

Theory, Solution Techniques and Applications of Singular Boundary Value Problems for Ordinary Differential Equations

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Abstract. In this paper we present an overview of analytical results and numerical methods for singular boundary value problems for ordinary differential equations with a singularity of the first kind. We also comment on some applications where these problems typically occur. Special attention is paid to the analysis of shooting methods, where the associated initial value problems are solved by the acceleration technique known as Iterated Defect Correction (IDeC) based on the backward Euler method, and on direct discretization using collocation schemes. Convergence, error estimation and mesh selection are discussed for both approaches. Moreover, we study the fixed point convergence of the IDeC iteration, where the fixed point corresponds to a collocation solution.

1 Analytical Properties

In this paper, we discuss nonlinear singular boundary value problems of the first order with a singularity of the first kind,

$$z'(t) = \frac{M(t)}{t}z(t) + f(t, z(t)), \quad t \in (0, 1] , \quad (1.1a)$$

$$B_{a2}z(0) + B_{b2}z(1) = \beta_2 , \quad (1.1b)$$

$$z \in C[0, 1] , \quad (1.1c)$$

where z, f are vector-valued functions of dimension n , M is an $n \times n$ matrix¹, B_{a2}, B_{b2} are $r \times n$ matrices and β_2 is a vector of dimension $r \leq n$. Analytical properties of the boundary value problem (1.1) were studied in full detail in [10]. It turns out that (1.1c) reduces to $n-r$ linearly independent conditions that $z(0)$ has to satisfy, and these are suitably augmented by (1.1b) to yield a well-posed problem². Thus, we usually write (1.1) in its equivalent form consisting of (1.1a) and the n linearly independent conditions

$$B_a z(0) + B_b z(1) = \beta . \quad (1.1d)$$

For a well-posed problem we now make the following assumptions:

¹ Throughout the paper we assume $M \in C^1[0, 1]$ and write $M(t) = M + tC(t)$, $C \in C[0, 1]$.

² It should be noted that every solution of a well-posed problem satisfies $Mz(0) = 0$.

1. Equation (1.1) has an isolated solution $z \in C[0, 1] \cap C^1(0, 1]$. With this solution and a $\rho > 0$ we associate the spheres

$$S_\rho(z(t)) := \{y \in \mathbb{R}^n : |z(t) - y| \leq \rho\}$$

and the tube

$$T_\rho := \{(t, y) : t \in [0, 1], y \in S_\rho(z(t))\}.$$

2. $f(t, z)$ is continuously differentiable with respect to z , and $\frac{\partial f(t, z)}{\partial z}$ is continuous on T_ρ .

For this situation, the following smoothness properties hold, for a proof see [10]:

Theorem 1.1. *Let f be p times continuously differentiable on T_ρ and $M \in C^{p+1}[0, 1]$. Then*

1. $z \in C^{p+1}(0, 1]$.
2. If all the eigenvalues of M have nonpositive real parts, then $z \in C^{p+1}[0, 1]$.
3. Let σ_+ denote the smallest of the positive real parts of the eigenvalues of M and n_0 the dimension of the largest Jordan box associated with the eigenvalue 0 in the Jordan canonical form of M . Then the following statements hold:
 - For $p < \sigma_+ < p + 1$, $|z^{(p+1)}(t)| \leq \text{const. } t^{\sigma_+ - p - 1} (|\ln(t)|^{n_0 - 1} + 1)$.
 - For $\sigma_+ = p + 1$, $|z^{(p+1)}(t)| \leq \text{const. } (|\ln(t)|^{n_0} + 1)$.
 - For $\sigma_+ > p + 1$, $z \in C^{p+1}[0, 1]$.

Note that the spectrum of M not only influences the smoothness of the solution of (1.1), but also determines how the boundary conditions have to be chosen to yield a well-posed problem³.

2 Applications

Singular problems arise in a wide range of research fields. Problems as different as the solution of differential equations posed on unbounded intervals (see [8]), the computation of connecting orbits or invariant manifolds for dynamical systems ([17]), differential-algebraic equations ([18]) or Sturm-Liouville eigenvalue problems ([6]), are in the scope of techniques for singular boundary value problems. Our special focus is on two types of applications.

