Collocation Methods for the Computation of Bubble-Type Solutions of a Singular Boundary Value Problem in Hydrodynamics

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1 Introduction

The singular boundary value problem we discuss here originates from the Cahn-Hillard theory, which is used in hydrodynamics to study the behavior of non-homogeneous fluids. In [3], the *density profile equation* for the description of the formation of microscopical bubbles in a non-homogeneous fluid (in particular, vapor inside one liquid) is derived. In the form of the equation derived in [9], a nonlinear boundary value problem for a scalar second order ordinary differential equation for the *density* ρ of the medium results. In dimensionless parameters this reads

$$\rho''(r) + \frac{N-1}{r}\rho'(r) = 4\lambda^2(\rho(r)+1)\rho(r)(\rho(r)-\xi), \tag{1a}$$

$$\rho'(0) = 0, \quad \rho(\infty) = \xi. \tag{1b}$$

Here, λ is a parameter which may be chosen as $\lambda = 1$ without restriction of generality. N denotes the dimension of the problem, which in the physically meaningful case is $N = 3$. Finally, $0 < \xi < 1$ is varied such as to reflect different physical situations.

We are interested in computing a monotonously increasing solution for $0 < r < \infty$ ("bubble-type solution"). When such a solution exists it has exactly one zero R in that interval (which can be interpreted as the bubble radius). Furthermore, it can be shown that $-1 < \rho(0) < 0$ and $-1 < \rho(r) < \xi,\ r > 0$, and that $\rho'(\infty) = 0$ and $|\rho(0)| < \infty$. Finally, it turns out that the solution features an interior layer, which gets sharpers as $\xi \to 1$. All these properties have been discussed in [9], see also [8].

2 Transformation to a Finite Interval

Here, we propose to solve (1) via transformation to a singular boundary value problem on a finite interval. To this end, two different approaches can be adopted: Transformation to a first order ODE via the Euler transformation, and subsequent transformation to the interval $[0, 1]$, or transformation of the second order problem to $[0, 1]$ and direct solution in the second order formulation. In both cases, we approximate the solution numerically using a collocation solver which is currently being developed for higher order ODEs [6]. We stress here, however, that the resulting singular problems of first and second order are not equivalent.

2.1 First Order Problem

First, we transform (1a) to first order by the Euler transformation $z(r) = (z_1(r), z_2(r)) = (\rho(r), r\rho'(r))$. Subsequently, we split the interval $(0, \infty) = (0, 1] \cup [1, \infty)$, and transform the second interval to $(0, 1]$. Thus, we obtain a singular boundary value problem for $z(s) = (z_1(s), z_2(s), z_3(s) = z_1(1/s), z_4(s) = z_2(1/s)),\ s \in (0, 1]$,

$$z'(s) = \begin{pmatrix} \frac{M}{s} & 0 \\ 0 & \frac{-M}{s} \end{pmatrix} z(s) + \begin{pmatrix} f(s, z_1(s), z_2(s)) \\ g(s, z_3(s), z_4(s)) \end{pmatrix}, \tag{2}$$

where

$$M = \begin{pmatrix} 0 & 1 \\ 0 & 2-N \end{pmatrix},$$
$$f(s, z_1, z_2) = \begin{pmatrix} 0 \\ 4\lambda^2 s(z_1+1)z_1(z_1-\xi) \end{pmatrix},$$
$$g(s, z_3, z_4) = \begin{pmatrix} 0 \\ -4\lambda^2 \frac{1}{s^3}(z_3+1)z_3(z_3-\xi) \end{pmatrix}.$$

The boundary conditions in the new variables read

$$z_2(0) = 0,\ z_3(0) = \xi,\ z_1(1) = z_3(1),\ z_2(1) = z_4(1). \tag{3}$$

The same transformation is carried out in detail for other boundary value problems on semi-infinite intervals in [2].

In order to discuss the well-posedness of (2), (3) within the framework of the theory of singular boundary value problems developed in [4] and [5], we linearize the problem at the exact solution (using certain properties derived in [9]). This results in

$$y'(s) = \begin{pmatrix} \frac{N(s)}{s} & 0 \\ 0 & \frac{A(s)}{s^3} \end{pmatrix} y(s), \tag{4}$$

where

$$N(s) = \begin{pmatrix} 0 & 1 \\ 4\lambda^2 s^2(3z_1^2(s) + 2(1-\xi)z_1(s) - \xi) & 2-N \end{pmatrix},$$
$$A(s) = \begin{pmatrix} 0 & -2s^2 \\ -4\lambda^2(3z_3^2(s) + 2(1-\xi)z_3(s) - \xi) & (N-2)s^2 \end{pmatrix},$$

and the boundary conditions the same as (3), but with the homogeneous boundary value $y_3(0) = 0$. From the boundary conditions for z it follows that

$$N(0) = M, \quad A(0) = \begin{pmatrix} 0 & 0 \\ -4\lambda^2\xi(\xi+1) & 0 \end{pmatrix}.$$

Consequently, $y_2(0) = y_3(0) = 0$ are necessary and sufficient conditions for a continuous solution of (4) to exist.

It is interesting to note at this point that alternatively to (1b), the boundary conditions

$$\rho'(0) = 0,\ \rho'(\infty) = 0 \tag{5}$$

are used in the literature [3]. In the first order formulation (2), these conditions do not yield a well-posed problem, as has been demonstrated above. This is not necessarily a contradiction, however, as the boundary condition may be admissible for the second-order problem nonetheless, see §2.2.

