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COMPARING SOME ASPECTS OF TWO CODES FOR TWO-POINT BOUNDARY-VALUE PROBLEMS

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Comparing some aspects of two codes for two-point boundary-value problems *)

by

P.W. Hemker, H. Schippers & P.M. de Zeeuw

ABSTRACT

For the numerical solution of two-point boundary-value problems the codes PASVAR and COLSYS have been tested on a variety of problems. These codes are compared primarily as how well they can handle difficulties caused by boundary layers, stiffness, non-linearity and mesh-selection. In particular it is considered how well they are able to find an appropriate mesh in the case of boundary-layers.

The criteria for the comparisons essentially are:

1. reliability,
2. number of coefficient function evaluations, etc.,
3. overhead costs (time and space consumption).

The problems and comparison criteria are specified carefully. At the end some remarks are made on the ease of use and on extra features of the two codes.

KEY WORDS & PHRASES: *Two-point boundary-value problems; codes; PASVAR; COLSYS; software evaluation*

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*) This report will be submitted for publication elsewhere.

CONTENTS

1. INTRODUCTION

Originally our interest was directed towards all promising codes for two-point boundary value problems, but after some time we realized that this aim was too ambitious. In general, the codes can be distinguished into two main classes: 1. codes based on methods for initial value problems (shooting- and orthogonalization-type methods) and 2. codes based on global methods (discretization-type methods). Although the dividing line between both cannot always be sharply determined, it appeared that the differences between both types were so large that any rigorous comparison between codes from both kinds would be too bold an enterprise. Therefore we restricted ourselves to the two codes that both use global methods: PASVA3 by LENTINI and PEREYRA [1977] and COLSYS by ASCHER, CHRISTIANSEN and RUSSELL [1977]. A number of useful remarks on other codes that are essentially based on initial value methods can be found in a paper by SCOTT and WATTS [1976].

We are aware of the fact that there are no best codes as soon as the variety in a class of problems is large enough (which is the case with the two-point boundary value problems considered). Hence, the aim of this paper is to establish the relative merits of the two codes under various different (difficult) circumstances.

The first one is the code named DD04AD from Harwell, Computer Science and System Division, AERE, Oxfordshire, England. It is a fully documented program, written in a most transportable FORTRAN (since it has passed the PFORT verifier). This code is the most recent (1978) version of PASVA3 (a code by Lentini and Pereyra), which has a long history (see PEREYRA [1978]) and of which a sequence of predecessors has been widely used for the last few years. The code uses a variable order method which is based on deferred corrections applied to the trapezoidal discretization rule.

The second code is a more recent one, developed by ASCHER, CHRISTIANSEN and RUSSELL [1978]. It is based on collocation with B-splines. In contrast with the first code it is able to handle higher order systems, without first reducing them to a system of first order equations. Both codes avail of fully automatic, adaptive, non-uniform mesh generating procedures.

2. ON PROBLEM SELECTION

First of all we should notice that there are no objective criteria to establish a "representative set of test problems". In compiling a set of problems nevertheless, we should essentially make a choice between two methodologies. Either:

1. one selects a (more or less chaotic) set of problems (a "test battery"), e.g. problems that arise from physical applications, and one observes how well the different methods perform, or:
2. one constructs a set of problems that all represent a specific difficulty, which can be parametrized: i.e. the problem contains a parameter which controls the degree of the difficulty involved.

Both methodologies have their disadvantages. In the first approach the knowledge of how a code performs on a particular complex real live problem hardly can be generalized (extrapolated) to other problems. Therefore, the success on such a particular problem can (only) improve the confidence in the behaviour of a code, rather than show how it performs generally. Using the second methodology one can derive firm statements of how well a code performs on the one particular type of difficulty, but in general one cannot extrapolate these statements to real live problems when difficulties pile up.

An extensive test battery of problems e.g. can be found in DIEKHOFF et. al. [1977] where it is used for the comparison of routines for the solution of initial value problems in multiple shooting.

For our purpose, however, we consider it to be more useful to follow the second approach and, hence, we select problems in which one particular difficulty arises. Furthermore, we introduce a controling parameter and we trace what difficulties up to what grade can be handled by the codes.

We select a set of ten problems, that are described in detail in the following sections. Seven problems concern with single second order equations and the other three are systems of equations. The controling parameter in the seven single equations is essentially the constant which multiplies the highest (second order) derivative. This implies that for small values of this parameter the differential equations are of singular perturbation type, so that its solution has boundary- or internal layers. The presence of these layers provides the facilities to test thoroughly the mesh-generating abilities

of the codes. The problems 8-10 represent more or less real live problems.

Most of our problems have been taken from well-known literature on this subject; thus we confirm a certain standardization which is growing.

3. QUANTITIES FOR EVALUATION AND COMPARISON

The following quantities have been measured for the comparison of the results and the performance:

MFIN - the final number of meshpoints,
MCH - the number of mesh-changes,
TIME - CP-time used on a CDC-CYBER 70/73 computer (this should be considered as a relative figure for the present comparison only!),
FEV - number of function evaluations,
JAEV - number of Jacobian evaluations,
SEDE - number of set-ups and decompositions of linear systems,
SLE - number of times a linear system was solved.

Making a fair comparison between both codes, one encounters the following difficulty with respect to the estimated accuracy and the allowed errors (the specified tolerances). For the code PASVAR, the user can specify an absolute tolerance, demanding a maximum *absolute* error for all components $z_i(.)$ and all meshpoints $\{x_k\}$ of the solution at once. For the code COLSYS, however, the user specifies a *relative* tolerance for each component separately. For each component and in all meshpoints both methods determine an estimate of the maximum absolute error:

$$\text{error}_i(x_k) = \left|\text{estimated absolute error in } z_i(x_k)\right|.$$

Both methods determine the solution of the two-point boundary-value problem (TPBVP) iteratively, adapting the meshpoint distribution and solving the corresponding non-linear equations. The stop-criteria of the algorithms are related to the tolerances (TOL) specified by the user. The stop-criterium of PASVAR is

$$\text{error}_i(x_k) \leq \text{TOL}, \qquad \text{for all components } i, \quad \text{for all meshpoints } x_k.$$

The stop-criterium of COLSYS is

$$\text{error}_i(x_k) \leq \text{TOL}_i * |z_i(x_k)| + \text{TOL}_i, \qquad \text{for all components } i, \quad \text{for all meshpoints } x_k.$$

On these grounds, to make a fair comparison we need test-problems of which the solutions satisfy the following conditions:

1.) the various components should not differ in order of magnitude,

2.) for all components $z_i(.)$ should be bounded by a constant which is of the order of unity.