³ In particular, for initial value problems (where $B_b = 0$), the absence of purely imaginary eigenvalues or eigenvalues with positive real parts, is necessary in order to formulate a problem having a unique, continuous solution $z(t)$. In this case, the condition $Mz(0) = 0$ is necessary and sufficient for $z \in C[0, 1]$ and provides $n - r$ linearly independent conditions which the initial value $z(0)$ has to satisfy. Here, r is the dimension of the kernel of M . This solution is unique iff the $r \times r$ matrix $B_{a2}\tilde{E}$ is nonsingular, where \tilde{E} is a basis of the kernel of M . For terminal value problems (where $B_a = 0$), we require the absence of purely imaginary eigenvalues, eigenvalues with negative real parts or a multiple eigenvalue 0, where the associated block in the Jordan canonical form is not diagonal. In that case, we need to pose n linearly independent terminal conditions at $t = 1$ to obtain a unique solution. For a discussion of these special cases of (1.1), see [12].

In the simulation of the run-up and run-out of dry-flowing avalanches, a leading-edge model due to McClung et al., cf. [19], is used to describe the avalanche’s dynamics. This yields an initial value problem for a scalar first order ordinary differential equation with a singularity of the first kind which describes the velocity $v(t)$ of the avalanche’s leading edge. Our aim is the development of an efficient numerical solution method for the associated initial value problem.

The density functional theory developed by Walter Kohn reduces some problems of *computational material science* to the single atom case with a suitably defined external potential, see [4]. In this context, the radial Schrödinger equation has to be solved. This is a singular ordinary differential equation of the second order with a singularity of the first kind, which can be equivalently expressed in the form (1.1a). Here, our main goal is the speed-up of numerical computations by applying approximation methods especially suited for singular problems, as an alternative to the approach currently adopted in standard codes.

3 Shooting Methods and Iterated Defect Correction

It was shown in [14] that shooting methods (see for example [1]) are stable for singular problems and retain the full convergence orders when the associated initial value problems are well-posed. However, this is a severe restriction in case of singularity — it is clear from §1 that a special structure of the spectrum of the matrix M is required (in order to obtain either a well-posed initial or terminal value problem). This means that the shooting approach can only be applied to solve a subclass of the possible problem range.

The crucial point for the numerical realization of these methods is the stable integration of the associated initial value problems, cf. [1]. Moreover, the common choice of shooting points for multiple shooting, see for example [20], may be unfavorable in this case. Whenever shooting points are allowed to approach $t = 0$, order reductions may occur, see [2]. However, when the first shooting point is suitably fixed, the usual strategies for the mesh selection seem to be applicable to the rest of the interval, where the initial value problems can be solved by standard methods like embedded explicit Runge-Kutta pairs. Since many standard methods suffer from order reductions near the singularity, we need a different strategy for the first interval. Our strategy for this region close to the singular point is the so-called “Iterated Defect Correction” Method (IDeC), which we describe below.

Consider (1.1a) with the (well-posed) initial condition $z(0) = \beta \in \ker M$. Moreover, we assume to know a first approximation $z_h^{[0]} := z_h = (z_0, \dots, z_N)$ obtained by some discretization method φ_h on an equidistant grid $\Delta_h := (\tau_0, \dots, \tau_N)$, $\tau_i = ih$, $h = \frac{1}{N}$. If we choose $N = mN_1$ with $m \in \mathbb{N}$ fixed and $N_1 \in \mathbb{N}$, we can use a continuous piecewise polynomial function $p^{[0]}(t)$ of maximal degree m to interpolate $z_h^{[0]}$. Using this interpolating function, we construct a “neighboring problem” associated with the original problem and solved exactly

by $p^{[0]}(t)$,

$$y'(t) = \frac{M(t)}{t}y(t) + f(t, y(t)) + d^{[0]}(t), \quad t \in (0, 1] , \quad (3.1a)$$

$$y(0) = p^{[0]}(0) = \beta , \quad (3.1b)$$

where

$$d^{[0]}(t) := p^{[0]'}(t) - \frac{M(t)}{t}p^{[0]}(t) - f(t, p^{[0]}(t)) . \quad (3.2)$$