2.2 Second Order Problem

If instead of transforming to a first order problem, we transform (1a) to the interval $[0, 1]$ in the second order formulation, we obtain (cf. [7])

$$z_2''(s) = \frac{N-3}{s} z_2'(s) + 4\lambda^2 \frac{1}{s^4} (z_2(s)+1) z_2(s) (z_2(s)-\xi). \tag{6}$$

Together with the original equation ($z_1 = \rho$) and the boundary conditions

$$z_1'(0) = 0,\ z_2(0) = \xi,\ z_1(1) = z_2(1),\ z_1'(1) = -z_2'(1) \tag{7}$$

we obtain a boundary value problem for a second order ODE with an essential singularity.

To check the well-posedness of this problem, no theory for second-order singular problems exists so far. Thus, we have to transform the linearized problem to the first order and discuss the resulting problem.

The linearization of problem (1a), (6) about the exact solution $z(s)$ reads

$$y''(s) = \frac{A_1(s)}{s} y'(s) + \frac{A_0(s)}{s^2} y(s), \tag{8}$$

where

$$\begin{aligned} A_1(s) &= \begin{pmatrix} 1-N & 0 \\ 0 & N-3 \end{pmatrix}, \\ A_0(s) &= \begin{pmatrix} s^2 c(s, z_1(s)) & 0 \\ 0 & \frac{1}{s^2} c(s, z_2(s)) \end{pmatrix}, \\ c(s, z) &= 4\lambda^2 (3z^2 + 2(1-\xi) z - \xi). \end{aligned}$$

If we now use the Euler transformation $x(s) = (y(s), sy'(s))$ to transform (8) to a first order equation, we obtain

$$x'(s) = \frac{C(s)}{s} x(s) = \frac{\tilde{C}(s)}{s^3} x(s), \tag{9}$$

with

$$C(s) = \begin{pmatrix} 0 & I \\ A_0(s) & I + A_1(s) \end{pmatrix}, \quad \tilde{C}(0) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & c(0) & 0 & 0 \end{pmatrix}.$$

Since $c(0) \neq 0$, we can conclude that $x_2(0) = 0$ is a necessary condition for the well-posedness of the problem, which corresponds to $y_2(0) = 0$. The condition $y_1'(0) = 0$ is not reflected in this formulation, however. This makes the approach outlined in this section unsatisfactory from a theoretical point of view. This does not imply that the second order formulation is of no practical use: We have to point out, that there is some freedom of choice in the transformation to first order. The standard transformation $x(s) = (y(s), y'(s))$ leads to the same boundary condition for the first order problem, however. As of yet, no standard way to analyze second order problems with an essential singularity has been developed. In any case, the formulation (9) appears to rule out the boundary conditions (5). Indeed, in [3] the condition is not explicitly used in the numerical solution of the boundary value problem, but rather a shooting approach is adopted and it is not apparent from the numerical results whether the formulation yields a well-posed problem. Thus, possibly (5) may indeed not lead to a well-posed singular problem on $[0, 1]$.

3 Numerical Results

We start the presentation of the numerical results obtained for problem (1) by collocation with the second order formulation (1a), (6) and (7). This problem statement turned out to be easier computationally, as there are fewer equations to solve, and hence fewer initial guesses are required for the solution of the collocation equations. Even though the wellposedness of the second order, singular problem on the interval $[0, 1]$ is not clear theoretically, our computations yielded promising results. For all the computation reported in this paper, we used `kollimplizitmix`, a new collocation solver for singular differential equations of arbitrary, mixed order in implicit form which is currently being developed at our institute [6]. For both the second order problem (1a), (6), (7) and the first order problem (2), we compare the results in the explicit formulations with a restatement of the differential equations in implicit form, where no negative powers of the independent variable appear in the right-hand side.

3.1 Numerical Results for the Second Order Problem

First, we discuss the problem formulation of (1a), (6) and (7) where the equation (6) is multiplied by s^4, $s \in (0, 1]$,

$$z_1''(s) = 4\lambda^2(z_1(s) + 1)z_1(s)(z_1(s) - \xi) - \frac{N-1}{s} z_1'(s), \tag{10a}$$

$$s^4 z_2''(s) = s^3(N-3)z_2'(s) + 4\lambda^2(z_2(s) + 1)z_2(s)(z_2(s) - \xi), \tag{10b}$$

which can – in that form – only be solved with implicit solvers. In this experiment, the singularity of the first kind which is present in (10a) is not removed. The first initial profile we used for the Newton solver of `kollimplizitmix` for $\xi = 0.5$ was

$$z_1(s) = -1 \quad \text{and} \tag{11a}$$

$$z_2(s) = -\frac{3}{2}s + \frac{1}{2}, \quad s \in (0, 1]. \tag{11b}$$

The computation (the tolerance on the Newton increment is always set to 1e−10) with two equidistant collocation points and 10 intervals was successful, and so we could use this approximate solution as initial profile (cf. Figure 1) for further computations with varying collocation points and number of collocation intervals.