To achieve this, we need to scale a problem. For this purpose, in a number of problems under consideration we introduced a *rescaling factor*. This factor was used, when an higher order equation was reformulated as a first order system. By the rescaling factor, the large derivatives (steep gradients in the solution) are reduced to an order of magnitude of the solution itself as follows. Let the original problem be

$$\begin{cases} y'' = f(t,y,y'), \\ y(t_0) = a, \; y(t_1) = b. \end{cases}$$

Then, with $\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} y \\ \alpha y' \end{pmatrix}$

we define the rescaled problem, with scaling factor α, by

$$y_1' = y' = \frac{1}{\alpha} y_2,$$

$$y_2' = \alpha f(t, y_1, \frac{1}{\alpha} y_2).$$

For each problem where rescaling was used, the rescaling factor is mentioned explicitly in the problem definition.

In order to compare the reliability of both codes we introduce the following quantities for each component z_i:

$$\text{desired error}_i = \begin{cases} \max_k (TOL_i * |z_i(x_k)| + TOL_i), & \text{for COLSYS,} \\ TOL, & \text{for PASVAR,} \end{cases}$$

$$\text{actual error}_i = \max_k |\text{error in } z_i(x_k)|,$$
(i.e. the actual, absolute error in component i),

$$\text{estimated error}_i = \text{The maximum absolute error as estimated by the code under consideration.}$$

Here, $\{x_k\}$ is the set of meshpoints in which we desire to know the solution.

In those cases where no explicit formula for the exact solution was available, the error in $z_i(x_k)$ was determined by first computing a sufficiently accurate reference solution and comparing this value with the computed result. Using COLSYS, we obtained values $z_i(x_k)$ by interpolation with the interpolation routine that is part of the COLSYS-package. The values $\{x_k\}$ always were included in the mesh that was used with PASVAR; hence the values $z_i(x_k)$ always were available after a call of PASVAR.

In a number of cases the actual error is larger than the error estimated by the code. These cases, where a code is unreliable, are denoted by (*) in the performance report.

Other abbreviations that are used in section 4 are:

H - the results obtained from computation by COLSYS; the problem being formulated as a high order equation (system of equations),

F - the results obtained by COLSYS; the problem formulated as a system of first order equations,

P - the results obtained by PASVAR; in this case the problem is always reformulated as a system of first order equations. (PASVAR cannot handle higher order equations directly).

cont = 0 results were obtained without continuation,

= 1/n/m results were obtained by continuation: first keeping TOL constant and taking n steps with varying parameter values

μ (i.e. the controling parameter); thereafter keeping μ constant varying TOL for m steps,

= */n/m the same as 1(n)m but no results could be obtained, even with n continuation steps for μ and m steps for the tolerance.

With respect to the space consumption of the codes, in the tests we have given COLSYS and PASVAR equal opportunities; we took

dimension (integer work space) = 5000,
dimension (real work space) = 15000.

In COLSYS a number of parameters can be set in order to influence the flow of computation. We didn't make any particular choice but we took the obvious default values. However, of course, if the problem was linear we set the relevant parameter(s). An initial mesh is given both to PASVAR and to COLSYS, it is the mesh on which the final solution is wanted. This mesh is given explicitly in the definition of each problem.

4. TEST PROBLEMS AND TEST RESULTS

In table 4.0 we first give a survey of the main characteristics of the problems selected.

no.	order	linear	operator-type	solution-type	main reference
1	2	yes	symmetric	2 boundary layers	Stoer & Bulirsch [1973]
2	2	yes	non-symm.	internal layer	Hemker [1977]
3	2	no	symmetric	1 boundary layer	Troesch [1960]
4	2	no	non-symm.	1 boundary layer	O'Malley [1974]
5	2	no	non-symm.	internal layer	Pearson [1968]
6	2	no	non-symm.	bound. & internal l.	Cole [1968]
7	2	no	non-symm.	internal layer	Cole [1968]
8	5	no	infinite interval	branch point	Zandbergen & Dijkstra [1977]
9	3	no	discont. coeffs.		Diekhoff et al. [1977]
10	4	no	singular coeffs.		Deuflhard et al. [1976]

Table 4.0 Main characteristics of the test problems.

PROBLEM 1.

$$y''(x) - \mu^2 y(x) = \mu^2 \cos^2(\pi x) + 2\pi^2 \cos(2\pi x)$$

$$y(0) = y(1) = 0,$$

with the exact solution

$$y(x) = \frac{e^{\mu(x-1)} + e^{-\mu x}}{1 + e^{-\mu}} - \cos^2(\pi x).$$

This problem is singularly perturbed with boundary layers of $O(\mu^{-1})$ at both end points.

To compute: $y(x_k)$, $x_k = 0.0(0.1)1.0$.
Rescaling factor: $\alpha = \mu$.

The results are given in table 4.1.

References: Stoer & Bulirsch [1973], Russell [1974], Scott & Watts [1976], Lentini & Pereyra [1977].

μ (i.e. the controling parameter); thereafter keeping μ constant varying TOL for m steps,

= */n/m the same as 1(n)m but no results could be obtained, even with n continuation steps for μ and m steps for the tolerance.

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8	5	no	infinite interval	branch point	Zandbergen & Dijkstra [1977]
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$$y(x) = \frac{e^{\mu(x-1)} + e^{-\mu x}}{1 + e^{-\mu}} - \cos^2(\pi x).$$

This problem is singularly perturbed with boundary layers of $O(\mu^{-1})$ at both end points.

