

ASC Report No. 11/2016

A Novel Approach to Singular Free Boundary Problems in Ordinary Differential Equations

P.M. Lima, M.L. Morgado, M. Schöbinger and E.B. Weinmüller

Institute for Analysis and Scientific Computing —
Vienna University of Technology — TU Wien
www.asc.tuwien.ac.at ISBN 978-3-902627-05-6

Most recent ASC Reports

- 10/2016 *M. Hanke, R. März, C. Tischendorf, E. Weinmüller, S. Wurm*
Least-Squares Collocation for Higher Index Differential-Algebraic Equations
- 9/2016 *A. Jüngel, P. Shpartko, and N. Zamponi*
Energy-transport models for spin transport in ferromagnetic semiconductors
- 8/2016 *C. Abert, M. Ruggeri, F. Bruckner, C. Vogler, A. Manchon, D. Praetorius, and D. Suess*
Predicting giant magnetoresistance using a self-consistent micromagnetic diffusion model
- 7/2016 *B. Düring, A. Jüngel, and L. Trussardi*
A kinetic equation for economic value estimation with irrationality and herding
- 6/2016 *M. Amrein, J.M. Melenk, and T.P. Wihler*
An hp -adaptive Newton-Galerkin finite element procedure for semilinear boundary value problems
- 5/2016 *M. Gualdani and N. Zamponi*
Spectral gap and exponential convergence to equilibrium for a multi-species Landau system
- 4/2016 *M. Halla*
Regular Galerkin approximations of holomorphic T-Gårding operator eigenvalue problems
- 4/2016 *L. Bian, G. Pang, S. Tang, A. Arnold*
ALmost EXact boundary conditions for transient Schrödinger-Poisson systems
- 2/2016 *A. Jüngel and N. Zamponi*
A cross-diffusion system derived from a Fokker-Planck equation with partial averaging
- 1/2016 *M. Kaltenböck*
Definitizability of normal operators on Krein spaces and their functional calculus

Institute for Analysis and Scientific Computing
Vienna University of Technology
Wiedner Hauptstraße 8–10
1040 Wien, Austria

E-Mail: admin@asc.tuwien.ac.at
WWW: <http://www.asc.tuwien.ac.at>
FAX: +43-1-58801-10196

ISBN 978-3-902627-05-6

© Alle Rechte vorbehalten. Nachdruck nur mit Genehmigung des Autors.



A Novel Computational Approach to Singular Free Boundary Problems in Ordinary Differential Equations

P.M. Lima

*CEMAT, Instituto Superior Técnico, Universidade de Lisboa
Av. Rovisco Pais, 1049 001 Lisboa, Portugal*

M.L. Morgado

Dep. Matemática, Universidade de Trás-os-Montes e Alto Douro, Vila Real, Portugal

M. Schöbinger and E.B. Weinmüller

Institute for Analysis and Scientific Computing, Vienna University of Technology, Vienna, Austria

Abstract

We study the numerical solution of a singular free boundary problem for a second order nonlinear ordinary differential equation, where the differential operator is the degenerate m -Laplacian. A typical difficulty arising in free boundary problems is that the analytical solution may become non-smooth at one boundary or at both boundaries of the interval of integration. A numerical method proposed in [18] consists of two steps. First, a smoothing variable transformation is applied to the analytical problem in order to improve the smoothness of its solution. Then, the problem is discretized by means of a finite difference scheme.

In the present paper, we consider an alternative numerical approach. We first transform the original problem into a special parameter dependent problem sometimes referred to as an ‘eigenvalue problem’. By applying a smoothing variable transformation to the resulting equation, we obtain a new problem whose solution is smoother, and so the open domain MATLAB collocation code `bvpsuite` [16] can be successfully applied for its numerical approximation.

Keywords: Degenerate Laplacian, singular free boundary problem, smoothing variable substitution, collocation methods.

2000 MSC: 65L05,34B16

1. Introduction

Many mathematical models in physics and mechanics can be formulated as the following free boundary problem (FBP): Find a real number $M > 0$ and a positive solution $C^1[0, M] \cap C^2(0, M)$ of the equation

$$(|y'(x)|^{m-2} y'(x))' + \frac{N-1}{x} |y'(x)|^{m-2} y'(x) + f(y(x)) = 0, \quad 0 < x < M, \quad (1)$$

such that y satisfies the boundary conditions

$$y'(0) = 0, \quad y(M) = y'(M) = 0. \quad (2)$$

Email addresses: `plima@math.ist.utl.pt` (P.M. Lima), `luisam@utad.pt` (M.L. Morgado), `e.weinmuller@tuwien.ac.at` (M. Schöbinger and E.B. Weinmüller)

Here, N is the space dimension ($N \geq 2$), $m > 1$, and

$$f(y) = ay^q - by^p, \quad (3)$$

where $p < q$ and $a, b > 0$. For $m = 2$, equation (1) reduces to

$$y''(x) + \frac{N-1}{x} y'(x) + f(y(x)) = 0, \quad 0 < x < M, \quad (4)$$

where the differential operator on the left-hand side corresponds to the radial part of the classical Laplacian operator. In the general case, when $m \neq 2$, this operator becomes the so-called degenerate m -Laplacian. Existence and uniqueness results for the solution of (4) can be found in [11].

This kind of problems arise in the context of radial solutions of

$$\Delta_m y = f(y),$$

in a ball $B(0, M) \subset \mathbb{R}^N$, where $\Delta_m y = \operatorname{div}(|Dy|^{m-2} Dy)$ is the degenerate m -Laplace operator in \mathbb{R}^N .

The FBP with $m = 2$ was extensively studied in the literature. For the case of a smooth forcing function f , the related results can be found in [12, 14, 19, 22]. For results covering singular functions f see [5, 6, 7, 8, 9, 10, 21] and references therein.