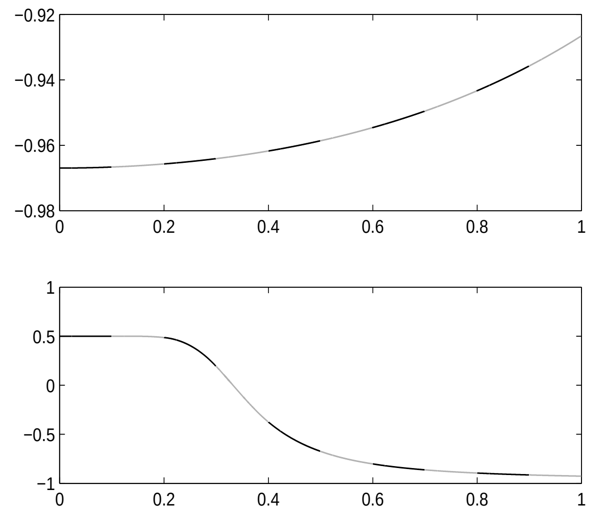

Figure 1: 10 intervals, two equidistant collocation points

3.1.1 Empirical Convergence Orders

First, we study the empirical convergence orders of our collocation methods for the case where $\xi = 0.5$. We define $z_p^{\{i\}}$, $p = 1, 2$, as the numerical solution of (10) computed at $4 \cdot 2^{i-1}$ intervals (with the exception of one collocation point, where $8 \cdot 2^{i-1}$ intervals were used). Let

$$konv\_est\_i := \frac{\ln\left(\frac{\|z_p^{\{i\}} - z_p^{\{i+1\}}\|}{\|z_p^{\{i+1\}} - z_p^{\{i+2\}}\|}\right)}{\ln 2},$$

where $\|\cdot\|$ denotes the maximum norm on the space of grid vectors (here, the solution values at the mesh points – the end points of the collocation intervals – are used only).

Tables 1–5 show that the convergence orders for the singular problem (10) correspond with the general theoretical results for collocation methods applied to regular boundary value problems. For Gaussian collocation points we even observe superconvergence, which is surprising in the case of a problem with an essential singularity (cf. Table 6).

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	7.706994e−03	1.00
2	3.834069e−03	1.79
3	1.102951e−03	1.94
4	2.869508e−04	1.98
5	7.239566e−05	1.99
6	1.813940e−05	—

i	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	6.734136e−02	2.02
2	1.655467e−02	1.76
3	4.869139e−03	1.92
4	1.282108e−03	1.98
5	3.241564e−04	1.99
6	8.124505e−05	—

Table 1: One equidistant collocation point

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	7.047587e−02	2.72
2	1.065506e−02	2.07
3	2.530996e−03	1.79
4	7.273203e−04	1.95
5	1.881034e−04	1.98
6	4.743891e−05	—

i	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	1.750105e−01	2.10
2	4.069410e−02	1.85
3	1.123480e−02	1.78
4	3.271116e−03	1.93
5	8.548392e−04	1.98
6	2.162979e−04	—

Table 2: Two equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	8.931855e−03	−0.12
2	9.714313e−03	5.03
3	2.952864e−04	4.40
4	1.391326e−05	3.97
5	8.828332e−07	3.99
6	5.538612e−08	—

i	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	8.436093e−02	0.88
2	4.575663e−02	5.03
3	1.394671e−03	4.36
4	6.756214e−05	3.98
5	4.281413e−06	3.99
6	2.685386e−07	—

Table 3: Three equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	4.052108e−02	2.86
2	5.564251e−03	7.91
3	2.302719e−05	2.89
4	3.094143e−06	3.93
5	2.026812e−07	3.98
6	1.281511e−08	—

i	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	1.796997e−01	2.57
2	3.025414e−02	8.13
3	1.079556e−04	2.85
4	1.490041e−05	3.92
5	9.797834e−07	3.98
6	6.201161e−08	—

Table 4: Four equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	7.508804e−03	7.57
2	3.930525e−05	1.59
3	1.300722e−05	7.57
4	6.822115e−08	5.96
5	1.095187e−09	5.99
6	1.722567e−11	—

i	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.977417e−02	4.94
2	9.676535e−04	3.79
3	6.965323e−05	7.53
4	3.747167e−07	5.96
5	5.983782e−09	5.98
6	9.451401e−11	—

Table 5: Five equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.454307e−02	6.22
2	3.277156e−04	5.12
3	9.418404e−06	8.22
4	3.154728e−08	5.93
5	5.161539e−10	5.98
6	8.155809e−12	—

i	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	8.369461e−02	5.50
2	1.846019e−03	5.19
3	5.044448e−05	8.18
4	1.737186e−07	5.94
5	2.821679e−09	5.97
6	4.475209e−11	—

Table 6: Three Gaussian collocation points

3.1.2 Varying the Value of ξ

For computing solutions with $\xi > 0.5$ we used a simple pathfollowing procedure, where the numerical solution obtained for a value of ξ is used as the initial profile for the solution of the collocation equations for the subsequent value of ξ. As the interior layer gets sharper for $\xi \to 1$, it becomes increasingly difficult to find a numerical solution of the problem. In that case the initial profile for the solution of the nonlinear collocation equations has to be chosen very carefully. However, pathfollowing worked very well in the interval $[0.5, 0.8]$ when increasing ξ with a stepsize $\Delta\xi = 0.1$. For $[0.8, 0.9]$ a stepsize $\Delta\xi = 0.01$ and a special grid with more grid points close to the layer was necessary (used grid: $[0 : 0.01 : 0.06, 0.061 : 0.0005 : 0.14, 0.15 : 0.01 : 1]$ at three Gaussian collocation points). Figure 2 gives an overview of the evolution of the solution for $\xi \to 0.9$.

