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Efficient collocation schemes for singular boundary value problems *

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We discuss an error estimation procedure for the global error of collocation schemes applied to solve singular boundary value problems with a singularity of the first kind. This a posteriori estimate of the global error was proposed by Stetter in 1978 and is based on the idea of Defect Correction, originally due to Zadunaisky. Here, we present a new, carefully designed modification of this error estimate which not only results in less computational work but also appears to perform satisfactorily for singular problems. We give a full analytical justification for the asymptotical correctness of the error estimate when it is applied to a general nonlinear regular problem. For the singular case, we are presently only able to provide computational evidence for the full convergence order, the related analysis is still work in progress. This global estimate is the basis for a grid selection routine in which the grid is modified with the aim to equidistribute the global error. This procedure yields meshes suitable for an efficient numerical solution. Most importantly, we observe that the grid is refined in a way reflecting only the behavior of the solution and remains unaffected by the unsmooth direction field close to the singular point.

Keywords: ordinary differential equations, singularity of the first kind, boundary value problems, numerical solution, collocation methods, global error estimation, mesh selection

AMS subject classification: 65L05

1. Introduction

In this paper, we consider the application of collocation methods and different ways to estimate their global error for the following class of nonlinear singular boundary value problems of the first order:

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

$$\widetilde{B}_0 z(0) + \widetilde{B}_1 z(1) = \tilde{\beta}, \tag{1.1b}$$

$$z \in C[0, 1], \tag{1.1c}$$

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where z and f are vector-valued functions of dimension n, M is a smooth $n \times n$ matrix, and $\widetilde{B}_0, \widetilde{B}_1 \in \mathbb{R}^{r \times n}$, $\tilde{\beta} \in \mathbb{R}^r$, $r \leqslant n$ are constant. In the sequel we will often use the shorthand notation

$$F\big(t, z(t)\big) := \frac{M(t)}{t} z(t) + f\big(t, z(t)\big)$$

for the right-hand side of (1.1a).

The analytical properties of (1.1) have been discussed in full detail in [18]. It turns out that the requirement (1.1c) is equivalent to $n - r$ linearly independent conditions which together with (1.1b) are necessary for the problem to be well-posed. Therefore, we usually write (1.1) in its equivalent form consisting of (1.1a) and the n linearly independent conditions

$$B_0 z(0) + B_1 z(1) = \beta. \tag{1.1d}$$

The investigation of numerical methods to be used as a basis for a reliable code taking into account the specific difficulties caused by the singularity is strongly motivated by applications from physics, [6,8] or [9], chemistry, cf. [30], and mechanics (buckling of spherical shells, [7,11]), as well as research activities in related areas, cf. [12,27–29].

Our decision to use collocation for the numerical solution of the underlying boundary value problem was motivated by its advantageous convergence properties (see section 2 for a recapitulation of classical results), whereas in presence of a singularity other direct higher order methods (finite differences) show order reductions and become inefficient. Moreover, the standard acceleration techniques like Iterated Defect Correction or extrapolation based on low-order methods do not work efficiently either, because in general, an asymptotic error expansion in the sense of [32, pp. 21–33] for the basic scheme does not exist, cf. [23].

Shooting methods can be shown to work satisfactorily for singular boundary value problems which can be posed in the form of an associated well-posed initial value problem having the same solution, provided an efficient solver for singular IVPs is available, see [4,24]. A reliable high order solver for singular initial value problems has been proposed in [25] as an alternative to explicit Runge–Kutta methods and multi-step methods, which show order reductions when they are used to solve singular initial value problems, see [19,21]. Unfortunately, it turns out that certain restrictions have to be imposed in order to obtain a well-posed initial value problem: for initial (or terminal) value problems all eigenvalues of the matrix $M(0)$ from (1.1) have to lie in the left (respectively right) half-plane, see [22]. In applications however, problems with a general spectrum are not uncommon and may still yield a well-posed boundary value problem (1.1).