It is worth mentioning that a closely related problem was analyzed in the recent paper [23], where the equation

$$\varepsilon^p r^{1-N} (r^{N-1} |\rho'(r)|^{p-2} \rho'(r))' - W'(\rho(r)) = 0, \quad r > 0, \quad (5)$$

was studied. Here, ε is an unknown parameter which has to be determined and the solution of equation (5) has to satisfy the boundary conditions,

$$\rho'(0) = \rho(R) = \rho'(R) = 0, \quad (6)$$

where R is a given constant. Under certain conditions on $W(\rho)$, p , and N , the existence and uniqueness of solutions to (5)–(6) can be shown.

In [18, 20], asymptotical properties of the solution to (1)–(2) were studied in full detail. Special attention was paid to the singularities at $x = 0$ and $x = M$. Asymptotic expansions of the solution at these points have been derived and on their basis, smoothing variable transformations were proposed [18]. Finally, the problem was numerically simulated using a finite difference scheme of order 2.

The aim of the present work is to solve (1)–(2) using the MATLAB solver `bvpsuite` based on high order collocation schemes and designed to deal with difficulties caused by singularities in the differential operators [16]. This code was in [13] applied to solve problems of type (1) posed on unbounded domains.

The first step in solving (1)–(2) is to rewrite (1) for a new variable $z = x/M$,

$$y''(z) + \frac{1}{m-1} \frac{N-1}{z} y'(z) + \frac{1}{m-1} \lambda \frac{f(y(z))}{|y'(z)|^{m-2}} = 0, \quad 0 < z < 1, \quad (7)$$

$$y'(0) = 0, \quad y(1) = y'(1) = 0, \quad (8)$$

where $\lambda = M^m$ is called the eigenvalue. Here, the aim is to find a real number λ , such that a positive solution of equation (7) exists, for which conditions (8) are satisfied. The next step is to apply the smoothing variable transformations [18] to obtain a final parameter dependent boundary value problem (BVP) which will be treated by `bvpsuite`.

The outline of the paper is as follows: In Section 2, we describe the variable transformations used to derive specific models of the form (7)–(8) for the numerical simulations. In Section 3, we describe the code `bvpsuite` in some detail and show that it can be directly applied to our model problems. Finally, numerical results are presented in Section 4 and conclusions in Section 5 complete the article.

2. Variable Substitution

In this article, we consider a function y to be singular (or non-smooth) at a certain point, if the second and higher derivatives of y are unbounded in a neighborhood of this point. Otherwise, we regard the function y to be regular (or smooth).

Several types of singularities may occur in problem (7)–(8). Since equation (7) can be equivalently written as

$$y''(z) = -\frac{1}{m-1} \left(\frac{N-1}{z} y'(z) + \lambda \frac{f(y(z))}{|y'(z)|^{m-2}} \right), \quad 0 < z < 1,$$

we may expect the problem to be singular at the origin due to the division by z in the first term on the right-hand side, and at both endpoints, when $m > 2$, due to the division by $|y'(z)|^{m-2}$ in the second term. On the other hand, the problem may also be singular at $z = 1$, whenever p or q are negative, see (3). Concerning these singularities, the following four different situations arise:

- Case A. If $m \leq 2$ and $p \geq m/2 - 1$: the solution is smooth at both endpoints.
- Case B. If $m \leq 2$ and $p < m/2 - 1$: the solution is regular at $z = 0$ and singular at $z = 1$.
- Case C. If $m > 2$ and $p \geq m/2 - 1$: the solution is singular at $z = 0$ and smooth at $z = 1$.
- Case D. If $m > 2$ and $p < m/2 - 1$: the solution is singular at both endpoints.

In order to provide a better understanding for the techniques used in this paper, we now recall results from [18] describing the asymptotic behaviour of the solutions of (1)–(2) and consequently, (7)–(8), near the singular points. In the following theorem the behaviour of the solutions near the origin is discussed.

Theorem 2.1. *Let $N \geq 2$, $m > 1$, and $-1 < p < q$. For each $y_0 > 0$, problem (1) subject to initial conditions $y(0) = y_0$, $y'(0) = 0$, has, in the neighborhood of $x = 0$, a unique holomorphic solution which can be represented by*

$$y(x, y_0) = y_0 - \frac{m-1}{m} \left(\frac{ay_0^q - by_0^p}{N} \right)^{\frac{1}{m-1}} z^{\frac{m}{m-1}} [1 + g_{0,1}(y_0) x^{\frac{m}{m-1}} + o(x^{\frac{m}{m-1}})], \quad (9)$$

where $g_{0,1}$ is a functions of y_0 that can be obtained by substituting (9) into (1).

Concerning the behaviour of the solutions near $x = M$, we have the following result.

Theorem 2.2. *Let $N \geq 2$, $m > 1$, $-1 < p < q$, and $m-1-p > 0$. For each $M > 0$, problem (1) subject to terminal conditions $y(M) = y'(M) = 0$, has in the neighborhood of $x = M$, a unique holomorphic solution which can be represented by*

$$y(x, M) = \left(\frac{b(m-1-p)^m}{m^{m-1}(m-1)(p+1)} \right)^{\frac{1}{m-1-p}} (M-x)^{\frac{m}{m-1-p}} \left[1 + \sum_{l=0, j=0, l+j \geq 1}^{\infty} G_{l,j} (M-x)^{l+j \frac{m(q-p)}{m-1-p}} \right],$$

where the coefficients $G_{l,j}$ can be uniquely determined.