In comparison to finding solutions for $\xi > 0.5$, the collocation equations are easy to solve for $\xi < 0.5$. E. g. for $\xi = 0.2$ our procedure even worked for initial profiles consisting of only straight lines, like $z_1(s) = -0.5, z_2(s) = -0.8s + 0.3,\ s \in (0, 1]$. Figure 3 gives a graphical overview for $\xi = [0.005, 0.1, 0.2, \ldots, 0.5]$. In Figure 4, all solutions given in Figures 2 and 3 are displayed in one plot. Figure 5 gives all the solution profiles transformed back to the original domain $[0, \infty)$. Table 7 shows for different values of ξ the values of $\rho(0)$ and the bubble radius R, computed numerically at 1000 intervals and five Gaussian points.

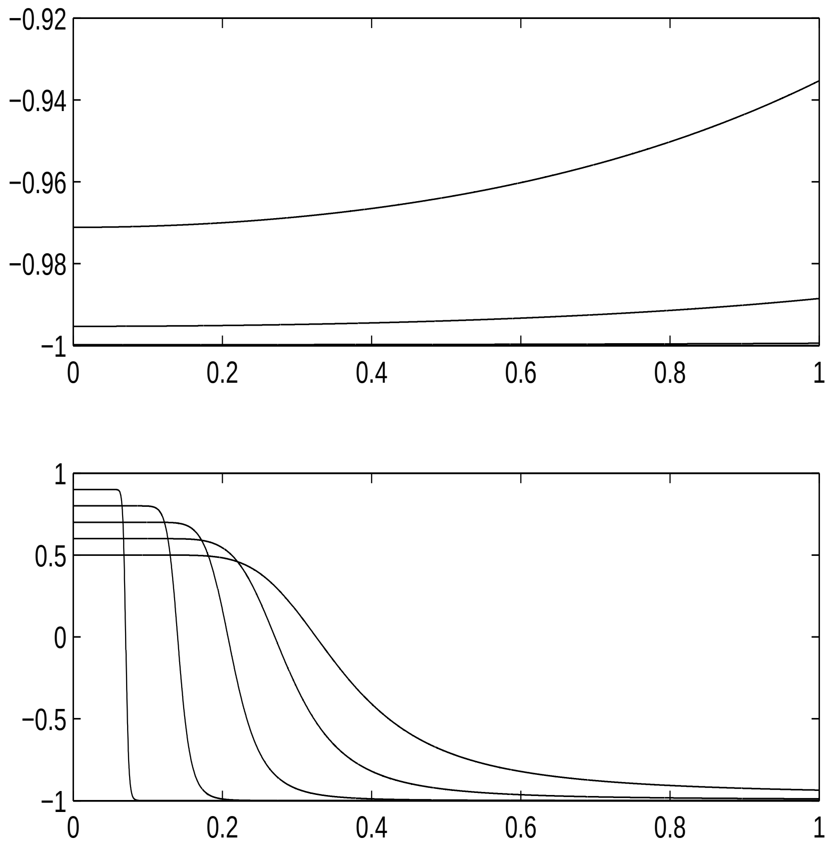

Figure 2: 1000 intervals, three Gaussian collocation points, $\xi = 0.5,\ 0.6,\ 0.7,\ 0.8,\ 0.9$

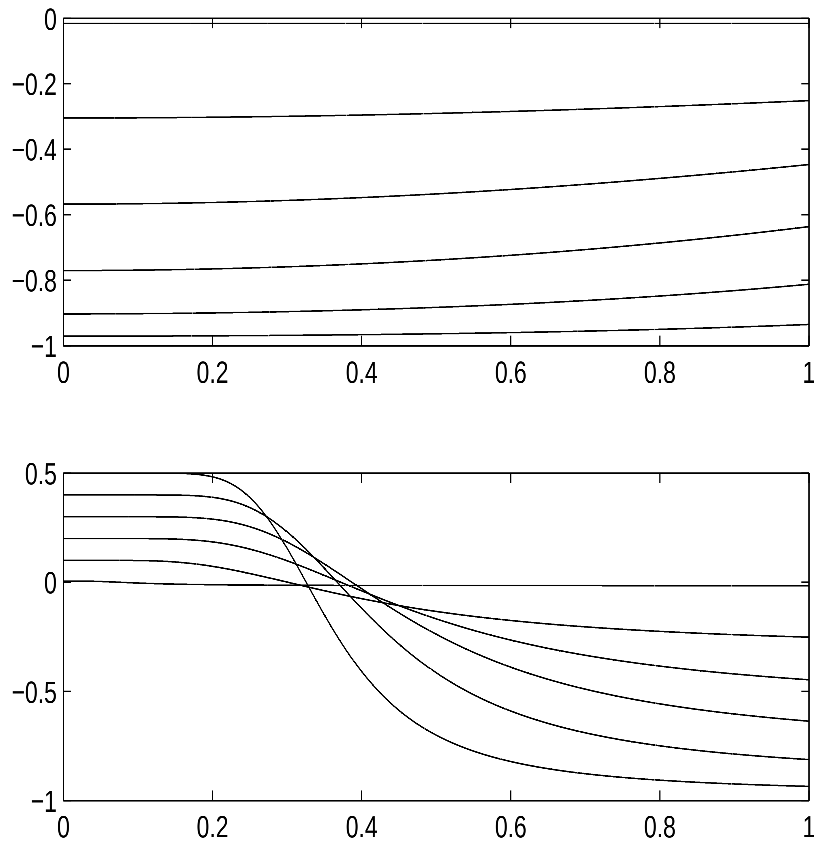

Figure 3: 1000 intervals, three Gaussian collocation points, $\xi = 0.005,\ 0.1,\ 0.2,\ 0.3,\ 0.4,\ 0.5$

