Applied Numerical Mathematics 13 (1993) 103–108
North-Holland



APNUM 428

# RWPM: a software package of shooting methods for nonlinear two-point boundary value problems

M. Hermann and D. Kaiser

*Institut für Angewandte Mathematik, Friedrich-Schiller-Universität, Jena, Leutragraben 1, D-07740 Jena, Germany*

Received 22 September 1992
Revised 14 December 1992
Accepted 18 January 1993

*Abstract*

Hermann, M. and D. Kaiser, RWPM: a software package of shooting methods for nonlinear two-point boundary value problems, Applied Numerical Mathematics 13 (1993) 103–108.

The aim of this paper is to present the numerical software package RWPM which solves linear and nonlinear two-point boundary value problems in ordinary differential equations. The package is based on multiple shooting and stabilized march techniques. Numerical examples demonstrating the efficiency of the package are presented.

*Keywords.* Two-point boundary value problems; shooting methods; software package.

## 1. Introduction

Consider the two-point boundary value problem (BVP) for a system of $n$ nonlinear ordinary differential equations

$$x'(t)=f(t, x(t)), \quad a<t<b, \tag{1.1}$$

subject to $n$ nonlinear boundary conditions

$$r(x(a), x(b))=0, \tag{1.2}$$

where $x(t) \in \mathbb{R}^n$, $f: \Omega_1 \to \mathbb{R}^n$, $\Omega_1 \subset (a, b) \times \mathbb{R}^n$, and $r: \Omega_2 \to \mathbb{R}^n$, $\Omega_2 \subset \mathbb{R}^n \times \mathbb{R}^n$. Assume that (1.1)–(1.2) has an isolated solution and for convenience that $f$ and $r$ are as smooth as desired.

In comparison with finite difference methods and collocation methods, shooting techniques for the solution of (1.1)–(1.2) have the advantages that: sophisticated software for the solution of initial value problems (IVPs) can be used, an initial guess for the solution is only required at

*Correspondence to*: M. Hermann, Institut für Angewandte Mathematik, Friedrich-Schiller-Universität Jena, Leutragraben 1, D-07740 Jena, Germany. E-mail: hermann@mathematik.uni-jena.dbp.de.

a few points in the interval $[a, b]$, and less storage is needed for problems which require many mesh points to get a sufficiently accurate solution. There are some good implementations of the multiple shooting method, for example BVPSOL [3], MUSN [13], TS [12], and RWPM [6].

In the last ten years our multiple shooting code RWPM has undergone a lot of significant changes. Doing this, we placed special emphasis on the reduction of the number of IVPs to be solved since in a shooting technique the numerical solution of IVPs requires the major part of the computational work. In [4] we have proposed a (nearly) nonlinear version of the stabilized march method which integrates only $q+1$ IVPs per Newton step. It can be used for BVPs with *linear* partially separated boundary conditions

$$\begin{pmatrix} B_a^{(1)} \\ B_a^{(2)} \end{pmatrix} x(a) + \begin{pmatrix} 0 \\ B_b^{(2)} \end{pmatrix} x(b) = \beta, \tag{1.3}$$

where $B_a^{(1)} \in \mathbb{R}^{p \times n}$, $B_a^{(2)}$, $B_b^{(2)} \in \mathbb{R}^{q \times n}$, $\beta \in \mathbb{R}^n$, and $p + q = n$. The corresponding algorithm can be found in [5]. A further improvement of RWPM has been achieved by developing a (fully) nonlinear stabilized march method for BVPs with *nonlinear* partially separated boundary conditions

$$r_p(x(a)) = 0, \qquad r_q(x(a), x(b)) = 0, \tag{1.4}$$

where $r_p : \Omega_3 \to \mathbb{R}^p$, $\Omega_3 \subset \mathbb{R}^n$, $r_q : \Omega_4 \to \mathbb{R}^q$, $\Omega_4 \subset \mathbb{R}^n \times \mathbb{R}^n$, and $n = p + q$. The method is based on a so-called *Generalized Brent Method* for the numerical treatment of the algebraic shooting equations (see [7]). At each step of the iteration this stabilized march technique requires the integration of $q+1$ IVPs instead of $n+1$ integrations in multiple shooting.