Note that Theorems 2.1 and 2.2 are formulated for problem (1)–(2), posed on $[0, M]$. Therefore, when applying these results to the problem (7)–(8), we have to restrict our attention to the case $M = 1$. Based on these two results, we now discuss Cases B, C and D in more detail. For each situation, there is a family of variable substitutions which smoothes the solution of the original problem [18]. Since Case D is the most general one, the corresponding family of variable substitutions contains the other ones. The variable substitutions for Case D read:

$$t = \left(1 - (1-z)^{\frac{k_2}{2}} \right)^{\frac{k_1}{2}}, \quad (10)$$

where $k_1 = \min(\frac{m}{m-1}, 2)$ and $k_2 = \min(\frac{m}{m-1-p}, 2)$. After introducing this variable substitution into equation (7), we obtain

$$\begin{aligned} a_1(t) |y'(t)|^{m-2} [b_1(t)y''(t) + c_1(t)y'(t)] + \lambda(ay(t)^q - by(t)^q) &= 0, \\ y'(0) = 0, \quad y(1) = y'(1) = 0, \end{aligned} \tag{11}$$

where

$$\begin{aligned} a_1(t) &= (m-1) \left(\frac{k_1 k_2}{4}\right)^{m-1} t^{\left(1-\frac{2}{k_1}\right)(m-1)} \left(1-t^{\frac{2}{k_1}}\right)^{\left(1-\frac{2}{k_2}\right)(m-1)}, \\ b_1(t) &= \frac{k_1 k_2}{4} t^{1-\frac{2}{k_1}} \left(1-t^{\frac{2}{k_1}}\right)^{1-\frac{2}{k_2}}, \\ c_1(t) &= \frac{1}{4} t^{-\frac{2}{k_1}} \left(1-t^{\frac{2}{k_1}}\right)^{-\frac{2}{k_2}} \left[4-2k_2 + \left(1-t^{\frac{2}{k_1}}\right)(-4+k_1 k_2)\right] + \frac{N-1}{(m-1) \left(1-\left(1-t^{\frac{2}{k_1}}\right)^{\frac{2}{k_2}}\right)}. \end{aligned}$$

Note that in (11) the prime denotes derivation with respect to the new variable t , while it denotes derivation with respect to z in equation (7). The variable substitutions to be applied in Cases B and C are particular cases of (10) with $k_1 = 2$ and $k_2 = 2$, respectively.

3. MATHAB Code `bvpsuite`

We use the open domain MATLAB code `bvpsuite` [16] to solve the model problems designed in Section 4. The basic solver of the code is based on polynomial collocation, a widely used and well-studied standard solution method for two-point BVPs, see for example [1] and the references therein. Moreover, for singular problems, many popular discretization methods like finite differences, Runge–Kutta or multistep methods show order reductions, thus making computations inefficient and prohibiting asymptotically correct error estimation and reliable mesh adaptation. Therefore, in our code development, we have chosen collocation as a high-order, robust, general-purpose numerical method. It is a new version of the general purpose MATLAB code `sbvp`, cf. [3, 15], which has already been successfully applied to a variety of problems, see for example [2, 4, 13, 15, 17]. The code is designed to solve implicit systems of differential equations whose order may vary¹. Here, as an example, we consider the problem

$$F(t, y^{(4)}(t), y^{(3)}(t), y''(t), y'(t), y(t)) = 0, \quad 0 < t \leq 1, \tag{12}$$

$$b(y^{(3)}(0), y''(0), y'(0), y(0), y^{(3)}(1), y''(1), y'(1), y(1)) = 0. \tag{13}$$

Problem (12) may also include unknown parameters to be calculated along with the solution y . In this case, appropriately many additional boundary conditions in (13) need to be prescribed. For this reason the problem at hand is in scope of `bvpsuite` and we can run the code with no further pre-handling.

The numerical approximation defined by collocation is computed as follows: On a grid

$$\Delta := \{\tau_i : i = 0, \dots, L\}, \quad 0 = \tau_0 < \tau_1 < \dots < \tau_L = 1,$$

we approximate each component of the analytical solution by a piecewise defined collocating function

$$p(s) := p_i(s), \quad s \in [\tau_i, \tau_{i+1}], \quad i = 0, \dots, L-1,$$

where we require $p \in C^{q-1}[0, 1]$ if the order of the underlying differential equation (or the highest derivative of the solution component) is $0 \leq q \leq 4$. Here, p_i are polynomials of maximal degree $k-1+q$ which satisfy the system (12) in the *collocation points*,

$$\{t_{i,j} = \tau_i + \rho_j(\tau_{i+1} - \tau_i), \quad i = 0, \dots, L-1, \quad j = 1, \dots, k\}, \quad 0 < \rho_1 < \dots < \rho_k < 1.$$

¹The order can also be zero, which means that algebraic constraints which do not involve derivatives are also admitted.

The associated boundary conditions (13) are also prescribed for p . Classical theory [1] predicts that the convergence order is at least $O(h^k)$, where h is the maximal stepsize, $h := \max_i |\tau_{i+1} - \tau_i|$. The same could be shown for the first order problems with a singularity of the first kind. Quite often, even the superconvergence order, in case of Gaussian points $O(h^{2k})$, can be observed in practice. In our case, the problem consists of a scalar equation which is parameter dependent, subject to linear boundary conditions,

$$F(t, y''(t), y'(t), y(t), \lambda) = 0, \quad 0 < t \leq 1, \quad y'(0) = y'(1) = y(1) = 0.$$

Therefore, we approximate y by a piecewise polynomial function p of a maximal degree $k + 1$, such that $p \in C^1[0, 1]$.

To make the computations more efficient, an adaptive mesh selection strategy based on an a posteriori estimate for the global error of the collocation solution has been implemented.