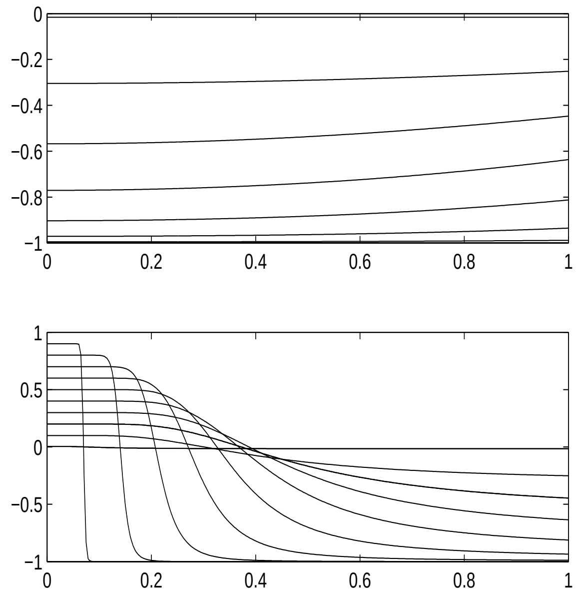

Figure 4: 100 intervals, three Gaussian collocation points, $\xi = 0.005,\ 0.1, \ldots, 0.9$

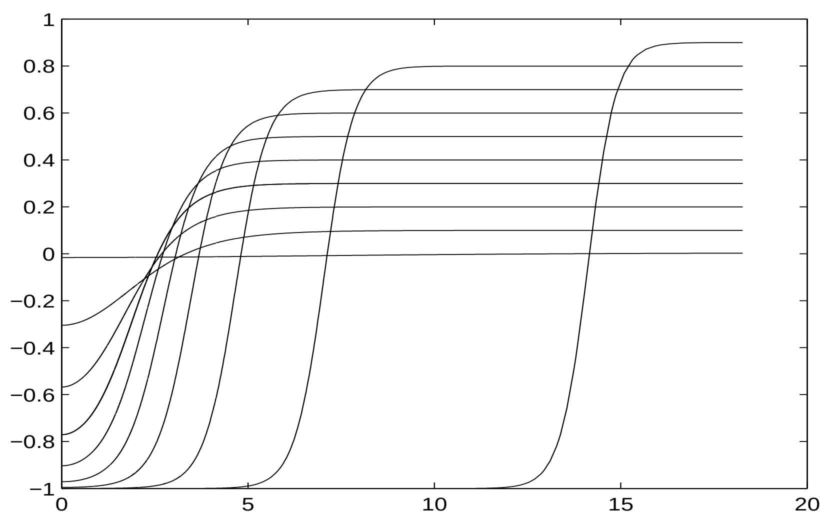

Figure 5: Solution transformed back to $[0, \infty)$, plotted on $[0, 18]$, $\xi = 0.005, 0.1, \ldots, 0.9$

ξ	$\rho(0)$	R
0.005	-0.0159289136828783	13.38832839442030
0.1	-0.3046629136033505	3.321895964695048
0.2	-0.5677637628759243	2.685731314320864
0.3	-0.7707036640421842	2.582331278753935
0.4	-0.9031250928005992	2.720986515873215
0.5	-0.9711193345410850	3.070009104044001
0.6	-0.9953000352050223	3.695885728344484
0.7	-0.9997788979966252	4.816886913795842
0.8	-0.9999995735610771	7.130991634435890
0.9	-0.9999999999999942	14.16875522106554

Table 7: Values computed with 1000 intervals and five Gaussian points. R denotes the *bubble radius*, i. e. $\rho(R) = 0$

3.1.3 Accuracy of the Computed Values

The convergence orders of the numerical approximations appear to be very stable, indicating that our results are reliable and accurate. In this section, we try to quantify the accuracy we can obtain, and also show the differences between the implicit formulation discussed so far and the explicit problem statement (1a), (6) and (7). The experiments reported in this section were computed for $\xi = 0.5$. It turns out that the accuracy of the solution (reflected in the differences between the solution approximations and the number of unaltered digits when the step-size is halved) is similar in both problem formulations. However, the condition numbers of the Jacobian of the collocation equations occurring for the solution approximation accepted by our Newton solver for each step-size, differ significantly. A possible reason why the large discrepancy in condition numbers does not seem to influence the obtained accuracy is given in [10]. Still, it should be advantageous to use the implicit formulation, since bad starting values for the nonlinear equations in conjunction with bad conditioning could lead to a failure of the nonlinear solver to converge at all, and the linear algebra may be unreliable in the presence of large condition numbers. Tables 8–10 give the values of $\rho(0)$, the bubble radius R, the condition numbers and their order as a function of h for the explicit and implicit formulations, and the implicit variant where equation (1a) is explicit with a singularity of the first kind. We observe that the maximally attainable accuracy is of the order of magnitude of round-off error in all cases, even though the condition numbers are $O(1/h^6)$ in the first case and $O(1/h^3)$ in the last case. If (1a) is also multiplied by s, then the condition numbers are $O(1/h^2)$, which is optimal for second order ODEs [1]. Thus, we observe a clear dependence of the condition number of the collocation equations on the order of the singular terms appearing in the equations.