The fact that in general $p^{[0]'} \notin C[0, 1]$ does not affect the following considerations. We now solve (3.1) by the same numerical method φ_h and obtain an approximate solution $p_h^{[0]}$ for $p^{[0]}(t)$. This means that for the solution of the neighboring problem (3.1) we know the global error which we can use to estimate the unknown error of the original problem and utilize this information to improve the solution⁴ z_h ,

$$z_h^{[1]} := z_h + \left(R_h(p^{[0]}) - p_h^{[0]} \right) . \quad (3.3)$$

We use these values to define a new interpolating function $p^{[1]}(t)$ by requiring $p^{[1]}(t_j) = z_j^{[1]}$, $j = 0, \dots, N$. Now $p^{[1]}(t)$ is used to define a neighboring problem in the same manner as for (3.1), where again the exact solution is known, and the numerical solution of this neighboring problem yields a further correction of z_h , $z_h^{[2]} := z_h + \left(R_h(p^{[1]}) - p_h^{[1]} \right)$. Clearly, this procedure can be iteratively continued.

If the backward Euler method is used as the basic method φ_h for the IDeC iteration, the level of accuracy of the successive iterates is improved as for regular problems. This result is formulated in the following theorem⁵, cf. [15]:

⁴ $R_h(z) := (z(t_0), \dots, z(t_N))$ for a continuous function z .

⁵ The result implies that we are in a position to use shooting methods in conjunction with IDeC based on the backward Euler method to obtain numerical solutions with an arbitrary convergence order for those problems (1.1) which can be equivalently expressed as initial value problems. Moreover, the successive updates also represent an asymptotically correct error estimate for the previous IDeC iterate which enables error control mechanisms that are robust with respect to the singularity. However, if we used a basic method of higher order, we could hope to apply IDeC even more efficiently: For regular problems, using a Runge-Kutta method of order p results in an order sequence $O(h^p)$, $O(h^{2p})$, \dots . Unfortunately, for singular problems this is not the case. It was shown in [16] that the use of neither the box scheme, the trapezoidal rule nor the computationally cheap forward Euler method yield the desired improvement in the accuracy in general. For terminal value problems, where eigenvalues with positive real parts occur, the size of these eigenvalues influences the order sequences that can be achieved. Under certain circumstances, however, a fixed point property of IDeC makes it possible to compute a high order solution even if the classical order sequence is not observed. This is the subject of §4.

Theorem 3.1. *Consider the IDeC method based on the backward Euler rule and on piecewise interpolation with polynomials of degree m for the numerical solution of a singular initial value problem. For the approximations obtained in the course of the iteration,*

$$\|z_h^{[j]} - R_h(z)\|_h := \max_{0 \leq l \leq N} |z_l^{[j]} - z(t_l)| = O(h^{j+1}), \quad j = 0, \dots, m-1, \quad (3.4)$$

holds provided that f and M are sufficiently smooth. In this case (polynomials of degree m are used for the interpolation), further iteration does not increase the asymptotic order of the approximation in general.

4 Fixed Points of IDeC and Collocation Methods

Apart from considering the asymptotics of IDeC as the discretization parameter h tends to zero, it also seems natural to investigate the asymptotic behavior of the iterates $z_h^{[j]}$ for $j \rightarrow \infty$. This may be especially attractive in the case where the classical improvement of the convergence order (with respect to h) is not observed, but nonetheless the IDeC iterates eventually tend towards a high order solution. Therefore, in this section we study the fixed point property of IDeC based on the backward Euler rule and the box scheme. Here, we do not restrict ourselves to the case of initial value problems, but also consider two-point boundary value problems. The definition of IDeC is fully analogous in this case. First, we require some notation. For a (not necessarily equidistant) grid Δ we assume $N = mN_1$ as in §3. We denote

$$t_i := \tau_{im}, \quad t_{ij} := \tau_{im+j} = t_i + \rho_j(t_{i+1} - t_i), \quad 0 < \rho_1 < \dots < \rho_m \leq 1 \quad (4.1)$$

for $j = 1, \dots, m$, $i = 0, \dots, N_1 - 1$. Fixed points of IDeC can be characterized as follows.