4. Numerical Examples

4.1. Example 1

As a first example, we consider the case $p = -\frac{1}{2}$, $q = 1$, $a = 1$, $b = 1$, $m = \frac{3}{2}$, and $N = 3$. Then, the original equation (7) has the form

$$y''(z) + \frac{4}{z} y'(z) + 2\lambda \left(y(z) - \frac{1}{\sqrt{y(z)}} \right) \sqrt{|y'(z)|} = 0, \quad (14)$$

and is subject to boundary conditions

$$y'(0) = y'(1) = y(1) = 0.$$

Since $p < m/2 - 1 = -1/4$ and $m < 2$, according to the classification in Section 2, this example corresponds to Case B, where the solution is not smooth at $z = 1$. More precisely, the first derivative of y is continuous at this point but the second and higher derivatives are unbounded, $y \in C^1[0, 1] \cap C^\infty[0, 1)$, cf. Theorem 2.2. Due to this non-smoothness, using `bvpsuite` to solve problem (14) was not successful. The Newton procedure did not converge, even when using starting values lying in a small vicinity of the exact solution. As a remedy, we use a variable substitution (10) with $k_1 = 2$ and $k_2 = 3/2$. This means that we apply $t = 1 - (1 - z)^{\frac{3}{4}}$ to (14) which yields the following modified BVP:

$$\frac{3\sqrt{3}}{16\sqrt{1-t}} y''(t) + \left(\frac{\sqrt{3}}{16(1-t)^{\frac{3}{2}}} + \frac{\sqrt{3}}{(1-t)^{\frac{1}{6}}(1-(1-t)^{\frac{3}{4}})} \right) y'(t) + \lambda \sqrt{|y'(t)|} \left(y(z) - \frac{1}{\sqrt{y(t)}} \right) = 0,$$

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

whose solution is smooth in the whole interval $[0, 1]$, in the sense that $y \in C^2[0, 1]$.

The collocation with one Gaussian point could be successfully applied to solve this problem. The numerical results are shown in Table 1. We list the absolute errors of the approximations for the eigenfunctions and eigenvalues. Since we do not know the exact solution, the errors are computed with respect to the reference solution $y_{ref}(t)$, obtained on a very fine grid with 12.800 subintervals. We calculate the maximal error in y by taking the discrete maximum of $|y(t) - y_{ref}(t)|$ over all grid and collocation points. In both cases, of eigenfunctions and eigenvalues, the numerical results suggest convergence of second order. This is the same convergence order that was obtained when solving the problem using the finite differences method [18]. For higher order collocation methods applied to solve the above model no convergence was observed. This may mean that in this case the algorithm is affected by numerical instability.

The graph of the numerical solution of the modified problem is shown in Figure 1.

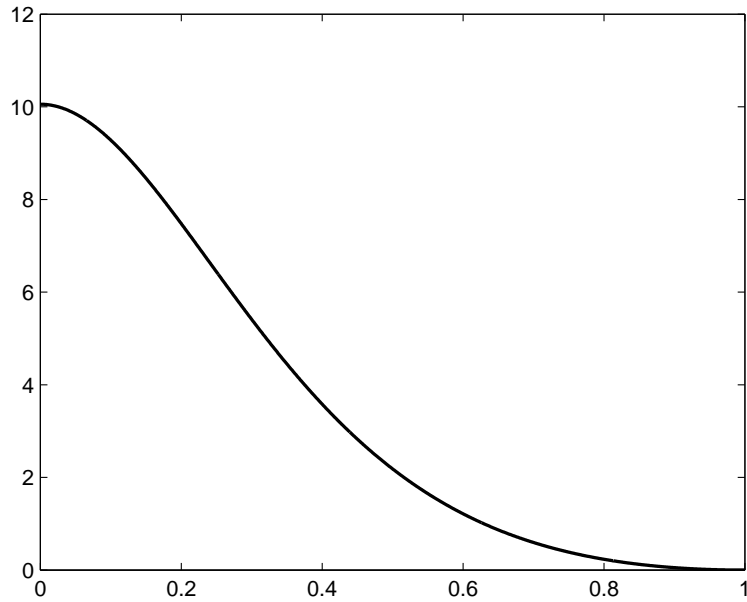


Figure 1: Example 1: Graph of the numerical solution of the modified problem.

| number of subintervals | maximal error in y | rate for y | error in λ | rate for λ |
|------------------------|----------------------|--------------|--------------------|--------------------|
| 101 | 1.4159e-3 | - | 7.7077e-4 | - |
| 201 | 3.7705e-4 | 1.9089 | 2.0018e-4 | 1.9450 |
| 401 | 9.8751e-5 | 1.9329 | 5.1658e-5 | 1.9542 |
| 801 | 2.5368e-5 | 1.9608 | 1.3163e-5 | 1.9725 |
| 1601 | 6.2294e-6 | 2.0258 | 3.2199e-6 | 2.0315 |

Table 1: Example 1: Convergence results for the modified problem based on collocation with one Gaussian point, $k = 1$. The maximal error in y is calculated using all grid and collocation points. The classical convergence order for the global error in y and for the Gaussian points is $O(h^{k+1})$ uniformly in t .

4.2. Example 2

We now consider the case $p = \frac{1}{2}$, $q = 1$, $a = 1$, $b = 1$, $m = 3$, and $N = 3$, where the original BVP has the form

$$y''(z) + \frac{1}{z} y'(z) + \frac{\lambda}{2} \frac{y(z) - \sqrt{y(z)}}{|y'(z)|} = 0, \quad y'(0) = y'(1) = y(1) = 0, \quad (15)$$

and its analytical solution is known,

$$y(z) = \left(2 - 2z^{\frac{3}{2}}\right)^2, \quad \lambda = 216, \quad y \in C^2(0, 1].$$

Since $p = m/2 - 1 = 1/2$ and $m > 2$, see Section 2, this example corresponds to Case C, where the solution is not smooth at $z = 0$. Again, the first derivative of y is continuous at the origin but the second and higher derivatives are unbounded, $y \in C^1[0, 1] \cap C^\infty(0, 1]$, see Theorem 2.1.

In order to deal with the singularity at $z = 0$ and improve the performance of the numerical methods, we introduce a variable substitution with $k_1 = 3/2$ and $k_2 = 2$. Then, according to (10), $t = z^{\frac{3}{4}}$, and (15) reduces to the form

$$\frac{27}{32t} y''(t) + \frac{27}{32t^2} y'(t) + \lambda \frac{y(t) - \sqrt{y(t)}}{|y'(t)|} = 0, \quad y'(0) = y'(1) = y(1) = 0, \quad (16)$$

It is easily seen that the exact solution of (16) is given by

$$y(t) = (2 - 2t^2)^2, \quad \lambda = 216, \quad y \in C^\infty[0, 1].$$

For Example 2, we could solve both, the original and the modified problem. As expected, when applying the collocation method to the modified problem, the accuracy of the results was significantly improved.