Collocation has been used in one of the best known and established standard codes for (regular) boundary value problems, COLSYS (COLNEW), see [1,2]. In COLSYS, (superconvergent) collocation at Gaussian points is used, cf. [10]. For a restricted[1] class of singular problems, it was shown in [20] that the convergence order of collocation

[1] In [20], the real parts of the eigenvalues of $M(0)$ are assumed to be nonpositive.

methods is at least equal to the *stage order* (see section 2) of the method, but superconvergence cannot be expected in general. By a suitable choice of the collocation nodes, the stage order can be (uniformly) improved by one power of h. These convergence results hold for a wide class of problems (1.1) typically occurring in applications, where $M(0)$ is diagonalizable. For the most general case however, the convergence order may be negatively affected by logarithmic terms. The results for second order problems given in [34] suggest that collocation applied to the general problem (1.1) shows a similar behavior. In the discussion of singular systems, where superconvergence does not hold in general, we restrict our attention to equidistant collocation. The convergence results for these collocation schemes will be recapitulated in section 2. Since it makes sense to generalize the ideas and techniques discussed here to non-equidistant collocation, comments on such a generalization will be made later in the text.

The reason why we propose to control the global error instead of monitoring the local error is the unsmoothness of the local error near the singular point and order reductions from which it often suffers. For an extensive discussion of this phenomenon and numerical experiments, see [16,26]: it turns out that grids generated via the equidistribution of the *local* error are usually very fine close to the singularity even when the solution is very smooth there.

The estimate of the global error we are interested in was proposed in its classical version by Stetter, cf. [33], and is based on an idea due to Zadunaisky, see [35], originally formulated for solutions obtained by Runge–Kutta schemes. This idea also became a basis for the acceleration technique known as *Iterated Defect Correction*, cf. [14,25]. The classical error estimate due to Stetter works satisfactorily at the mesh points (i.e., when the solution values at the collocation points are disregarded) but fails to be asymptotically correct for finer grids including collocation points, see section 3. Here, we propose a modification which enables us to provide an asymptotically correct error estimate for the full grid, enhancing the efficiency of the estimate and the grid flexibility. Experimental results illustrating this approach for singular problems and its analysis for the regular case (where $M \equiv 0$ in (1.1)) can be found in section 4. In section 5, we present an outline of the mesh selection strategy and demonstrate its performance.

Throughout the paper, the following notation is used. We denote by $\mathbb{C}^n$ the space of complex-valued vectors of dimension n and use $|\cdot|$,

$$|x| = \left|(x_1, x_2, \dots, x_n)^{\mathrm{T}}\right| := \max_{1 \leqslant i \leqslant n} |x_i|,$$

to denote the maximum norm in $\mathbb{C}^n$. $C_n^p[0,1]$ is the space of complex vector-valued functions which are p times continuously differentiable on $[0,1]$. For functions $y \in C_n^0[0,1]$, we define the maximum norm,

$$\|y\|_\infty := \max_{0 \leqslant t \leqslant 1} \left|y(t)\right|.$$

$C_{n\times n}^p[0,1]$ is the space of complex-valued $n \times n$ matrices with columns in $C_n^p[0,1]$. Where there is no confusion, we will omit the subscripts n and $n \times n$ and denote $C = C[0,1] = C^0[0,1]$.

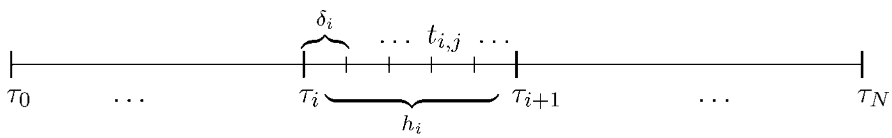

Figure 1. The computational grid.