Theorem 4.1. *A grid vector z_h^* is the fixed point of IDeC based on the backward Euler method on an equidistant grid Δ_h iff z_h^* is the solution of a collocation method of order m on a grid of the form (4.1) with $\rho_j = \frac{j}{m}$, $j = 1, \dots, m$. If the box scheme serves as basic method, the same holds with $\rho_j = \frac{2j-1}{2m}$, $j = 1, \dots, m$.*

Proof. Obviously, z_h^* is a fixed point of IDeC iff the defect (3.2) vanishes in the points where the right-hand side of (1.1) is evaluated for the numerical method φ_h . See also [9]. \square

Theorem 4.1 does not state under which circumstances the IDeC iteration indeed approaches a fixed point. The following examples and some theoretical considerations show, however, that we may quite frequently expect such convergence to take place.

Consider the singular boundary value problem

$$z'(t) = \frac{1}{t} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} z(t) + \begin{pmatrix} 0 \\ 3t \cos(t) - t^2 \sin(t) \end{pmatrix}, \quad t \in (0, 1], \quad (4.2a)$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ \sin(1) \end{pmatrix}, \quad (4.2b)$$

with exact solution $z(t) = (z_1(t), z_2(t))^T = (t \sin(t), t \sin(t) + t^2 \cos(t))^T$. Since here the eigenvalues of M are ± 1 , there exists no equivalent well-posed initial value problem, and consequently, Theorem 3.1 is not applicable. Indeed, the order sequence of IDeC based on the backward Euler method and a Zadunaisky polynomial of degree 6 reduces to $O(h)$, $O(h^2)$, $O(h^2)$, \dots , see Table 1. The reasons why such order reductions occur were examined in [16].

Table 1. Order sequence of the backward Euler method for (4.2)

h	err ₀	p_0	err ₁	p_1	err ₂	p_2	err ₃	p_3
0.0833	2.6e-02		8.9e-03		1.0e-03		1.3e-03	
0.0417	1.2e-02	1.09	2.3e-03	1.95	2.1e-04	2.28	3.4e-04	1.89
0.0208	6.0e-03	1.03	5.8e-04	1.98	5.2e-05	1.97	8.7e-05	1.96
0.0104	3.0e-03	1.01	1.4e-04	1.99	1.4e-05	1.85	2.2e-05	1.98

If we continue the IDeC iteration, however, we find that eventually a fixed point is approached. This can be observed in Table 2, where $\|z_h^{[j]} - z_h^{[j-1]}\|_h$ is given for four different step-sizes and some values of j . Note that the fixed point is approached faster for smaller h . From Theorem 4.1 it is clear that this fixed point is a collocation solution with a convergence order $O(h^6)$.

Table 2. Fixed point convergence of the backward Euler method for (4.2)

iterate j	$h = 0.1667$	$h = 0.0417$	$h = 0.0104$	$h = 0.0025$
1	1.3e-01	1.5e-02	3.5e-03	8.6e-04
5	7.0e-03	5.9e-04	3.8e-05	2.4e-06
10	2.3e-04	1.0e-05	6.1e-07	3.8e-08
15	1.4e-05	7.7e-07	4.7e-08	3.0e-09
20	6.7e-07	3.6e-08	2.2e-09	1.4e-10
25	3.5e-08	1.9e-09	1.1e-10	7.2e-12