We have run the following variants of the collocation method: Collocation with $k = 1, 2, 3$ Gaussian points and $k = 2$ equidistant points. Here, the degree of the corresponding collocation polynomial is always $k + 1$. The performance of these algorithms is illustrated with respect to the numerical approximations of λ in Figure 2. The graphs of the numerical solutions to the original and modified problems are displayed in Figure 3. Note that we are using the same horizontal axis for different independent variables, z , in case of the original problem, and t , in case of the modified one.

4.3. Example 3

This model arises for $p = 1 - \alpha = -\frac{1}{2}$, $q = 1$, $a = 1$, $b = \frac{1}{\alpha} = \frac{2}{3}$, $m = 2$, and $N = 1$, and the original BVP reads:

$$y''(z) + \lambda \left(y(z) - \frac{2}{3\sqrt{y(z)}} \right) = 0, \quad y'(0) = y'(1) = y(1) = 0. \quad (17)$$

As in the previous case, the exact solution is known,

$$y(z) = \left(\frac{8}{3}\right)^{\frac{2}{3}} \left(\cos\left(\frac{\pi}{2}z\right)\right)^{\frac{4}{3}}, \quad \lambda = \left(\frac{2\pi}{3}\right)^2, \quad y \in C^2[0, 1).$$

Since $p < m/2 - 1 = 0$ and $m = 2$, this example again corresponds to Case B, with a solution which is not smooth at $z = 1$. According to Theorem 2.2 the second and higher derivatives of y are unbounded at $z = 1$, $y \in C^1[0, 1] \cap C^\infty[0, 1)$. When the collocation method was applied to solve (17), numerical solutions could be found, but due to the solution structure, the convergence rate was poor.

Here, we choose $k_1 = 2$ and $k_2 = 4/3$ and consequently, see (10), we use the variable substitution $t = 1 - (1 - z)^{\frac{2}{3}}$ to reduce (17) to its modified version,

$$\frac{4}{9(1-t)} y''(t) + \frac{2}{9(t-1)^2} y'(t) + \lambda \left(y(t) - \frac{2}{3\sqrt{y(t)}} \right) = 0, \quad y'(0) = y'(1) = y(1) = 0,$$

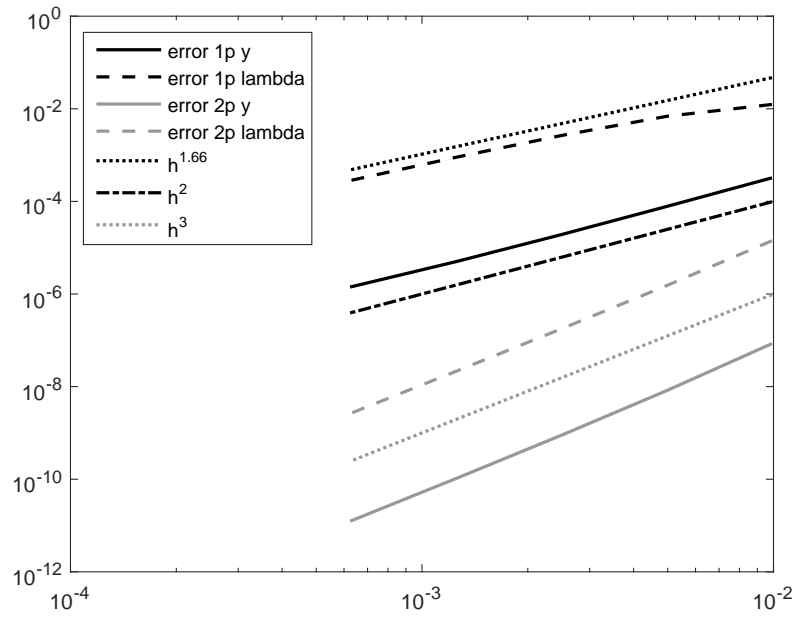


Figure 2: Example 2: Maximal absolute errors in the approximations for the eigenfunction y and in the approximations of the eigenvalue λ plotted as a function of the stepsize. The graphs are related to collocation at one and two Gaussian points.

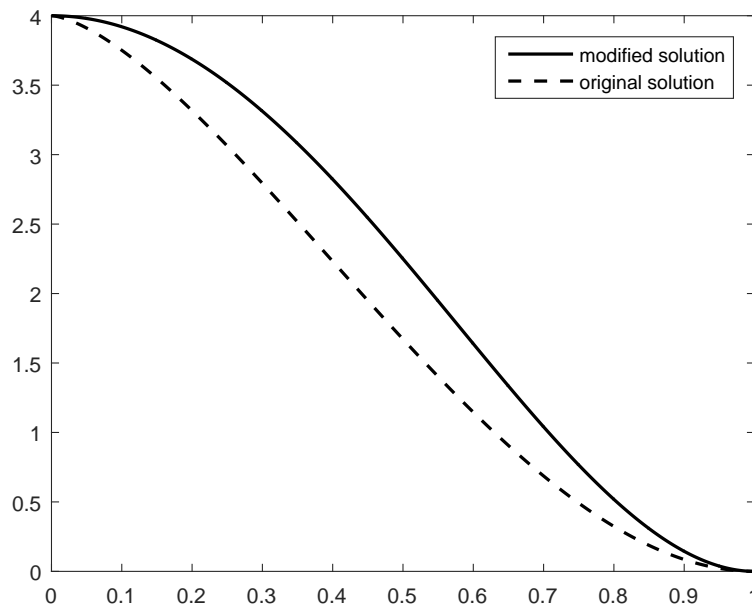


Figure 3: Example 2: Numerical solutions of the original and modified problems.