In this paper we describe the actual version of the package RWPM. The code is implemented in Microsoft FORTRAN 5.0 and can be run on a PC. The computation process is graphically depicted (graphic cards like Hercules, CGA, EGA, VGA can be used). The package can be ordered from the authors for a nominal handling charge (please send two 3.5″ or 5.25″ diskettes).

## 2. The package RWPM

The package RWPM consists of two essential parts:

- a *multiple shooting* technique for BVPs of the form (1.1)–(1.2) (including problems with partially separated endconditions (1.4) and pure IVPs),
- a *stabilized march* technique for BVPs of the special form (1.1) and (1.4).

The user has the option to choose one of the above-mentioned methods by a control variable. This variable is also used to distinguish between linear and nonlinear BVPs. The solution of the BVP is computed at $m$ given output points

$$a = t_1 < t_2 < \cdots < t_m = b. \tag{2.1}$$

The nonlinear algebraic shooting equations are solved

- *in multiple shooting*: by a damped and regularized Newton method [6],
- *in stabilized march*: by a damped version of the Generalized Brent Method [10].

In the Newton method damping is given the priority. Only in cases where the method doesn't find an acceptable descent or the Jacobian of the system is (nearly) singular, a regularization strategy is added. Both nonlinear equation solvers are based on difference approximations of the derivatives. The user has the option to compute also rank-1 approximations of the Jacobian.

In case of linear BVPs the Jacobian is computed only at the first iteration step. It can happen that more than one step is necessary to achieve a prescribed precision. These (additional) steps can be interpreted as an iterative refinement known from matrix computations.

The numerical stability of a shooting method strongly depends on the linear equation solver (see e.g. [1,18]). Therefore, Gaussian elimination with column pivoting and row scaling is implemented. The sparsity of the system matrix is taken into consideration by using a packed form of storage. If the boundary conditions are completely separated the associated Jacobian is a (block) banded matrix that has upper bandwidth 1. Then, the linear system is solved by back substitution (without fill-in).

The IVP-solvers used in RWPM are entries from a systematized collection of codes for solving IVPs in ordinary differential equations. This collection contains e.g.

- for *nonstiff* problems: explicit Runge–Kutta methods of order 5(6) and 7(8) (see [17]), explicit Runge–Kutta method of order 7(8) (see [14,16]), Gragg–Bulirsch–Stoer extrapolation method (see [9]);
- for *stiff* problems: ROW method of order 6 (see [11]), semi-implicit extrapolation method (see [2]).

In RWPM the net of shooting points is automatically generated. The user has the following three possibilities: to start with the desired output points (2.1) as initial net, to start with the net $\{a, b\}$—which means *simple shooting*—or to start with a net consisting of the boundary points and the midpoint of the interval $[a, b]$. New shooting points are added to the net in several situations, e.g. when the IVP-solver fails or $\| G_i \|$ is larger than a given threshold, where $G_i$ denotes a block matrix in the associated Jacobian of the shooting equations. The user has a lot of options to enter an initial trajectory. In particular, approximations of the solution of the BVP can be prescribed either at all shooting points of the initial net or at an endpoint of the interval $[a, b]$.

The input of RWPM contains only one precision parameter EPS. Based on this parameter EPS all other tolerances are internally constructed, e.g. tolerances in the stepsize strategy of the IVP-solvers, tolerances in the stopping criteria of the nonlinear equation solvers and tolerances for the stepsizes in difference approximations.

The most important stopping criteria for the iteration process (Newton method or Brent method) are: the norm of the defect of the nonlinear system is less than ESP (regular termination), the maximum number of iterations is exceeded (irregular termination), and the nonlinear equation solver terminates at a stationary point (irregular termination).

Finally, it should be mentioned that RWPM generates an approximation of the solution of the BVP at the output points (2.1) as well as a listing and/or a graphic display of the computation process. The package RWPM has been used successfully in the study of continuation and bifurcation problems in BVPs [8].

## 3. Numerical results

In this section we summarize some numerical experiments with the software package RWPM. In particular, we show that the stabilized march technique (denoted by RWPS) requires indeed fewer IVP calls than the traditional multiple shooting technique (denoted by RWPM). All computations were executed on a 386-AT in Microsoft FORTRAN 5.0 carrying a mantissa of 16 significant digits. The interval [0, 1] was subdivided into 10 and 20 equidistributed segments. The resulting IVPs were solved by a semi-implicit extrapolation method SIMPRS [2].