Tables 3 and 4 give the same information on the order sequence and the fixed point convergence for the problem

$$z'(t) = \frac{1}{t} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(t) - \begin{pmatrix} 0 \\ 9t \cos(3t) + 3 \sin(3t) \end{pmatrix}, \quad t \in (0, 1], \quad (4.3a)$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ \cos(3) \end{pmatrix}, \quad (4.3b)$$

with exact solution $z(t) = (\cos(3t), -3t \sin(3t))^T$. In this case the box scheme is used as the basic method for IDeC. It turns out that the classical order sequence is not observed in this case either, although M has a double eigenvalue 0 and the problem is equivalent to a well-posed initial value problem. Why IDeC fails in this case and even the basic order may be reduced by a logarithmic term (which is apparently the case in Table 3) is explained in [16]. Although the first two

iterations fail to improve the order of the solution (Table 3), we suddenly observe the convergence order $O(h^6)$ after the third iteration step. Table 4 shows that at least in the asymptotic regime a fixed point was reached (up to roundoff errors). It is clear from Theorem 4.1 why the reached level of accuracy is $O(h^6)$ – the fixed point of the iteration coincides with a collocation method of this order.

Table 3. Order sequence of the box scheme for (4.3)

h	err ₀	p_0	err ₁	p_1	err ₂	p_2	err ₃	p_3
0.0833	3.4e-02		1.7e-03		8.8e-05		4.7e-05	
0.0417	1.0e-02	1.70	4.4e-04	1.93	1.3e-05	2.8016	4.6e-07	6.65
0.0208	3.1e-03	1.75	1.1e-04	1.97	3.2e-06	2.0032	6.6e-09	6.13
0.0104	8.9e-04	1.79	2.8e-05	1.99	8.0e-07	1.9905	1.3e-10	5.63

Table 4. Fixed point convergence of the box scheme for (4.3)

iterate j	$h = 0.1667$	$h = 0.0417$	$h = 0.0104$	$h = 0.0025$
1	1.4e-01	1.4e-02	1.2e-03	9.7e-05
2	5.4e-03	6.0e-04	3.8e-05	2.4e-06
3	1.8e-04	1.7e-05	1.1e-06	7.1e-08
4	1.1e-05	2.3e-08	9.0e-11	8.3e-12
5	1.6e-08	2.2e-11	3.7e-12	8.9e-12
6	7.4e-13	1.7e-12	3.9e-12	9.1e-12

Finally, we are going to analyze the application of the IDeC iteration based on the backward Euler method to the linear initial value problem with a constant coefficient matrix,

$$z'(t) = \frac{M}{t}z(t) + f(t), \quad t \in (0, 1] , \quad (4.4a)$$

$$z(0) = \beta . \quad (4.4b)$$

We assume that only one polynomial of degree m is used for the interpolation⁶. We choose a starting vector $z_h^{[0]} = (\beta, z_1^{[0]}, \dots, z_m^{[0]})$, where $\tilde{z}_h^{[0]} := (z_1^{[0]}, \dots, z_m^{[0]})$ are arbitrary vectors. Again we denote by $p^{[0]}(t)$ the interpolant of $z_h^{[0]}$ and define the defect and neighboring problem as in (3.2) and (3.1). We now use the numerical solution $p_h^{[0]}$ of (3.1) to “improve” the solution z_h obtained by the backward Euler method. Using a representation of the solution given in [13], we find

$$z_j^{[1]} = z_j + z_j^{[0]} - p_j^{[0]}$$

⁶ This means that the analysis is relevant for coarse step-sizes, but the behavior near the singularity is described for an arbitrary step-size.

$$\begin{aligned}
&= \sum_{l=1}^j \prod_{k=l}^j \left(I - \frac{M}{k} \right)^{-1} hf(t_l) + z_j^{[0]} + \sum_{l=1}^j \prod_{k=l}^j \left(I - \frac{M}{k} \right)^{-1} \frac{M}{l} z_l^{[0]} - \\
&\quad - \sum_{l=1}^j \prod_{k=l}^j \left(I - \frac{M}{k} \right)^{-1} \sum_{s=0}^m W_{ls} z_s^{[0]}, \quad j = 1, \dots, m, \quad (4.5)
\end{aligned}$$

where the weights W_{ls} are defined in such a way that

$$p^{[0]'}(t_l) = \frac{1}{h} \sum_{s=0}^m W_{ls} z_s^{[0]} .$$

Formula (4.5) describes an affine mapping $\tilde{z}_h^{[0]} \mapsto \tilde{z}_h^{[1]}$. Analogously, we can write