To compute: $y(x_k)$, $x_k = 0.0(0.1)1.0$.
Rescaling factor: $\alpha = \mu$.

The results are given in table 4.1.

References: Stoer & Bulirsch [1973], Russell [1974], Scott & Watts [1976], Lentini & Pereyra [1977].

μ	C	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
	H	.16-3	.18-8	.12-6	21	2	0.7	94	94	2	2	0	
2	F	.16-3	.23-12	.37-7	21	2	1.2	124	124	2	2	0	
	P	.10-3	.11-4	.11-4	19	2	0.4	152	34	2	7	0	
	H	.16-5	.27-10	.36-8	41	3	1.6	216	216	3	3	0	
2	F	.16-5	.23-12	.37-7	21	2	1.2	124	124	2	2	0	
	P	.10-5	.34-6	.33-6	19	2	0.6	194	34	2	9	0	
	H	.15-3	.71-8	.16-5	21	2	0.7	94	94	2	2	0	
10	F	.15-3	.61-10	.50-6	21	2	1.2	124	124	2	2	0	
	P	.10-3	.71-4	.77-4	19	2	0.4	152	34	2	7	0	
	H	.15-5	.30-11	.21-8	81	4	3.4	458	458	4	4	0	
10	F	.15-5	.61-10	.50-6	21	2	1.2	124	124	2	2	0	
	P	.10-5	.78-6	.85-6	19	2	0.7	236	34	2	11	0	
	H	.19-3	.92-7	.61-6	81	7	4.2	584	584	7	7	0	
10^2	F	.19-3	.48-4	.16-4	19	5	2.5	266	266	5	5	0	*
	P	.10-3	.81-6	.19-4	107	3	1.8	628	205	3	6	0	
	H	.19-5	.11-8	.25-8	161	9	9.5	1300	1308	9	9	0	
10^2	F	.19-5	.64-6	.54-6	39	5	3.7	398	398	5	5	0	*
	P	.10-5	.20-6	.90-6	107	3	2.3	846	205	3	8	0	
	H	.19-3	.66-8	.19-7	141	15	13.5	1905	1905	15	15	0	
10^3	F	.19-3	.12-5	.75-5	41	7	7.4	774	774	7	7	0	
	P	.10-3	.46-5	.40-4	314	10	15.3	5157	1302	10	25	0	
	H	.19-5	.67-9	.17-8	223	15	23.9	3360	3360	15	15	0	
10^3	F	.19-5	.62-6	.36-6	47	8	9.5	1008	1008	8	8	0	*
	P	.10-5	.78-7	.91-6	409	12	25.6	8841	2018	12	32	0	

Table 4.1. Numerical results for problem 1.

(* means: the actual error is larger than the estimated error).

PROBLEM 2.

$$y'' + \mu^2 xy' = -\pi^2 \cos(\pi x) - \mu^2 \pi x \sin(\pi x),$$

$$y(-1) = 2,\ y(1) = 0,$$

with the exact solution

$$y(x) = \cos(\pi x) + \frac{\operatorname{erf}(\mu x/\sqrt{2})}{\operatorname{erf}(\mu/\sqrt{2})}$$

The solution has a transition layer of thickness $\theta(\mu^{-1})$ at the point $x = 0$.

To compute: $y(x_k)$, $x_k = -1.0(0.2)1.0)$.
Rescaling factor, $\alpha = \mu$.

The results are given in table 4.2.

Notes to table 4.2:

- In those cases where no results could be obtained immediately, the following continuation sequences were used $(tol_0 | \mu_0, \ldots, \mu_n | tol_1, \ldots, tol_m)$.

  (1): (.10-1|100|.10-3).
  (2): (.10-1|100|.10-3,.10-5),
  (3): (.10-1|100,1000|.10-3),
  (4): (.10-1|100,325,550,775,1000|.10-3),
  (5): (.10-1|100,1000|.10-3,.10-5),
  (6): (.10-1|100,325,550,775,1000|.10-3,.10-5).

References: Hemker [1977].

μ	c	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
	H	.30-3	.76-8	.27-6	21	2	0.7	94	94	2	2	0	
2	F	.30-3	.18-10	.83-7	21	2	1.2	124	124	2	2	0	
	P	.10-3	.78-4	.80-4	19	3	0.8	227	54	3	11	0	
	H	.30-5	.12-9	.82-8	41	3	1.6	216	216	3	3	0	
2	F	.30-5	.18-10	.83-7	21	2	1.2	124	124	2	2	0	
	P	.10-5	.29-6	.27-6	29	3	1.1	334	69	3	13	0	
	H	.30-3	.19-5	.18-5	41	4	1.8	248	248	4	4	0	
10	F	.30-3	.41-6	.25-4	21	2	1.2	124	124	2	2	0	
	P	.10-3	.11-6	.14-4	112	5	2.4	791	251	5	11	0	
	H	.30-5	.26-8	.46-8	99	7	6.8	935	935	7	7	0	
10	F	.30-5	.19-8	.24-6	33	4	3.0	320	320	4	4	0	
	P	.10-5	.78-7	.11-6	112	5	4.5	1475	251	5	17	0	
	H	.30-3	.83-8	.92-8	119	8	11.1	1528	1528	8	8	0	
10^2	F	.30-3	.65-5	.25-4	29	6	4.4	468	468	6	6	0	
	P	.10-3	.41-5	.79-4	197	9	8.8	3087	987	9	18	1/0/1	(1)
	H	.30-5	.20-8	.21-8	161	7	10.1	1424	1424	7	7	0	
10^2	F	.30-5	.40-6	.34-6	43	7	6.7	706	706	7	7	0	
	P	.10-5	-	-	-	-	-	-	-	-		*/0/2	(2)
	H	.30-3	.19-8	.17-7	201	13	25.3	3476	3476	13	13	1/1/1	(3)
10^3	F	.30-3	.90-6	.58-5	101	10	19.2	1952	1952	10	10	0	
	P	.10-3	.26-5	.26-5	394	16	30.2	10515	4416	21	39	1/4/1	(4)
	H	.30-5	.44-9	.14-8	261	22	59.5	8168	8168	22	22	1/1/2	(5)
10^3	F	.30-5	.25-7	.53-7	101	10	20.5	2060	2060	10	10	0	
	P	.10-5	.52-8	.22-7	394	16	32.6	11307	4416	21	41	1/4/2	(6)

Table 4.2. Numerical results for problem 2. For the abbreviations see section 3. For the notes see the text in section 4.