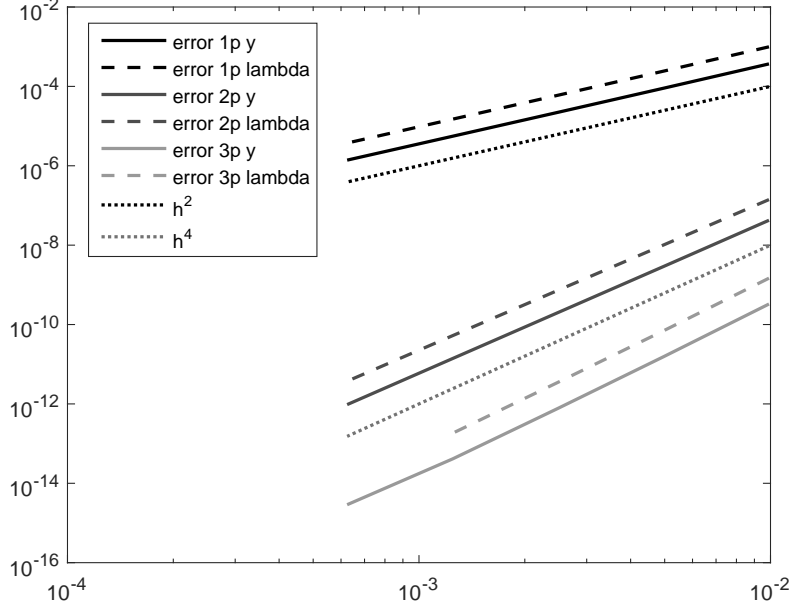


Figure 4: Example 3: Maximal absolute errors in the approximations for the eigenfunction y and in the approximations of the eigenvalue λ plotted as a function of the stepsize. The graphs are related to collocation at one, two, and three Gaussian points.

whose exact solution is

$$y(t) = \left(\frac{8}{3}\right)^{\frac{2}{3}} \left(\cos\left(\frac{\pi}{2}\left(1 - (1-t)^{\frac{3}{2}}\right)\right)\right)^{\frac{4}{3}}, \quad \lambda = \left(\frac{2\pi}{3}\right)^2, \quad y \in C^\infty[0, 1].$$

We observe that the smoothing variable substitution results in a significant improvement of the accuracy of the numerical results. The different variants of the method, specified in Example 2, are compared in Figure 4 and the graphs of the solutions to the original and modified problem can be found in Figure 5.

4.4. Example 4

In the final model, we choose $p = 0$, $q = 1$, $a = 1$, $b = 1$, $m = 3$, and $N = 3$, to obtain

$$y''(z) + \frac{1}{z} y'(z) + \frac{\lambda}{2} \frac{y(z)-1}{|y'(z)|} = 0, \quad y'(0) = y'(1) = y(1) = 0. \quad (18)$$

Here, since $p < m/2 - 1 = 1/2$ and $m > 2$, we deal with Case D, where the solution is not smooth at both interval endpoints. More precisely, $y \in C^1[0, 1] \cap C^\infty(0, 1)$, which means the all higher derivatives are unbounded in the neighborhood of $z = 0$ and $z = 1$, see Theorems 2.1 and 2.2. As in Example 1, the collocation fails to solve the original problem (18) while the modified version of (18) can be solved successfully. In this case, $k_1 = k_2 = 3/2$, and we have to use $t = \left(1 - (1-z)^{\frac{3}{4}}\right)^{\frac{3}{4}}$, to arrive at the modified problem having quite an involved form,

$$\frac{729}{2048t(1-t^{\frac{4}{3}})} y''(z) + \left(\frac{81}{512t^{\frac{2}{3}}(1-t^{\frac{4}{3}})^2} - \frac{243}{2048t^2(1-t^{\frac{4}{3}})} + \frac{81}{128t^{\frac{2}{3}}(1-t^{\frac{4}{3}})^{\frac{2}{3}}(1-(1-t^{\frac{4}{3}})^{\frac{4}{3}})} \right) y'(z) + \lambda \frac{y(z)-1}{|y'(z)|} = 0, \\ y'(0) = y'(1) = y(1) = 0. \quad (19)$$

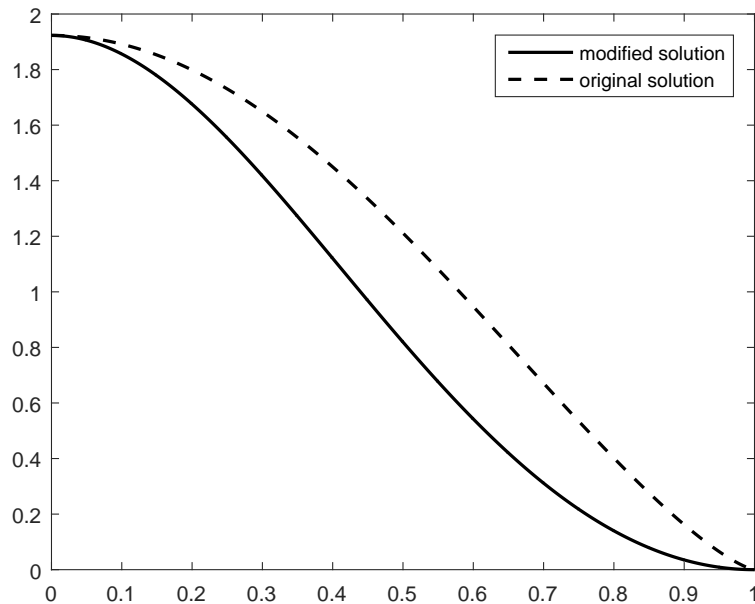


Figure 5: Example 3: Numerical solutions of the original and modified problems.

The solution of the modified problem (19) is smooth on the whole interval $[0, 1]$ and therefore, collocation applied to (19) is more efficient and accurate. The performance of the collocation method with one, two, and three Gaussian points can be found in Figure 6 and the related graph of the numerical solution to the modified problem in Figure 7.