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.454307e−02	6.22	8.369461e−02	5.50
2	3.277156e−04	5.12	1.846019e−03	5.19
3	9.418404e−06	8.22	5.044448e−05	8.18
4	3.154728e−08	5.93	1.737186e−07	5.94
5	5.161539e−10	5.98	2.821679e−09	5.97
6	8.155809e−12	5.99	4.475209e−11	5.99
7	1.277867e−13	5.64	7.011614e−13	5.95
8	2.553513e−15	—	1.126876e−14	—

i	$\rho(0)$	R	$cond\_est_i$	$cond\_conv_i$
1	−0.9595766144502999	2.932241252321063	9.911998e+04	−3.01
2	−0.9712771815045127	3.072004143210495	8.043081e+05	−3.00
3	−0.9711237599349815	3.070093397609374	6.500439e+06	−2.99
4	−0.9711193495594734	3.070010564060050	5.210324e+07	−2.99
5	−0.9711193347866662	3.070009059103224	4.164876e+08	−2.99
6	−0.9711193345449642	3.070009102148822	3.328048e+09	−2.99
7	−0.9711193345411442	3.070009104088092	2.660230e+10	−2.99
8	−0.9711193345410848	3.070009104042217	2.127149e+11	—
9	−0.9711193345410852	3.070009104043983	1.701274e+12	—

Table 8: Conditioning and accuracy for three Gaussian points, implicit formulation (10)

3.2 Numerical Results for the First Order Problem

The computations for the first order problem (2) also worked well with `kollimplizitmix`. Unfortunately it was more difficult to find a suitable initial profile, as there are more equations to solve than in the second order problem, and moreover we also require a guess for the profile of the solution's derivative. Finally, the interior layer is even more pronounced for the variable corresponding to the first derivative. We could not find a first guess containing only straight lines over the whole interval where the Newton solver converged, which does not mean that none exists. But we were successful with straight lines for z_1 and z_2 and a polynomial interpolation of only 3 points for z_3 and z_4, cf. Figure 6, computed with 3 Gaussian collocation points and 10 intervals ($\xi = 0.5$). First, the points $z_3(0) = 0.5, z_3(0.5) = 0, z_3(1) = -1, z_4(0) = 0, z_4(0.5) = 0.5, z_4(1) = 0$ were interpolated by a quadratic polynomial, and subsequently this polynomial was interpolated on 10 subintervals with collocation polynomials defined for three Gaussian points. A plot of the solution found with this starting profile is given in Figure 7. We can use this solution as an initial profile for further computations.

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.454307e−02	6.22	8.369461e−02	5.50
2	3.277156e−04	5.12	1.846019e−03	5.19
3	9.418404e−06	8.22	5.044448e−05	8.18
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5	5.161539e−10	5.98	2.821679e−09	5.97
6	8.155476e−12	5.99	4.475120e−11	5.99
7	1.282308e−13	5.71	7.024936e−13	5.95
8	2.442491e−15	—	1.132427e−14	—

i	$\rho(0)$	R	$cond\_est_i$	$cond\_conv_i$
1	−0.9595766144502999	2.932241252321063	1.431590e+04	−1.98
2	−0.9712771815045126	3.072004143210495	6.631216e+04	−2.00
3	−0.9711237599349814	3.070093397609374	2.715011e+05	−2.00
4	−0.9711193495594735	3.070010564060050	1.095890e+06	−1.99
5	−0.9711193347866661	3.070009059103223	4.395917e+06	−1.99
6	−0.9711193345449644	3.070009102148822	1.759544e+07	−1.99
7	−0.9711193345411442	3.070009104088092	7.038791e+07	−1.99
8	−0.9711193345410848	3.070009104042218	2.815440e+08	—
9	−0.9711193345410850	3.070009104043981	1.126140e+09	—

Table 9: Conditioning and accuracy for three Gaussian points, fully implicit formulation, where (10a) is multiplied by s

3.2.1 Empirical Convergence Orders

To determine the empirical convergence orders for the first order problem with $\xi = 0.5$, we define $z_p^{\{i\}}$, $p = 1, 2$, as the numerical solution computed at $8 \cdot 2^{i-1}$ intervals (exception: one collocation point, where $16 \cdot 2^{i-1}$ intervals are used). Again, we observe the classical convergence orders and even superconvergence is present.