$$\tilde{z}_h^{[j+1]} = S_m(M) \tilde{z}_h^{[j]} + g_m(M) . \quad (4.6)$$

For the analysis of (4.6) we use the usual definition of an analytical matrix function $\varphi(M)$,

$$\varphi(M) = \frac{1}{2\pi i} \int_{\Gamma} \varphi(\lambda) (\lambda I - M)^{-1} d\lambda , \quad (4.7)$$

where Γ is a sufficiently smooth closed positively oriented curve enclosing all eigenvalues of M , cf. [7]. Now, $S_m(\lambda)$ is a matrix defined by⁷

$$(S_m(\lambda))_{ij} = \begin{cases} - \sum_{l=1}^i \prod_{k=l}^i \left(1 - \frac{\lambda}{k} \right)^{-1} W_{lj}, & 1 \leq i < j \leq m, \\ \delta_{ij} - \sum_{l=1}^i \prod_{k=l}^i \left(1 - \frac{\lambda}{k} \right)^{-1} W_{lj} + \prod_{k=j}^i \left(1 - \frac{\lambda}{k} \right)^{-1} \frac{\lambda}{j}, & 1 \leq j \leq i \leq m, \end{cases}$$

and $g_m(\lambda)$ is given by

$$(g_m(\lambda))_j = \sum_{l=1}^j \prod_{k=l}^j \left(1 - \frac{\lambda}{k} \right)^{-1} hf(t_l) - \sum_{l=1}^j \prod_{k=l}^j \left(1 - \frac{\lambda}{k} \right)^{-1} W_{l0} \beta, \quad j = 1, \dots, m .$$

Since M has no eigenvalue with positive real part, Γ can be chosen such that $(1 - \lambda/k)^{-1}$ is analytical for all $k \in \mathbb{N}$ and therefore the above definitions are meaningful. For moderate m (which is the case relevant in practice), the matrix $S_m(\lambda)$ can easily be analyzed. For $m = 2, \dots, 14$ its spectral radius can be computed using MAPLE. It turns out that all eigenvalues of $S_m(\lambda)$ are equal to zero and thus the matrix is nilpotent of index at most m . By computing the Jordan canonical form for $m = 2, \dots, 6$ it could be verified that the index is indeed equal to m . Consequently, using the reasoning from [7, Lemma VII.3.13], it follows that the iteration (4.6) converges to the fixed point

$$\tilde{z}_h^* = \sum_{l=0}^{m-1} S_m^l(M) g_m(M)$$

⁷ Here, δ_{ij} is the Kronecker symbol.

in a finite number of steps⁸ for any starting vector $z_h^{[0]}$.

Fixed point convergence can be also observed for nonlinear problems. As an example consider the “Emden differential equation”,

$$z'(t) = \frac{1}{t} \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} z(t) - \begin{pmatrix} 0 \\ tz_1^5(t) \end{pmatrix}, \quad t \in (0, 1], \quad (4.8a)$$

$$z(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (4.8b)$$

with exact solution $z(t) = (1/\sqrt{1+t^2/3}, -t^2/(3\sqrt{(1+t^2/3)^3}))^T$. In Table 5 the results for the backward Euler method are shown. Note that, according to Theorem 3.1, a 6th order approximation is obtained after 5 steps of the IDeC procedure. The asymptotic quality of further iterates does not improve, and the fixed point (a collocation solution) of the same order $O(h^6)$ is gradually approached.

Table 5. Fixed point convergence of the backward Euler method for (4.8)

iterate j	$h = 0.1667$	$h = 0.0417$	$h = 0.0104$	$h = 0.0025$
1	1.6e-02	5.6e-03	1.5e-03	3.9e-04
2	4.8e-03	4.0e-04	2.6e-05	1.6e-06
3	9.7e-04	1.7e-05	3.4e-07	5.1e-09
4	2.9e-04	3.9e-06	2.0e-08	9.2e-10
5	2.4e-04	4.0e-07	2.5e-10	3.3e-10
6	1.2e-04	4.6e-08	3.3e-11	1.3e-10
7	3.1e-05	7.8e-09	5.9e-12	9.8e-12

5 Collocation Methods

The results presented in the previous section suggest that high order solutions of singular boundary value problems can be obtained by means of an IDeC iteration converging to a collocation solution. In this section we recapitulate convergence results for collocation schemes applied to singular boundary value problems in order to demonstrate their robustness with respect to the singularity.