PROBLEM 3. (Troesch's equation).

$$y'' = \mu \sinh(\mu y),$$

$$y(0) = 0,\ y(1) = 1.$$

By means of continuation Deuflhard has obtained results up to $\mu = 17$.

To compute: $y(x_k)$, $x_k = 0.0(0.1)1.0$.
Rescaling factor: $\alpha = \exp(\mu/2)$.

The results are given in table 4.3.

Notes to table 4.3: The following continuations were used

(1): (.20-1|5,6.5,8.25,10|.20-3),
(2): (.20-1|5,6.5,8.25,10|.20-3,.20-5),
(3): (.20-1|5,6.6,8.7,11.5,15.2),
*: actual error > predicted error.

Remark: If we did increase the parameter value μ to 30, also with COLSYS we were not able to obtain a solution.

References: Troesch [1960], Scott [1975], Scott & Watts [1976], Deuflhard et al. [1976].

μ	c	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
	H	.20-3	.78-8	.38-6	33	4	4.0	682	270	6	13	0	
5	F	.20-3	.25-5	.74-5	11	3	3.7	444	232	6	13	0	
	P	.20-3	.62-4	.93-4	63	2	2.7	988	273	9	19	0	
	H	.20-5	.48-8	.64-8	41	5	6.1	1058	406	8	18	0	
5	F	.20-5	.20-6	.16-6	19	5	7.2	964	422	9	20	0	
	P	.20-5	.15-6	.16-6	84	4	4.7	1483	438	11	22	0	
	H	.20-3	.40-6	.11-5	33	6	7.5	1460	530	13	35	0	
10	F	.20-3	.13-5	.14-5	21	8	13.6	2036	818	19	51	0	
	P	.20-3	.88-4	.14-3	106	10	15.2	4356	2609	51	73	1/3/1	(1)
	H	.20-5	.13-9	.93-9	161	8	20.6	4024	1354	17	47	0	
10	F	.20-5	.22-6	.25-6	29	7	16.2	2568	932	18	50	0	
	P	.20-5	.91-6	.11-5	147	13	21.0	6096	3009	54	84	1/3/2	(2)
	H	.20-3	.27-5	.84-6	63	11	31.5	6355	2373	51	131	0	*
20	F	.20-3	.62-6	.28-5	41	11	59.7	8418	3906	53	126	0	
	P	.20-3	-	-								*/5/0	(3)
	H	.20-5	.20-9	.11-8	263	13	61.7	12335	4353	57	149	0	
20	F	.20-5	.65-7	.30-7	81	13	68.6	9936	4376	56	137	0	*
	P	.20-5	-	-								*/5/0	(3)

Table 4.3. Numerical results for problem 3.

PROBLEM 4.

$$y'' + \mu e^{y} y' - \mu \frac{\pi}{2} \sin\left(\frac{\pi x}{2}\right) e^{2y} = 0,$$

$$y(0) = 0,\ y(1) = 0.$$

This problem is quasi-linear. The asymptotic solution for $\mu \to \infty$ is given by:

$$y(x) = -\log\{(1+\cos\left(\frac{\pi x}{2}\right))(1-\tfrac{1}{2}e^{-\mu x/2})\}.$$

To compute: $y(x_k)$, $x_k = 0.0(0.1)1.0$.
Rescaling factor: $\alpha = \mu$.

The results are given in table 4.4.

Notes to table 4.4: the following continuations were used

(1): (.15-1|20,100|.15-3),
(2): (.15-1|20,100|.15-3,.15-5),
(3): (.10-1|100,550,1000|.10-3),
(4): (.15-1|20,100,215,475,1000|.15-3),
(5): (.10-1|100,550,1000|.10-3,.10-5),
(6): (.15-1|20,100,215,475,1000|.15-3,.15-5).
* : actual error > estimated error.

References: O'Malley [1974].

μ	c	Error			MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
		Desired	Actual	Estimated									
	H	.12-3	.33-8	.19-7	21	2	2.4	346	190	5	10	0	
2	F	.12-3	.48-10	.37-9	21	2	3.1	332	208	4	7	0	
	P	.15-3	.67-5	.68-5	11	1	0.2	78	26	2	6	0	
	H	.12-5	.64-10	.11-8	21	2	2.9	410	254	7	14	0	
2	F	.12-5	.48-10	.37-9	21	2	3.1	332	208	4	7	0	
	P	.15-5	.41-7	.34-7	11	1	0.4	156	26	2	12	0	*
	H	.15-3	.35-6	.83-6	15	3	3.4	457	291	9	18	0	
10	F	.15-3	.42-6	.67-6	11	3	3.6	402	232	6	12	0	
	P	.15-3	.70-4	.12-3	15	3	0.8	271	72	5	15	0	
	H	.15-5	.14-8	.82-8	41	4	7.3	1032	568	14	28	0	
10	F	.15-5	.18-6	.32-6	13	3	3.9	438	244	6	12	0	
	P	.15-5	.35-7	.46-7	46	5	1.8	514	153	7	18	0	
	H	.17-3	.73-5	.13-5	29	6	8.3	1334	588	15	34	0	*
10^2	F	.17-3	.72-5	.26-4	11	5	5.1	616	296	8	17	0	
	P	.15-3	.67-4	.91-4	39	7	2.7	797	358	14	25	1/1/1	(1)
	H	.17-5	.98-8	.19-8	161	8	26.7	4454	1760	25	56	0	
10^1	F	.17-5	.80-8	.14-6	41	5	9.9	1362	538	9	21	0	
	P	.15-5	.32-7	.34-7	131	11	7.6	2121	731	18	37	1/1/2	(2)
	H	.17-3	.15-5	.10-5	41	9	20.5	4076	1334	22	58	0	*
10^3	F	.17-3	.62-5	.48-4	15	13	23.4	2880	1540	42	90	1/2/1	(3)
	P	.15-3	.69-5	.95-5	106	13	7.5	2095	1046	24	38	1/4/1	(4)
	H	.17-5	.36-8	.23-8	161	9	34.2	6828	2154	27	72	0	
10^3	F	.17-5	.10-7	.45-7	53	19	33.5	4432	2058	49	106	1/2/2	(5)
	P	.15-5	.29-6	.10-5	106	14	9.4	2743	1154	25	44	1/4/2	(6)