4.5. Summary of the Numerical Results

In the previous section, we discussed the results obtained using collocation method to solve certain models from the class of singular FBPs (1)–(2). In particular, we observed that the performance of the numerical method improves after applying the smoothing variable substitution. To complete the picture, in Table 2, we list the estimated convergence orders for the approximations to the solutions of the modified problems. The orders are estimated using coherent grids with stepsizes $h = 1/100, 1/200, \dots, 1/1600$. The classical convergence order for the Gaussian points is $O(h^{k+1})$ uniformly in t , and for the equidistant points $O(h^k)$ uniformly in t . These orders can be observed in most of the situations, when the solution is sufficiently smooth. Is this not the case, slight order reductions occur, as in Example 4, when two Gaussian points are used. Moreover, we observe, that we may have no convergence in the original formulation, see Example 4, while for the modified problem the method is convergent and produces dependable results. Example 1 seems to be really difficult to solve successfully with methods of higher order. It would be interesting to find out if this is only due to the lack of smoothness in the higher solution derivatives or other reasons.

5. Conclusions

We have implemented a new numerical method for the computation of approximate solutions to singular FBPs in ordinary differential equations. To this end, we used the open domain MATLAB code `bvpsuite`. Our numerical approach is based on smoothing variable transformations which transform the original problem whose solution has endpoint singularities into a new problem, with a solution which is smooth in the whole interval.

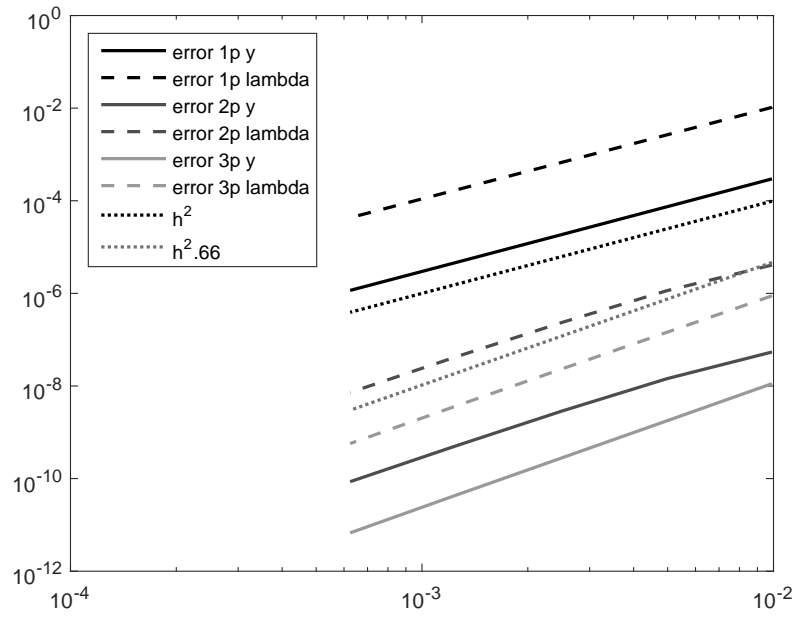


Figure 6: Example 4: Maximal absolute errors in the approximations for the eigenfunction y and in the approximations of the eigenvalue λ plotted as a function of the stepsize. The graphs are related to collocation at one, two, and three Gaussian points.

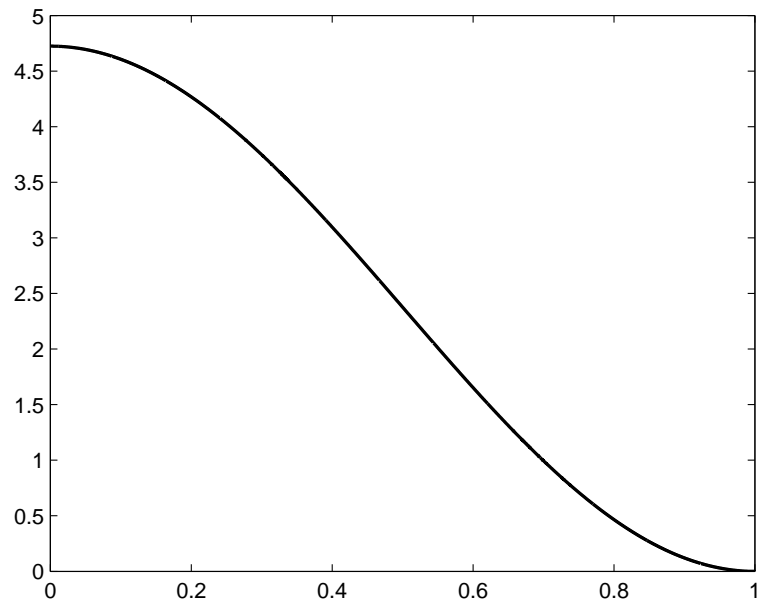


Figure 7: Example 4: Numerical solution of the modified problem.

| | Example 1 | Example 2 | Example 3 | Example 4 |
|--------------------------------|----------------|-----------|-----------|----------------|
| original, Gaussian, $k = 1$ | no convergence | 2 | 1 | no convergence |
| modified, Gaussian, $k = 1$ | 2 | 2 | 2 | 2 |
| modified, Gaussian, $k = 2$ | no convergence | 3.0 | 3.8 | 2.5 |
| modified, equidistant, $k = 2$ | no convergence | 2 | 2 | 2 |

Table 2: Estimated convergence orders for the absolute global errors in the eigenfunctions of the original and modified problems. We used Gaussian and equidistant collocation points. The maximal error is calculated using all grid and collocation points.

As illustrated by the numerical examples, when solving the modified problem the performance of the collocation method is always better than if it is applied to solve the original one. Even in the cases in which the numerical method fails to approximate the original problem, accurate results are obtained after applying the variable transformation.