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$	$\|\|z_2^{\{i\}} - z_2^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.454307e−02	6.22	8.369461e−02	5.50
2	3.277156e−04	5.12	1.846019e−03	5.19
3	9.418404e−06	8.22	5.044448e−05	8.18
4	3.154728e−08	5.93	1.737186e−07	5.94
5	5.161540e−10	5.98	2.821680e−09	5.97
6	8.155476e−12	5.99	4.475131e−11	5.99
7	1.282308e−13	5.85	7.022716e−13	5.98
8	2.220446e−15	—	1.110223e−14	—

i	$\rho(0)$	R	$cond\_est_i$	$cond\_conv_i$
1	−0.9595766144502999	2.932241252321063	4.913215e+09	−6.01
2	−0.9712771815045126	3.072004143210495	3.181393e+11	−6.00
3	−0.9711237599349814	3.070093397609374	2.060489e+13	−6.00
4	−0.9711193495594734	3.070010564060050	1.323525e+15	−5.99
5	−0.9711193347866662	3.070009059103223	8.472849e+16	−5.99
6	−0.9711193345449644	3.070009102148822	5.419582e+18	−5.99
7	−0.9711193345411442	3.070009104088092	3.466736e+20	−5.99
8	−0.9711193345410848	3.070009104042218	2.217985e+22	—
9	−0.9711193345410849	3.070009104043982	1.419253e+24	—

Table 10: Conditioning and accuracy for three Gaussian points, explicit formulation (1a), (6), (7)

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	9.607730e−03	2.12
2	2.199805e−03	2.02
3	5.387899e−04	2.00
4	1.340242e−04	2.00
5	3.346432e−05	2.00
6	8.363478e−06	—

i	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
1	5.567328e−02	2.18
2	1.227883e−02	2.04
3	2.970350e−03	2.00
4	7.383994e−04	2.00
5	1.842405e−04	2.00
6	4.604018e−05	—

Table 11: One equidistant collocation point

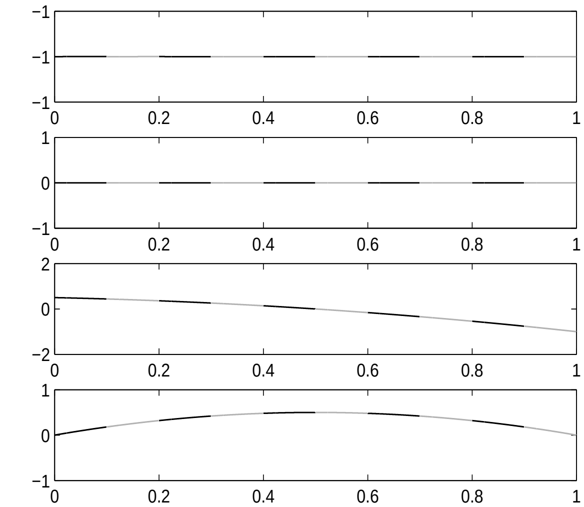

Figure 6: Initial profile: 10 intervals, three Gaussian collocation points

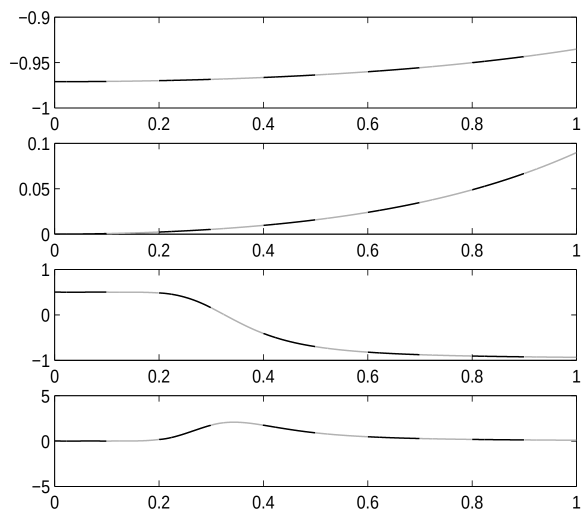

Figure 7: Solution: 10 intervals, three Gaussian collocation points, computed with simple initial profile

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	5.799088e−04	−1.67
2	1.849743e−03	1.53
3	6.365167e−04	1.89
4	1.710856e−04	1.97
5	4.355464e−05	1.99
6	1.093821e−05	—

i	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
1	3.492535e−02	1.58
2	1.165759e−02	1.65
3	3.690005e−03	1.88
4	9.999764e−04	1.98
5	2.530033e−04	1.99
6	6.351223e−05	—

Table 12: Two equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	6.275580e−03	4.45
2	2.861610e−04	4.10
3	1.665095e−05	3.96
4	1.067475e−06	3.99
5	6.713025e−08	3.99
6	4.202072e−09	—

i	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
1	3.027723e−02	4.38
2	1.444260e−03	4.00
3	9.014665e−05	3.96
4	5.771089e−06	3.98
5	3.642802e−07	3.99
6	2.279059e−08	—

Table 13: Three equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.941775e−03	7.40
2	1.737611e−05	2.68
3	2.708693e−06	3.89
4	1.826766e−07	3.97
5	1.163050e−08	3.99
6	7.302531e−10	—

i	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
1	1.492555e−02	6.22
2	1.992681e−04	3.32
3	1.982639e−05	3.95
4	1.277575e−06	3.98
5	8.043811e−08	3.99
6	5.036571e−09	—

Table 14: Four equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	4.033415e−04	5.29
2	1.028982e−05	7.12
3	7.377518e−08	5.94
4	1.196874e−09	5.98
5	1.887557e−11	5.99
6	2.952083e−13	—

i	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.189038e−03	5.36
2	5.315586e−05	6.74
3	4.948354e−07	6.03
4	7.555642e−09	6.00
5	1.175035e−10	5.99
6	1.843414e−12	—

Table 15: Five equidistant collocation points

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$
1	2.955559e−04	4.78
2	1.074934e−05	6.49
3	1.189372e−07	5.96
4	1.900909e−09	5.99
5	2.986944e−11	5.99
6	4.674039e−13	—

i	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
1	1.680902e−03	4.84
2	5.850010e−05	5.98
3	9.258769e−07	5.85
4	1.594605e−08	5.93
5	2.597591e−10	5.99
6	4.081291e−12	—

Table 16: Three Gaussian collocation points

3.2.2 Varying the Value of ξ

For $\xi \in (0, 1)$ we obtain similar values as for the second order problem. However, the solution for $\xi = 0.9$ is more difficult to calculate, so we do not give these results here. Table 17 gives the values of $\rho(0)$ and R for the respective values of ξ. For comparison, we give the values computed for the second order problem in brackets.