Table 4.4. Numerical results for problem 4.

PROBLEM 5.

$$Ayy'' - \mu\left(\frac{1+\gamma}{2} - \frac{A'}{\mu}\right)yy' + \mu\frac{y'}{y} + \mu\frac{A'}{A}\left(1 - \frac{\gamma-1}{2}y^2\right) = 0,$$

$$y(0) = 0.9129,\ y(1) = 0.375,$$

$$A = 1 + x^2,\ \gamma = 1.4.$$

The solution of this problem contains an internal shock-layer near the place where $y(x,\mu) = 1/\sqrt{1.2}$, i.e. the location of the shock-layer depends on the solution. For $\mu \to \infty$ the layer is near $x = 0.63$.

To compute: $y(x_k)$, x_k = 0.0(0.1)0.6,0.62(0.002)0.64,0.7(0.1)1.0.
Rescaling factor: $\alpha = \sqrt{\mu}$.

Both with PASVAR and with COLSYS, we did not find a solution if no initial guess of the solution was feeded to the code. The following piecewise linear approximation was used as an initial approximant:

$$\begin{aligned} y_0(x) &= x/6 + 0.9129, && x \in [0.0,0.6), \\ y_0(x) &= -5x + 4.013, && x \in [0.6,0.7], \\ y_0(x) &= -0.46x + 0.835, && x \in (0.7,1.0]. \end{aligned}$$

The results are given in table 4.5.

Notes to table 4.5; the following continuations were used:

(1): (.10-1|1000|.10-3),
(2): (.10-1|300,650,1000|.10-3),
(3): (.20-1|100,135,146),
(4): (.10-1|1000,5500,10000|.10-3),
(5): (.10-1|300,650,2700,10000|.10-3).

References: Pearson [1968], Hemker [1977].

μ	c	Error			MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
		Desired	Actual	Estimated									
	H	.20-3	.47-7	.10-6	23	3	3.8	634	363	6	12	0	
10	F	.20-3	.10-7	.14-7	23	3	5.8	838	394	5	11	0	
	P	.15-3	.16-4	.15-4	52	3	1.8	594	234	7	15	0	
	H	.20-5	.15-8	.33-8	43	3	5.2	904	453	6	12	0	
10	F	.20-5	.10-7	.14-7	23	3	6.8	924	480	6	13	0	
	P	.15-5	.78-7	.80-7	86	3	2.7	928	296	7	17	0	
	H	.23-3	.92-7	.95-7	77	5	10.9	2060	860	10	23	0	
10^2	F	.23-3	.16-5	.24-5	23	5	13.1	1898	874	11	27	0	
	P	.15-3	.21-4	.33-4	125	5	4.9	1749	640	12	22	0	
	H	.24-3	.37-5	.25-6	69	16	57.1	9332	4685	46	105	1/0/1	(1),*
10^3	F	.24-3	-	-								*/2/1	(2)
	P	.24-3	-	-								*/2/0	(3)
	H	.24-3	.18-6	.11-6	125	37	181.0	28600	14902	131	287	1/2/1	(4),*
10^4	F	.24-3	-	-								*/3/1	(5)
	P	.24-3	-	-								*/2/0	(3)

Table 4.5 Numerical results for problem 5

PROBLEM 6.

$$y'' + \mu y y' - \mu y = 0,$$
$$y(0) = 1,\ y(1) = 1/3.$$

The solution of this problem strongly depends on the boundary values. For the above values the solution has a boundary-layer at $x = 0$ and a corner layer at $x = 2/3$. In problem 7 we have the same equation, but other boundary values. In that case the solution has an internal shock layer at $x = 1/3$.

To compute: $y(x_k)$, $x_k = 0.0(0.1)1.0$.
Rescaling factor: $\alpha = \mu$.

The results are given in table 4.6.

Notes to table 4.6; the following continuations were used:

(1): (.15-1|20,50,100|.15-3),
(2): (.15-1|20,50,100|.15-3,.15-5),
(3): (.10-1|200,1000|.10-3),
(4): (.15-1|20,50,100,200,1000|.15-3),
(5): (.10-1|200,1000|.10-3,.10-5),
(6): (.15-1|20,50,100,200,1000|.15-3,.15-5).

References: Cole [1968], O'Malley [1968], Hemker [1977].