In [11], polynomial collocation with maximal degree $m \in \mathbb{N}$ for linear singular problems is considered. This means that we seek to approximate the analytical solution by a continuous collocating function $p(t) := p_i(t)$, $t \in [t_i, t_{i+1}]$, $i = 0, \dots, N_1 - 1$, where p_i is a polynomial of maximal degree m , which satisfies the differential equation (1.1a) in a finite number of points which are given as in (4.1), and the boundary conditions (1.1d). The resulting relations are called *collocation*

⁸ We observed that the fixed point is reached after only $m - 1$ iterations if the approximation computed by the backward Euler method, $z_h^{[0]} = z_h$, is used as a starting vector. Moreover, for the general case (1.1) the use of an arbitrary starting vector slows down the convergence to the fixed point, but for small h it still takes place.

equations. In this setting, a convergence order of $O(h^m)$ can be guaranteed for regular problems with appropriately smooth data. However, when the collocation nodes are chosen to satisfy

$$\int_0^1 \tau^l w(\tau) d\tau = 0, \quad l = 0, \dots, \nu < m, \quad w(t) := \prod_{j=1}^m (t - \rho_j), \quad (5.1)$$

even a (super-)convergence order $O(h^{m+\nu+1})$ holds, see [5].

In [11], the treatment is restricted to the case where the initial value problem equivalent to (1.1) is well-posed. For these problems the following theorem holds (n_0 is defined as in Theorem 1.1).

Theorem 5.1. *Let $M \in C^{m+1}[0, 1]$, $f \in C^m[0, 1]$ and let (1.1) have a unique solution. Then, for sufficiently small h , the collocation equations have a unique solution $p(t)$ which satisfies*

$$|p(t) - z(t)| = O(h^m), \quad t \in [0, 1].$$

If in addition $M \in C^{m+2}[0, 1]$, $f \in C^{m+1}[0, 1]$ and (5.1) holds (for $0 \leq \nu < m$), then

$$|p(t) - z(t)| = O(h^{m+1} |\log(h)|^{n_0-1}), \quad t \in [0, 1].$$

The latter estimate cannot be improved in general.

Theoretical results for singular second order problems given in [21] and the experimental evidence in [3], indicate that Theorem 5.1 also holds for a general spectrum of M (with σ_+ sufficiently large) and for nonlinear problems.

Moreover, in [3] a novel estimate of the global error, based on the defect correction idea, is introduced. The numerical solution obtained by a collocation scheme with $\rho_m < 1$ is used to define a neighboring problem similar to (3.1). The original and the neighboring problem are solved using the backward Euler method in the (not necessarily equidistant) points $t_{i,j}$, $j = 1, \dots, m$ and t_{i+1} , $i = 0, \dots, N_1 - 1$, and the difference between these two solutions is used as an estimate of the global error of the collocation solution. Instead of the defect (3.2) evaluated at the points specified above, we use a locally integrated defect⁹ given by

$$\bar{d}_{i,j} := \frac{p(t_{i,j}) - p(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \sum_{k=1}^{m+1} \alpha_{j,k} \left(\frac{M(t_{i,k})}{t_{i,k}} p(t_{i,k}) + f(t_{i,k}, p(t_{i,k})) \right), \quad (5.2)$$

with suitably chosen weights $\alpha_{j,k}$. It turns out that this yields an asymptotically correct error estimate for regular problems, cf. [3]. (The analogous procedure based on the “classical” defect $d(t_{i,j})$ does not provide such a correct estimate.) There is a strong experimental evidence that this is also the case for singular problems and a proof of this result is currently in preparation.

Finally, in [3] we also demonstrate that the error estimate described above can be used as a basis for a mesh selection algorithm that is robust with respect to the singularity.

⁹ Here, we use the shorthand notation $t_{i,m+1} := t_{i+1}$.

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