ξ	$\rho(0)$	R
0.005	-0.01592891368292191	13.38832839441593
	(-0.0159289136828783)	(13.38832839442030)
0.1	-0.3046629136033470	3.321895964695049
	(-0.3046629136033505)	(3.321895964695048)
0.2	-0.5677637628759235	2.685731314320865
	(-0.5677637628759243)	(2.685731314320864)
0.3	-0.7707036640421850	2.582331278753934
	(-0.7707036640421842)	(2.582331278753935)
0.4	-0.9031250928005982	2.720986515873215
	(-0.9031250928005992)	(2.720986515873215)
0.5	-0.9711193345410835	3.070009104044001
	(-0.9711193345410850)	(3.070009104044001)
0.6	-0.9953000352050234	3.695885728344480
	(-0.9953000352050223)	(3.695885728344484)
0.7	-0.9997788979966253	4.816886913796069
	(-0.9997788979966252)	(4.816886913795842)
0.8	-0.9999995735610769	7.130991634436940
	(-0.9999995735610771)	(7.130991634435890)

Table 17: Values computed with 1000 intervals and five Gaussian points, where R denotes the *bubble radius*, i. e. $\rho(R) = 0$. The values in brackets are the ones computed for the second order problem

3.2.3 Accuracy of the Computed Values

To conclude the presentation of our numerical results, we discuss the attainable accuracy and conditioning of the collocation equations for the first order formulations. Again, the results are computed for $\xi = 0.5$. As for the second order problem, the accuracy is similar for the implicit and explicit formulations, but the order of the condition numbers is different. In this case, we observe condition numbers $O(1/h^2)$ for the implicit formulation where no singular terms appear in the right-hand side of the ODEs. In this case, it is not possible to obtain the optimal rate $O(1/h)$ [1] by choosing an implicit formulation. How this could be effected, or if it is impossible to obtain the optimal results in this case, has to be further investigated. In the explicit formulation (2), (3), the condition numbers are $O(1/h^5)$.

i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
2	2.955559e−04	4.78	1.680902e−03	4.84
3	1.074934e−05	6.49	5.850010e−05	5.98
4	1.189372e−07	5.96	9.258769e−07	5.85
5	1.900909e−09	5.99	1.594605e−08	5.93
6	2.986944e−11	5.99	2.597591e−10	5.99
7	4.674039e−13	6.03	4.081291e−12	5.99
8	7.105427e−15	—	6.394885e−14	—

i	$\rho(0)$	R	$cond\_est_i$	$cond\_conv_i$
2	−0.9712627938698611	3.071620838990447	3.232161e+04	−1.98
3	−0.9711244247561622	3.070238049496702	1.321965e+05	−1.99
4	−0.9711193911408309	3.070002169646523	5.283813e+05	−1.99
5	−0.9711193354454427	3.070009388355330	2.110837e+06	−1.99
6	−0.9711193345552939	3.070009093948309	8.434144e+06	−1.99
7	−0.9711193345413068	3.070009102324399	3.370697e+07	−1.99
8	−0.9711193345410869	3.070009104095078	1.347424e+08	—
9	−0.9711193345410842	3.070009104034930	5.387348e+08	—

Table 18: Three Gaussian points, implicit formulation

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i	$\|\|z_1^{\{i\}} - z_1^{\{i+1\}}\|\|$	$konv\_est_i$	$\|\|z_3^{\{i\}} - z_3^{\{i+1\}}\|\|$	$konv\_est_i$
2	2.955559e−04	4.78	1.680902e−03	4.84
3	1.074934e−05	6.49	5.850010e−05	5.98
4	1.189372e−07	5.96	9.258769e−07	5.85
5	1.900909e−09	5.99	1.594605e−08	5.93
6	2.986955e−11	5.99	2.597591e−10	5.99
7	4.677370e−13	6.13	4.081291e−12	5.99
8	6.661338e−15	—	6.394885e−14	—

i	$\rho(0)$	R	$cond\_est_i$	$cond\_conv_i$
2	−0.9712627938698613	3.071620838990447	2.208019e+09	−4.99
3	−0.9711244247561621	3.070238049496702	7.141985e+10	−4.99
4	−0.9711193911408309	3.070002169646523	2.271353e+12	−4.99
5	−0.9711193354454427	3.070009388355330	7.240639e+13	−4.99
6	−0.9711193345552939	3.070009093948309	2.311632e+15	−4.99
7	−0.9711193345413068	3.070009102324397	7.386262e+16	−4.99
8	−0.9711193345410869	3.070009104095078	2.361397e+18	—
9	−0.9711193345410842	3.070009104034930	7.552049e+19	—

Table 19: Three Gaussian points, explicit formulation

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