μ	c	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
2	H	.20-3	.50-10	.15-7	21	2	2.0	314	158	4	8	0	
	F	.20-3	.35-10	.49-8	21	2	3.3	414	208	4	8	0	
	P	.15-3	.47-5	.51-5	11	1	0.4	130	39	3	10	0	
2	H	.20-5	.50-10	.15-7	21	2	2.0	314	158	4	8	0	
	F	.20-5	.35-10	.49-8	21	2	3.3	414	208	4	8	0	
	P	.15-5	.39-6	.40-6	14	3	0.8	275	70	5	16	0	
10	H	.20-3	.15-6	.14-5	17	3	2.5	388	204	6	12	0	
	F	.20-3	.73-6	.16-5	11	3	3.6	444	232	6	13	0	
	P	.15-3	.46-4	.50-4	29	4	1.0	329	119	7	15	0	
10	H	.20-5	.68-10	.89-9	81	5	8.8	1534	586	8	16	0	
	F	.20-5	.12-6	.41-6	15	3	4.0	516	256	6	13	0	
	P	.15-5	.13-5	.13-5	72	5	1.9	614	214	8	16	0	
10^2	H	.20-3	.37-6	.24-5	35	6	6.6	1263	443	10	26	0	
	F	.20-3	.70-6	.12-4	21	6	7.8	1136	462	11	28	0	
	P	.15-3	.44-4	.42-4	69	9	4.1	1389	645	26	43	1/2/1	(1)
10^2	H	.20-5	.60-9	.16-8	103	9	19.8	3745	1271	16	41	0	
	F	.20-5	.21-6	.27-6	29	6	10.4	1602	590	11	29	0	
	P	.15-5	.12-5	.12-5	69	10	5.6	1957	716	27	51	1/2/2	(2)
10^3	H	.20-3	.31-8	.14-6	113	10	42.1	6986	3505	62	148	0	
	F	.20-3	.23-4	.50-4	21	12	27.6	3418	1854	37	85	1/1/1	(3)
	P	.15-3	.70-5	.11-4	148	14	8.8	3065	1387	35	54	1/4/1	(4)
10^3	H	.20-5	.14-8	.20-8	161	9	49.6	8444	4028	64	152	0	
	F	.20-5	.13-6	.51-6	41	17	38.3	5090	2426	43	98	1/1/2	(5)
	P	.15-5	.92-6	.15-5	148	15	11.0	3965	1537	36	60	1/4/2	(6)

Table 4.6 Numerical results for problem 6.

PROBLEM 7.

$$y'' + \mu y y' - \mu y = 0,$$

$$y(0) = -7/6,\ y(1) = 3/2.$$

The equation is the same as in problem 6; only the boundary conditions differ. In this case the solution has an internal shock layer at x = 1/3.

To compute: $y(x_k)$, $x_k = 0.0(0.1)1.0$.
Rescaling factor: $\alpha = \sqrt{\mu}$.

The results are given in table 4.7.

Notes to table 4.7; the following continuations were used:

(1): (.20-1|20,50,100|.20-3),
(2): (.20-1|20,50,100|.20-3,.20-5),
(3): (.10-1|200,600,1000|.10-3),
(4): (.10-1|200,600,700),
(5): (.20-1|20,50,100,250,500,1000|.20-3).

References: Cole [1968], O'Malley [1968], Hemker [1977].

μ	c	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
	H	.25-3	.33-9	.70-8	21	2	2.0	314	158	4	8	0	
2	F	.25-3	.33-9	.23-8	21	2	3.3	414	208	4	8	0	
	P	.15-3	.21-4	.21-4	11	1	0.4	130	39	3	10	0	
	H	.25-5	.33-9	.69-8	21	2	2.3	346	190	5	10	0	
2	F	.25-5	.33-9	.23-8	21	2	3.8	456	250	5	10	0	
	P	.15-5	.27-6	.26-6	26	3	1.1	328	92	5	16	0	
	H	.25-3	.20-7	.12-5	21	2	2.7	410	222	6	13	0	
10	F	.25-3	.42-6	.37-9	21	2	5.1	666	334	7	17	0	*
	P	.15-3	.81-5	.79-5	71	4	1.8	607	205	8	17	0	
	H	.25-5	.35-9	.13-8	81	4	8.8	1534	618	9	19	0	
10	F	.25-5	.37-9	.42-6	21	2	5.6	708	376	8	19	0	
	P	.15-5	.81-7	.79-7	93	4	2.5	887	235	8	19	0	
	H	.25-3	.99-7	.12-6	85	8	21.2	3494	1744	35	81	0	
10^2	F	.25-3	.96-8	.22-5	41	8	22.3	3094	1420	28	68	0	
	P	.20-3	.32-5	.45-4	95	10	7.0	2641	1044	28	52	1/2/1	(1)
	H	.25-5	.87-8	.67-7	121	9	28.1	4840	2172	36	84	0	
10^2	F	.25-5	.15-8	.19-7	81	8	27.7	4078	1654	27	70	0	
	P	.20-5	.88-7	.17-6	215	14	18.5	6600	1711	32	73	1/2/2	(2)
	H	.25-3	.40-9	.12-6	113	33	81.9	14206	6540	114	268	1/2/1	(3)
10^3	F	.25-3										*/2/0	(4)
	P	.20-3	.40-9	.74-6	226	15	21.6	7647	3572	47	75	1/5/1	(5)

Table 4.7 Numerical results for problem 7.

PROBLEM 8.

$$f''' + 2ff'' = (f')^2 + s^2 - g^2,$$

$$g'' + 2fg' = 2f'g,$$

$$f(0) = f'(0) = f'(\infty) = 0,\ g(0) = 1,\ g(\infty) = s.$$

These equations describe the problem of rotating fluid above an infinite disk which is itself rotating. There exists a branching point for $s = -0.16054$; multiple solutions exist for $s < 0.07$.

To compute: $f(x_k)$, $g(x_k)$, $x_k = 0.0(1.0)16.0$.

We have fixed infinity at a finite value $x = \ell$. For $\ell = 16$ the reference solutions have been obtained by the COLSYS-code with TOL = 10^{-8}. For $s = -0.1$ it occurred that the H- and F- approach delivered two different solutions of the same problem, as is illustrated in table 4.8.1. Furthermore, in this table we compare the produced solution with the results of Zandbergen & Dijkstra [1977, table 4.1]. As far as the results coincide, they are underlined. Apparently for $s \leq -0.1$ the choice of $\ell = 16$ is too small to obtain an approximation to the solution of the original problem with unbounded domain.

	s	2f(ℓ)	f"(0)	-g'(0)
H & F	0.5	0.54568268	0.39083916	0.41768942
H & F	0.0	0.88445548	0.51023253	0.61592195
H	-0.1	-0.21525735	0.52686128	0.60449849
F	-0.1	0.59428832	0.49128306	0.60828491
H & F	-0.15	-0.20636382	0.53606657	0.61139430
H & F	-0.155	-0.20165568	0.53840936	0.61322735

Table 4.8.1 Numerical results of the COLSYS-code with TOL = 10^{-8}, Infinity was fixed at $\ell = 16$.
(As far as the results coincide with those of Zandbergen & Dijkstra they are underlined).