*Problem* (see e.g. [15]):

$$\begin{aligned}
&x_1' = a \cdot \frac{x_1}{x_2}(x_3 - x_1), \qquad x_2' = -a \cdot (x_3 - x_1)\\
&x_3' = \frac{1}{x_4}\{0.9 - 1000 \cdot (x_3 - x_5) - a \cdot x_3(x_3 - x_1)\},\\
&x_4' = a \cdot (x_3 - x_1), \qquad x_5' = -100 \cdot (x_5 - x_3),\\
&x_1(0) = x_2(0) = x_3(0) = 1, \qquad x_4(0) = -10, \qquad x_3(1) = x_5(1),\\
&a = 100.
\end{aligned} \tag{3.1}$$

Here, $n = 5$, $q = 1$, and $p = 4$ (see formula (1.3)).

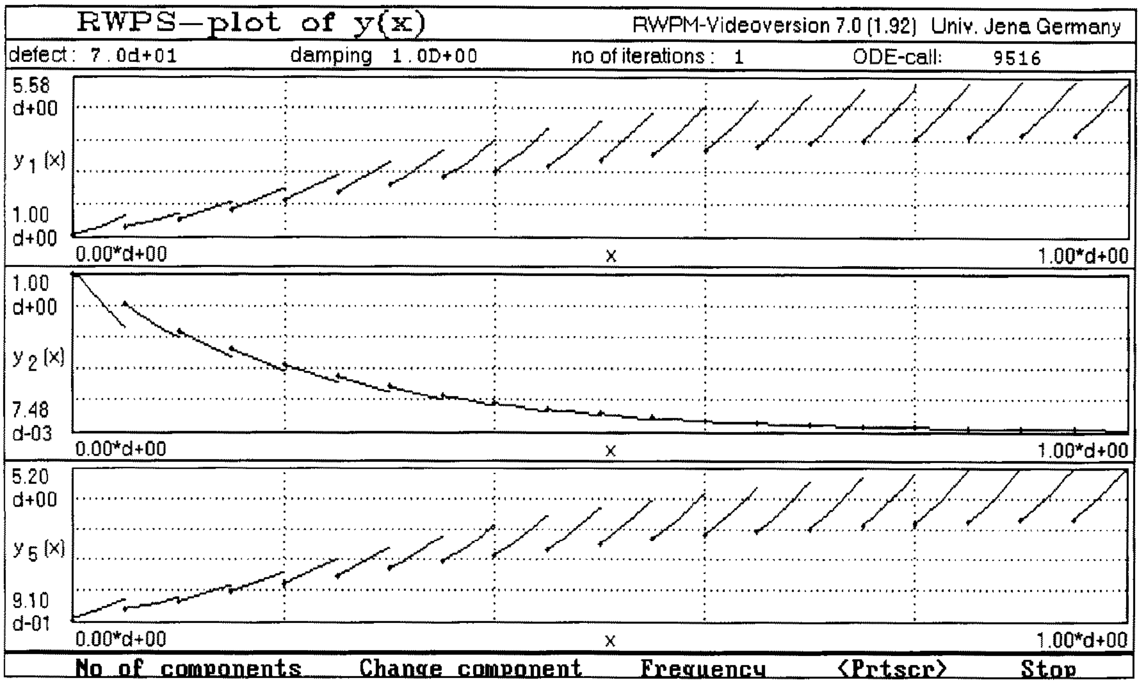


Fig. 1. Display of the first iterate: problem (3.1).

Table 1
10 equidistributed segments

| Code | $a=0$ | | | $a=100$ | | |
|---|---|---|---|---|---|---|
| | it | nivp | node | it | nivp | node |
| RWPM | 1 | 70 | 3430 | 6 | 370 | 88706 |
| RWPS | 1 | 40 | 1124 | 5 | 120 | 15224 |

Table 2
20 equidistributed segments

| Code | $a=0$ | | | $a=100$ | | |
|---|---|---|---|---|---|---|
| | it | nivp | node | it | nivp | node |
| RWPM | 1 | 140 | 6860 | 6 | 740 | 125066 |
| RWPS | 1 | 80 | 2076 | 4 | 200 | 17018 |

*Accuracy*: EPS $= 10^{-6}$.