For the numerical analysis, we define meshes of the form

$$\Delta := (\tau_0, \tau_1, \dots, \tau_N),$$

and $h_i := \tau_{i+1} - \tau_i$, $i = 0, \dots, N-1$, $\tau_0 = 0$, $\tau_N = 1$, $\mathbf{h} := \max_{0 \leqslant i \leqslant N-1} h_i$, and corresponding grid vectors

$$u_\Delta := (u_0, \dots, u_N) \in \mathbb{C}^{(N+1)n}.$$

The norm on the space of grid vectors is given by

$$\|u_\Delta\|_\Delta := \max_{0 \leqslant k \leqslant N} |u_k|.$$

For a continuous function $x(t) \in C[0,1]$, we denote by R_Δ the pointwise projection onto the space of grid vectors,

$$R_\Delta(x) := \big(x(\tau_0), \dots, x(\tau_N)\big).$$

For the collocation, m equidistantly spaced points are inserted in each subinterval $J_i := [\tau_i, \tau_{i+1}]$. This yields the (fine) grid[2]

$$\Delta^m := \big\{t_{i,j} \colon t_{i,j} = \tau_i + j\delta_i,\ i = 0, \dots, N-1,\ j = 0, \dots, m+1\big\}, \tag{1.2}$$

with

$$\delta_i := \frac{h_i}{m+1}. \tag{1.3}$$

For such a grid, u_{Δ^m}, $\|\cdot\|_{\Delta^m}$ and R_{Δ^m} are defined accordingly.

2. Collocation methods

In this section, we recapitulate classical results for the numerical solution of (1.1) obtained by a collocation scheme, cf. [3, pp. 218–226], which are important for the considerations in section 3 and the proof of theorem 4.1. Moreover, some numerical examples are given that illustrate the situation. For reasons explained earlier, we restrict our attention to collocation with continuous piecewise polynomial functions of degree $\leqslant m$ and equidistantly spaced collocation points. We sometimes refer to m as the *stage order* of the collocation method, which is a term commonly used in the context of Runge–Kutta methods (note that collocation schemes are equivalent to certain Runge–Kutta one-step methods). For any collocation method with stage order m, the convergence order is at

[2] For convenience, we denote τ_i by $t_{i,0} \equiv t_{i-1,m+1}$, $i = 1, \dots, N$.

least m. Now, we consider a grid Δ^m given in (1.2) and require the collocating function $p(t) := p_i(t),\ t \in J_i,\ i = 0, \dots, N-1$, where p_i is a polynomial of degree $\leqslant m$, to satisfy

$$p_i'(t_{i,j}) = F\big(t_{i,j}, p_i(t_{i,j})\big), \quad i = 0, \dots, N-1,\ j = 1, \dots, m, \tag{2.1a}$$

$$p_i(\tau_i) = p_{i-1}(\tau_i), \quad i = 1, \dots, N-1, \tag{2.1b}$$

$$B_0 p_0(0) + B_1 p_{N-1}(1) = \beta. \tag{2.1c}$$

For regular problems with sufficiently smooth data, the following convergence result holds (for a proof see [3, pp. 224–226]).

Theorem 2.1. Let $z(t)$ be an isolated solution of (1.1) with $M \equiv 0$. Then for any collocation scheme of the form (2.1) there exist constants $\rho,\ h_0 > 0$ such that the following statements hold for all meshes Δ with $\mathbf{h} \leqslant h_0$:

- There exists a unique solution $p(t)$ of (2.1) in a tube of radius ρ around $z(t)$.
- This solution can be computed by Newton's method which converges quadratically provided that the initial guess $p^{[0]}(t)$ is sufficiently close to $z(t)$.
- The following error estimates hold:

$$\big\| R_\Delta(p) - R_\Delta(z) \big\|_\Delta = \mathrm{O}\big(\mathbf{h}^{m+\nu}\big), \tag{2.2a}$$

$$\| p - z \|_\infty = \mathrm{O}\big(\mathbf{h}^{m+\nu}\big), \tag{2.2b}$$

$$\big\| p^{(l)} - z^{(l)} \big\|_\infty = \mathrm{O}\big(\mathbf{h}^{m+1-l}\big), \quad l = 1, \dots, m, \tag{2.2c}$$

where $\nu = 0$ if m is even and $\nu = 1$ if m is odd.

