k^b(a)$ is determined as that zero of the equation $\tau = 0$ which satisfies $z_k^{l-2}(a) < (>) \hat{z}_k^b(a) < (>) z_k^l(a)$. Finally, an approximation $\hat{\lambda}^b$ of λ^b is computed interpolating with the formula

$$\lambda = d_1 z_k(a)^2 + d_2 z_k(a) + d_3. \quad (28)$$

And so it follows

$$\hat{\lambda}^b = d_1 \hat{z}_k^b(a)^2 + d_2 \hat{z}_k^b(a) + d_3. \quad (29)$$

Remark 1:

$\tau(y)$ defined in (25) clearly depends on the actual homotopy index and the number of shooting points used in the last step. Thus, in order to accomplish a correct interpolation, we have to compute the values τ^{l-2} , τ^{l-1} , τ^l at the same index k with the same number and localization of the shooting points.

A repeated application of the interpolation formulas (27) and (28) results in an indirect method for the determination of bifurcation points; see **Algorithm II**.

Algorithm II

Step 1:

$$\text{Set } z^{(1)} := z^{l-2}, z^{(2)} := z^{l-1}, z^{(3)} := z^l, z^{(4)} := z^{(2)};$$

$$\tau^{(1)} := \tau^{l-2}, \tau^{(2)} := \tau^{l-1}, \tau^{(3)} := \tau^l, \text{ intval} := 2, j := 0;$$

Choose $\varepsilon_{\text{abs}} > 0$, $\varepsilon_{\text{rel}} > 0$, $itmax > 0$.

Step 2:

$$j := j + 1; \eta := \hat{z}_k^b(a);$$

Compute $z^{(0)}$ as the solution of (21); Compute $\tau^{(0)}$ according to (25).

Step 3:

$$\text{IF } |z_k^{(0)}(a) - z_k^{(4)}(a)| / |z_k^{(0)}(a)| < \varepsilon_{\text{rel}}$$

THEN $z^b := z^{(0)}$ and **Stop**;

$$\text{IF } |\lambda^{(0)} - \lambda^{(4)}| / |\lambda^{(0)}| < \varepsilon_{\text{rel}}$$

THEN $z^b := z^{(0)}$ and **Stop**;

$$\text{IF } |\tau^{(0)}| < \varepsilon_{\text{abs}}$$

THEN $z^b := z^{(0)}$ and **Stop**;

$$\text{IF } j > itmax$$

THEN **Stop**.

Step 4:

$$\text{IF } \text{intval} = 1$$

THEN

```

IF       $\tau^{(0)} \cdot \tau^{(1)} < 0$ 
THEN    $\tau^{(2)} := \tau^{(0)}, z^{(2)} := z^{(0)}$ 
ELSE    $\tau^{(1)} := \tau^{(0)}, z^{(1)} := z^{(0)}$ 
END IF
ELSE
IF       $\tau^{(0)} \cdot \tau^{(3)} < 0$ 
THEN    $\tau^{(2)} := \tau^{(0)}, z^{(2)} := z^{(0)}$ 
ELSE    $\tau^{(3)} := \tau^{(0)}, z^{(3)} := z^{(0)}$ 
END IF
END IF;
 $z^{(4)} := z^{(0)}$ .

```

Step 5:

```

IF       $\tau^{(1)} \cdot \tau^{(2)} < 0$ 
THEN    $intval := 1$ 
ELSE    $intval := 2$ 
END IF;

```

Accomplish the interpolations (27) and (28) with $z^{(1)}, z^{(2)}$ and $z^{(3)}$ for $z_k^{(0)}$ with $z_k^{(1)} < (>) z_k^{(0)} < (>) z_k^{(3)}$ and go to **Step 2**.

Remark 2:

The disadvantage of **Algorithm II** is that the Jacobian of (21) is singular at a bifurcation point. Therefore, bifurcation points can only be computed with a restricted accuracy.

In RWPKV the user has the following options to compute singular points:

- (i) the approximation of the singular point with a restricted accuracy using an indirect method (**Algorithm I** or **Algorithm II**),
- (ii) the computation of the singular point with an extended system (see e.g. Section 4)
- (iii) the combination of the above two strategies, i.e. the improvement of the result obtained with the indirect method by the subsequent solution of an extended system.

We have studied the equations (1) – (3) on the basis of strategy (ii). Further, in order to eliminate the regular singularity of the equations (2), the change of variables (7) has to be performed before the code RWPKV is run.

7. Numerical results

The bifurcation diagrams shown in the Figures 1 – 3 have been generated with the numerical techniques explained above. The simple turning points which have been computed with **Algorithm I** are tabulated in Table II.

All computations were executed on an EC 1056 computer in double precision arithmetic carrying a mantissa of 16 significant digits.