The numerical simulation suggests that in most of the cases the collocation method, combined with the variable substitution, shows classical convergence order in errors of the solutions and the eigenvalues. Sometimes, it is not possible to recover the optimal convergence order of the collocation method, as it was previously observed in the case of BVPs with the p -Laplacian [13].

This is the case in Examples 1 and 4. It is not surprising, because the solution of the modified problem is smoother than the solution of the original one, but it is not necessarily infinitely smooth. Therefore, it may not be sufficiently smooth to obtain the optimal convergence orders in the case of two or more Gaussian points. In such a case, it should be possible to improve the convergence rate of higher order methods by introducing new types of variable substitutions which further increase the smoothness of the solution. This question is left to future investigations.

Comparing the performance of the present algorithm, based on collocation methods, with the finite difference scheme from [18], we recall that in all examples presented here the finite difference method guarantees second order of convergence. This is the same order that is obtained in the present work, when using one Gaussian point or two equidistant points. By increasing the degree of the collocation polynomial, the accuracy of the approximations can be significantly improved, see Examples 2 and 3. To illustrate this fact, we rerun Example 3 whose solution is in $C^\infty[0, 1]$ using four equidistant and four Gaussian points and observed the convergence order $O(h^4)$ and $O(h^8)$, respectively. The latter order means the full superconvergence order of the Gaussian scheme.

In the future work, we intend to carry out a detailed convergence analysis of the collocation scheme in order to better understand its behaviour.

References

- [1] U. Ascher, R. M. M. Mattheij, and R. D. Russell, *Numerical solution of boundary value problems for ordinary differential equations*, Prentice-Hall, Englewood Cliffs, New York, 1988.
- [2] W. Auzinger, O. Koch, and E.B. Weinmüller, *Efficient collocation schemes for singular boundary value problems*, Numer. Algorithms **31** (2002), 5–25.
- [3] W. Auzinger, G. Kneisl, O. Koch, and E.B. Weinmüller, *A collocation code for boundary value problems in ordinary differential equations*, Numer. Algorithms **33** (2003), 27–39.
- [4] C. J. Budd, O. Koch, and E.B. Weinmüller, *Self-similar blow-up in nonlinear PDEs*, AURORA TR-2004-15 Institute for Analysis and Scientific Computing, Vienna University of Technology, Austria, 2004.
- [5] H. Chen, *Analysis of blow-up for a nonlinear degenerate parabolic equation*, J. Math. Anal. Appl. **192** (1995), 180–193.
- [6] H. Chen, *On a singular nonlinear elliptic equation*, Nonlin. Anal., TMA **29** (1997), 337–345.
- [7] M.G. Crandall, P.H. Rabinowitz, and L. Tartar, *On a Dirichlet problem with a singular nonlinearity*, Comm. PDE **2** (1977), 193–222.
- [8] J.I. Diaz, J.M. Morel, and L. Oswald, *An elliptic equation with singular nonlinearity*, Comm. PDE **12** (1987), 1333–1344.
- [9] A.M. Fink, J.A. Gatica, G.E. Hernandez, and P. Waltman, *Approximation of solutions of singular second order boundary value problems*, SIAM J. Math. Anal. **22** (1991), 440–462.
- [10] J.A. Gatica, V. Olikier, and P. Waltman, *Singular nonlinear boundary value problems for second-order ordinary differential equations*, J. Diff. Eqns **79** (1990), 62–78.
- [11] F. Gazzola, J. Serrin, and M. Tang, *Existence of ground states and free boundary problems for quasilinear elliptic operators*, Advances in Differential Equations **5** (2000), 1–30.

- [12] B. Gidas, W.M. Ni, and L. Nirenberg, *Symmetry and related properties via the maximum principle*, Comm. Math. Phys. **68** (1979), 209–243.
- [13] G. Hastermann, P.M. Lima, M.L. Morgado, and E.B. Weinmüller, *Density profile equation with p -Laplacian: analysis and numerical simulation*, Applied Mathematics and Computation **225** (2013) 550–561.
- [14] H.G. Kaper and M.K. Kwong, *Free boundary problems for Emden-Fowler equations*, Diff. Int. Eqns **3** (1990), 353–362.
- [15] G. Kitzhofer, *Numerical treatment of implicit singular BVPs*, Ph.D. Thesis, Institute for Analysis and Scientific Computing, Vienna University of Technology, Austria, 2013.
- [16] G. Kitzhofer, O. Koch, G. Pulverer, Ch. Simon, and E. Weinmüller, *The new Matlab code `bvpsuite` for the solution of singular implicit BVPs*, J. Numer. Anal. Indust. Appl. Math. **5** (2010), 113–134.
- [17] G. Kitzhofer, O. Koch, P. Lima; and E.B. Weinmüller, *Efficient Numerical Solution of the Density Profile Equation in Hydrodynamics*, J. Sci. Comput. **32** (2007) pp. 411–424.
- [18] P.M. Lima and M.L. Morgado, *Efficient computational methods for singular free boundary problems using smoothing variable substitutions*, J. Comp. Appl. Math. **236** (2012), 2981–2989.
- [19] P.L. Lions, *On the existence of positive solutions of semilinear elliptic equations*, SIAM Rev. **24** (1982), 441–467.
- [20] M.L. Morgado and P.M. Lima, *Numerical solution of a class of singular free boundary problems involving the m -Laplace operator*, J. Comp. Appl. Math. **234** (2010), 2838–2847.
- [21] D. O’Regan, *Existence of positive solutions to some singular and nonsingular second order boundary value problems*, J. Diff. Eqns **84** (1990), 228–251.
- [22] J.A. Smoller and G. Wasserman, *Existence, uniqueness, and nondegeneracy of positive solutions of semilinear elliptic equations*, Comm. Math. Phys. **95** (1984), 129–159.
- [23] P. Takac, *Stationary radial solutions for a quasilinear Cahn-Hilliard model in N space dimensions*, Electr. J. Diff. Eqns., Conf. **17** (2009), 227–254.