Remark 1: PASVAR failed for all of the parameter values s.

Remark 2: If s = 1.0 the problem becomes a very simple one, for the solution reads: $g \equiv 1$, $f \equiv 0$. Nevertheless, both PASVAR and COLSYS (H & F) failed.

For s = 0,5, 0.0 and -0.1, respectively, the results of COLSYS are given in table 4.8.2.

Notes to table 4.8.2; the following continuations were used:

(1) - $(s_0=0.0, tol_0=0.1\text{-}1)$, $(s_1=0.5, tol_1=0.1\text{-}3)$,
(2) - $(s_0=0.0, tol_0=0.1\text{-}1)$, $(s_1=0.5, tol_1=0.1\text{-}5)$.

Reference: Zandbergen & Dijkstra [1977].

s	c	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
0.5	$H^{(f)}$	.13-3	.54-9	.12-9	33	4	43.1	3015	1670	14	35	0	
	$_{(g)}$	.20-3	.42-9	.79-9									
0.5	$F^{(f)}$	.13-3	.76-7	.12-6	17	5	65.2	2199	1277	25	60	1/1/0	(1)
	$_{(g)}$	.20-3	.87-7	.30-6									
0.5	$H^{(f)}$	.13-5	.80-9	.16-9	33	4	46.0	3148	1803	15	37	0	
	$_{(g)}$	.20-5	.61-9	.93-9									
0.5	$F^{(f)}$	.13-5	.76-7	.12-6	17	5	66.8	2236	1314	26	62	1/1/0	(2)
	$_{(g)}$	.20-5	.87-7	.30-6									
0.0	$H^{(f)}$	.14-3	.31-7	.57-7	17	3	21.2	1353	865	13	29	0	*
	$_{(g)}$	.20-3	.14-6	.89-7									
0.0	$F^{(f)}$	.14-3	.12-6	.36-6	17	3	38.9	1215	727	11	25	0	
	$_{(g)}$	.20-3	.15-6	.46-6									
0.0	$H^{(f)}$	.14-5	.15-7	.30-7	19	3	21.5	1389	877	13	29	0	
	$_{(g)}$	.20-5	.60-7	.48-7									
0.0	$F^{(f)}$	.14-5	.16-6	.18-6	19	3	43.0	1320	808	12	27	0	
	$_{(g)}$	.20-5	.17-6	.27-6									
-0.1	$H^{(f)}$	.16-3	.13-6	.40-6	17	3	19.6	1284	796	12	27	0	
	$_{(g)}$	.20-3	.31-6	.57-6									
-0.1	$F^{(f)}$	.13-3	.27-6	.24-6	17	3	50.9	1560	1003	15	34	0	
	$_{(g)}$	.20-3	.42-6	.51-6									

Table 4.8.2 Numerical results for problem 8.
The reference solution has been obtained by COLSYS (H and F) with TOL = 10^{-8}.

PROBLEM 9.

$$p' = \nu(\alpha x - \tfrac{1}{2}\nu e^{t/T}),$$
$$x' = -bx\nu,$$
$$\lambda' = \nu(\lambda b - a), \qquad t \in [0,1],$$
$$P(0) = 1,\ x(0) = 1,\ \lambda(1) = 0,$$

and $\tilde{\nu}(t) = e^{-t/T} x(\alpha - \lambda b)$,

$$\nu(t) = \underline{\text{if}}\ \tilde{\nu} < 0\ \underline{\text{then}}\ 0\ \underline{\text{else}}$$
$$\underline{\text{if}}\ \tilde{\nu} > 1\ \underline{\text{then}}\ 1\ \underline{\text{else}}\ \tilde{\nu}\ .$$

The equations originate from an optimal control problem of a mass production. The equations have discontinuous derivatives in their coefficients.

To compute: $p(t_k)$, $x(t_k)$, $\lambda(t_k)$, $t_k = 0.0(0.125)1.0$.

In table 4.9 we give numerical results for the set of parameters $\alpha = 2.0$, $b = 0.08$, $T = 10.0$.

Reference: Diekhoff et al [1977].

c	Error			MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT
	Desired	Actual	Estimated								
(p)	.20-3	.48-10	.38-14								
F(x)	.20-3	.49-10	.79-15	17	2	4.9	411	207	5	11	0
(λ)	.29-3	.48-9	.24-14								
(p)	.10-3	.16-4	.15-4								
P(x)	.10-3	.62-6	.62-6	9	1	0.3	84	48	4	5	0
(λ)	.10-3	.15-4	.15-4								
(p)	.20-5	.48-10	.38-14								
F(x)	.20-5	.49-10	.79-15	17	2	4.8	411	207	5	11	0
(λ)	.29-5	.48-9	.24-14								
(p)	.10-5	.42-9	.38-9								
P(x)	.10-5	.53-10	.15-10	9	1	0.4	120	48	4	8	0
(λ)	.10-5	.24-9	.38-9								

Table 4.9 Numerical results for problem 9. (α = 2.0, b = 0.08, T = 10.0).

PROBLEM 10. (thin shallow spherical shell).

$$f'' = -\mu^2 g + fg - 3f'/x - 2\gamma,$$

$$g'' = \mu^2 f - \tfrac{1}{2}f^2 - 3g'/x,$$

$$f'(0) = g'(0) = f(1) = g'(1) + (1-\nu)g(1) = 0.$$

The equations have singular coefficients at $x = 0$.

To compute: $f(x_k)$, $g(x_k)$, $x_k = 0.0(0.1)1.0$.