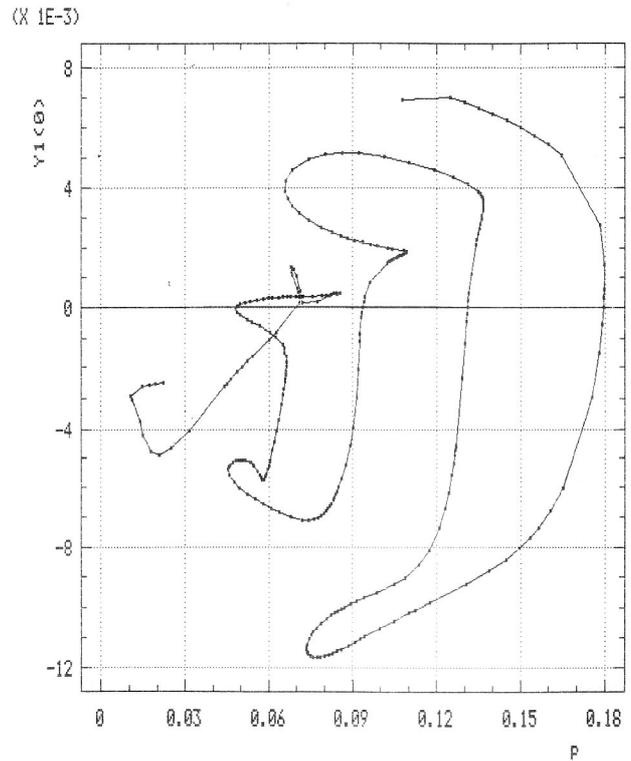


Figure 1
Bifurcation diagram of problem (1) – (3). $y_1(0)$ as a function of the load $P = \lambda$.

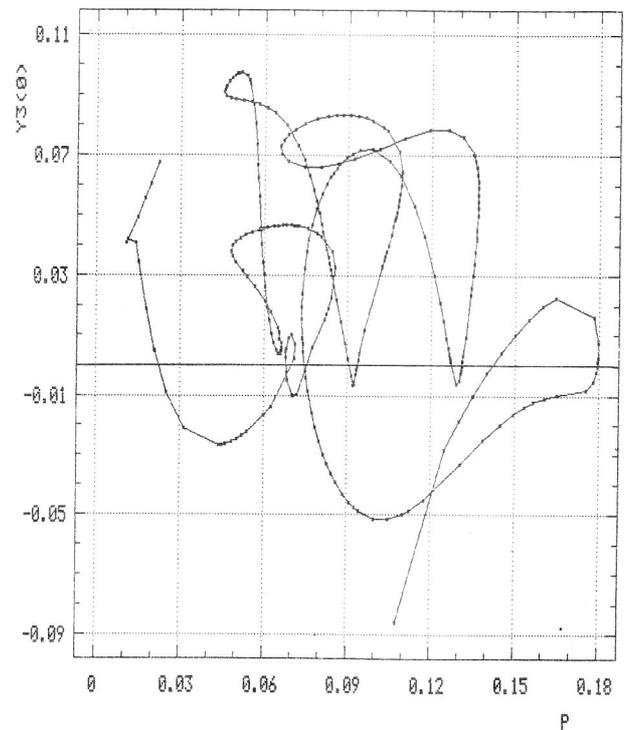


Figure 2
Bifurcation diagram of problem (1) – (3). $y_3(0)$ as a function of the load $P = \lambda$.

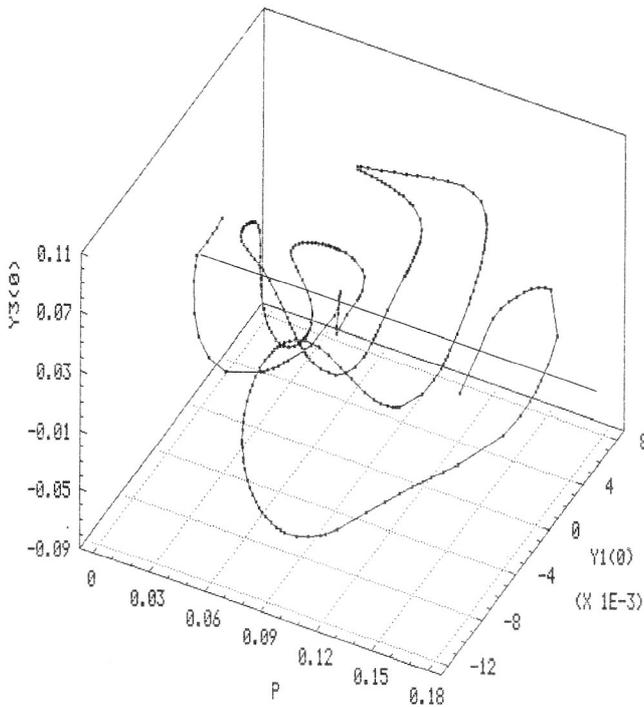


Figure 3
Bifurcation diagram of problem (1) – (3). $y_1(\theta)$ and $y_3(\theta)$ as functions of the load $P = \lambda$ (3D-plot).

Table II
Simple Turning Points of Problem (1) – (3)

i	Simple Turning Point Computed with Algorithm I λ_i	i	Simple Turning Point Computed with Algorithm I λ_i
1	1.044 966 606 D-2	8	1.092 588 536 D-1
2	6.783 193 893 D-2	9	6.565 326 428 D-2
3	7.126 531 645 D-2	10	1.366 385 960 D-1
4	8.557 434 714 D-2	11	7.359 173 869 D-2
5	4.822 184 831 D-2	12	1.795 044 640 D-1
6	6.629 468 586 D-2	13	1.053 265 914 D-1
7	4.540 166 680 D-2	14	3.062 204 680 D-1

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Anschrift der Verfasser:

Doz. Dr. M. Hermann
Universität Dortmund
Fachbereich Mathematik
Postfach 500500
W-4600 Dortmund 50

Thomas Ullmann
Klaus Ullrich
Friedrich-Schiller-Universität Jena
Mathematische Fakultät
UHH, 17. OG
O-6900 Jena