*Starting trajectory*: In a first step we set $a = 0$ in (3.1) and solved this reduced problem with RWPM and RWPS using the following starting trajectory:

$$x_1(t)=x_2(t)=x_3(t)\equiv 1, \qquad x_4(t)\equiv -10, \qquad x_5(t)\equiv 0.91. \tag{3.2}$$

In the second step the solution of the reduced problem was taken as starting trajectory for the given problem.

*Computational results*: See Tables 1 and 2 and Fig. 1. In the tables the following abbreviations are used: it = number of iteration steps, nivp = number of IVP-solver calls, node = number of ODE calls.

## References

[1] U.M. Ascher, R.M.M. Mattheij and R.D. Russell, *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations* (Prentice-Hall, Englewood Cliffs, NJ, 1988).
[2] G. Bader and P. Deuflhard, A semi-implicit midpoint rule for stiff systems of ODE's, *Numer. Math.* 41 (1983) 373–398.
[3] P. Deuflhard and G. Bader, Multiple shooting techniques revisited, in: P. Deuflhard and E. Hairer, eds., *Numerical Treatment of Inverse Problems in Differential and Integral Equations* (Birkhäuser, Boston, 1983) 74–94.
[4] M. Hermann, Efficient shooting algorithms for solving nonlinear TPBVPs with separated endconditions, in: P. Rózsa and G. Stoyan, eds., *Numerical Methods*, Colloquia Mathematica Societatis János Bolyai 50 (North-Holland, Amsterdam, 1986) 269–285.
[5] M. Hermann, Shooting algorithms for two-point BVPs, in: K. Strehmel, ed., *Numerical Treatment of Differential Equations (NUMDIFF-4)* (Teubner, Leipzig, 1988) 74–83.
[6] M. Hermann and H. Berndt, RWPM, a multiple shooting code for nonlinear two-point boundary value problems: version 4, Report N/82/67-N/82/69, Friedrich Schiller University Jena, Germany (1982).
[7] M. Hermann and D. Kaiser, Shooting methods for two-point BVPs with partially separated endconditions, Part I, Report 100, Dortmund University (1990); Part II, Report 120, Dortmund University (1992).
[8] M. Hermann and K. Ullrich, RWPKV: a software package for continuation and bifurcation problems in two-point boundary value problems, *Appl. Math. Lett.* 5 (1992) 57–61.

[9] H.G. Hussels, Schrittweitensteuerung bei der Integration gewöhnlicher Differentialgleichungen mit Extrapolationsverfahren, Diplomarbeit, Köln University (1973).
[10] D. Kaiser, Zur numerischen Behandlung von partiell separierten Zweipunktrandwertproblemen mit Schießmethoden, Thesis, Friedrich Schiller University Jena, Germany (1992).
[11] P. Kaps and G. Wanner, A study of Rosenbrock-type methods of high order, *Numer. Math.* 38 (1981) 279–298.
[12] M.E. Kramer, Aspects of solving non-linear boundary value problems numerically, Thesis, Eindhoven University of Technology, Eindhoven, Netherlands (1992).
[13] R.M.M. Mattheij and G. Staarink, Implementing multiple shooting for nonlinear BVP, RANA Report 87-14, Eindhoven University of Technology, Eindhoven, Netherlands (1987).
[14] P.J. Prince and J.R. Dormand, High order embedded RKF's, *J. Comput. Appl. Math.* 7 (1981) 67–75.
[15] M.R. Scott and H.A. Watts, A systemalized collection of codes for solving two-point boundary value problems, in: L. Lapidus and W.E. Schiesser, eds., *Numerical Methods for Differential Systems* (Academic Press, New York, 1976).
[16] L.F. Shampine and C. Baca, Fixed vs. variable order Runge–Kutta, Report 84-1410, Sandia National Laboratories, Albuquerque, NM (1984).
[17] J.H. Verner, Explicit Runge–Kutta methods with estimates of the local truncation error, Report 92, University of Auckland, New Zealand (1976).
[18] W. Wallisch and M. Hermann, *Schießverfahren zur Lösung von Rand- und Eigenwertaufgaben* (Teubner, Leipzig, 1985).