In table 4.10 we give the numerical results for $\nu = 1/3$, $\mu = 11$ and $\gamma = 2000,5000,10000$.

Remark: For this problem PASVAR failed since it was not able to cope with the singularity at $x = 0$; it is clear that PASVAR is unable to cope with problems for which either the coefficients in the equation or the coefficients in the Jacobian are singular at the meshpoints used.

References: Deuflhard et al [1976], Stoer & Bulirsch [1973].

γ	c	Error: Desired	Error: Actual	Error: Estimated	MFIN	MCH	TIME	FEV	JAEV	SEDE	SLE	CONT	Notes
2.10^3	$H^{(f)}$	.22-3	.34-6	.49-5	21	2	3.1	328	166	4	8	0	
	$H^{(g)}$	.35-2	.76-6	.45-5									
	$F^{(f)}$	.22-3	.22-9	.15-5	21	2	7.8	428	216	4	8	0	
	$F^{(g)}$	.35-2	.48-8	.96-6									
	$H^{(f)}$	.22-5	.13-9	.62-8	81	4	12.2	1466	568	7	14	0	*
	$H^{(g)}$	.35-4	.46-8	.33-8									
	$F^{(f)}$	.22-5	.20-7	.72-7	33	4	16.2	1028	416	6	12	0	
	$F^{(g)}$	.35-4	.12-7	.45-7									
5.10^3	$H^{(f)}$	.43-3	.13-7	.40-6	41	3	6.4	734	324	6	12	0	
	$H^{(g)}$	.85-2	.27-7	.21-6									
	$F^{(f)}$	.43-3	.53-9	.35-5	21	2	9.2	472	260	5	10	0	
	$F^{(g)}$	.85-2	.46-8	.20-5									
	$H^{(f)}$	.43-5	.37-9	.47-8	101	6	22.7	2840	1026	9	18	0	*
	$H^{(g)}$	.85-4	.49-8	.17-8									
	$F^{(f)}$	.43-5	.75-7	.26-6	33	4	17.5	1072	460	7	14	0	
	$F^{(g)}$	.85-4	.59-7	.96-7									
10^4	$H^{(f)}$	.86-3	.26-7	.59-6	41	3	6.6	768	324	6	13	0	
	$H^{(g)}$	.17-1	.59-7	.45-6									
	$F^{(f)}$	.86-3	.57-8	.56-5	21	2	9.4	516	260	5	11	0	
	$F^{(g)}$	.17-1	.50-7	.46-5									
	$H^{(f)}$	.86-5	.38-9	.86-8	91	6	21.9	2739	981	9	19	0	*
	$H^{(g)}$	.17-3	.45-7	.31-7									
	$F^{(f)}$	.86-5	.22-6	.36-6	33	4	17.8	1116	460	7	15	0	
	$F^{(g)}$	.17-3	.23-6	.38-6									

Table 4.10 Numerical results for problem 10. ($\nu = 1/3$, $\mu = 11$).

5. FINAL REMARKS

Scaling (user convenience)

Using the code PASVAR, one can specify only absolute tolerances; with the code COLSYS, however, the user specifies relative tolerances. The latter is an advantage in the case of components with different orders of magnitude or components that differ in magnitude over the interval of definition. Moreover, providing an array of tolerances is often more convenient for the user than rescaling the problem.

Continuation

The possibility of continuation has been widely used, but only in those cases where no results could be obtained without it. Continuation was used both in the sense of parametrizing the problem and going from large to small tolerances. Using continuation both codes gained a lot of robustness, i.e. they were able to handle problems with rather extreme parameters and with small tolerances.

Initial estimate of the solution

The possibility offered by COLSYS to give an approximate solution by means of a subroutine (SOLUTN) turned out to be useful. In some cases it was not possible to find a solution without this feature.

Robustness

Looking over the results (especially problems 2,3,5,10), we perceive that COLSYS is generally more able than PASVAR to handle problems with thin boundary layers. To find solutions, PASVAR had to use continuation in far more cases than COLSYS. The built-in continuation of PASVAR alone was often not sufficient and an additional continuation was needed for extreme parameter values.

Costs

Generally, the code PASVAR is somewhat cheaper both in use of storage and in CP-time consumption. Moreover, COLSYS is a more substantial program than PASVAR is.

	COLSYS	PASVAR
FORTRAN LINES (without comment)	1732	1109
OBJECT CODE (words after compilation by the FTN 4.8 compiler on the CDE CYBER 70/73 computer)	6851	5694

Singular coefficients

Due to the basic discretization that was used (the trapezoidal rule) PASVAR was not able to cope with the coefficient that was singular at the end point (problem 10), whereas COLSYS (collocation at Gaussian points) can handle this kind of singularities of which the location is known beforehand.

Reliability

We perceive that both codes are reliable in the sense that the real errors are always smaller than the specified tolerances. However, frequently the real error is larger than the estimate of the error. PASVAR more accurately predicts the error than COLSYS does.

Interpolation

In our tests we always asked for the solution at a (small) number of points, that were included in the initial mesh which was supplied to the

codes. The COLSYS-package has been provided with an interpolation routine which can be used if a COLSYS-solution has been obtained. It is not clear how a sufficiently accurate interpolation can be constructed for PASVAR.

6. CONCLUSIONS

Considering the results of our tests, we draw the following conclusions:

1) COLSYS is more robust than PASVAR.
2) PASVAR is somewhat cheaper in time and space consumption than COLSYS.
3) Both codes deliver reliable results, but the error estimates are to be trusted only in order of magnitude. PASVAR is more accurate about this point.
4) Both methods gain a lot of robustness by an additional -user provided- continuation (i.e. continuation both by parametrizing the problem and by going from large to small tolerances).

In this paper we have tested the codes PASVAR and COLSYS on a set of problems; most of these problems contain a controling parameter. For extreme values of this parameter the problems were of singular perturbation type. It is our experience that the COLSYS-package performs well on singular perturbation problems, whereas PASVAR often needs additional continuation, which, however, was not sufficient to solve the problems 5, 8 and 10.

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