Earlier theoretical results and numerical experience suggest that the situation in the singular case is more or less the same as in theorem 2.1. In [20], linear problems (1.1) where all eigenvalues of $M(0)$ have nonpositive real parts have been analyzed. In this case there exists a unique solution of the collocation scheme in a tube around the (unique) analytical solution, and the estimates (2.2a) and (2.2b) hold. In the case where $M(0)$ has a multiple eigenvalue 0 and the associated invariant subspace is not the eigenspace of $M(0)$, logarithmic terms may appear in the estimates (2.2) when m is odd. Since additionally for odd m the error estimate proposed in section 4 is not asymptotically correct (even in the case where the full convergence order without logarithmic terms holds) we assume m to be even in the sequel. Investigations for second order problems, cf. [34], indicate that an analogous result holds for a general spectrum of $M(0)$ provided that the positive real parts of the eigenvalues of $M(0)$ are sufficiently large. Numerical experience strongly supports this hypothesis, and the correctness of (2.2c).

Table 1
Uniform convergence of collocation for (2.3), $m = 4$.

h	err	ord	const
5.0000E−01	1.0495E−04		
2.5000E−01	6.7037E−06	3.96E+00	1.64E−03
1.2500E−01	4.2098E−07	3.99E+00	1.69E−03
6.2500E−02	2.6342E−08	3.99E+00	1.71E−03
3.1250E−02	1.6469E−09	3.99E+00	1.72E−03
1.5625E−02	1.0279E−10	4.00E+00	1.73E−03
7.8125E−03	6.1565E−12	4.06E+00	2.22E−03

Table 2
Convergence of first derivative for (2.3), $m = 4$.

h	err	ord	const
5.0000E−01	4.9248E−04		
2.5000E−01	6.3952E−05	2.94E+00	3.79E−03
1.2500E−01	4.1330E−06	3.95E+00	1.53E−02
6.2500E−02	2.7012E−07	3.93E+00	1.48E−02
3.1250E−02	1.7135E−08	3.97E+00	1.66E−02
1.5625E−02	1.0756E−09	3.99E+00	1.75E−02
7.8125E−03	6.7300E−11	3.99E+00	1.79E−02

As an example of our numerical evidence which supports the hypothesis that the convergence behavior stated in theorem 2.1 is also valid for general, nonlinear singular problems, we consider the so-called Emden Differential Equation, cf. [18],

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} z(t) - \begin{pmatrix} 0 \\ t z_1^5(t) \end{pmatrix}, \tag{2.3a}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} z(0) + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} z(1) = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}. \tag{2.3b}$$

The exact solution of this problem is

$$z(t) = \big(z_1(t), z_2(t)\big)^{\mathrm{T}} = \left(\frac{1}{\sqrt{1 + t^2/3}}, \quad -\frac{t^2}{3\sqrt{(1 + t^2/3)^3}} \right)^{\mathrm{T}}.$$

In tables 1–3, the convergence results for the collocation polynomial and its derivatives are given. By h we denote the equidistant step-size of the grid, by ‘err’ the maximal global error of the numerical solution on Δ^m, and ‘ord’ and ‘const’ are the empirical convergence rate and error constant, respectively.

Table 4 demonstrates the convergence of Newton’s method. The value ‘inc’ is the size of the Newton increment, from which the empirical convergence rate ‘ord’ is com-

Table 3
Convergence of second derivative for (2.3), $m = 4$.

h	err	ord	const
5.0000E−01	1.2833E−02		
2.5000E−01	2.7610E−03	2.21E+00	5.96E−02
1.2500E−01	3.4762E−04	2.98E+00	1.74E−01
6.2500E−02	4.4698E−05	2.95E+00	1.63E−01
3.1250E−02	5.6429E−06	2.98E+00	1.75E−01
1.5625E−02	7.0694E−07	2.99E+00	1.82E−01
7.8125E−03	8.8546E−08	2.99E+00	1.83E−01

Table 4
Convergence of Newton iteration for (2.3), $m = 4$, $h = 3.125\text{E–}02$.

inc	err	ord	const
1.1819E+00	3.4647E−02		
3.4445E−02	2.3161E−04		
2.3155E−04	5.9238E−08	1.41E+00	2.71E−02
5.7591E−08	1.6469E−09	1.65E+00	6.18E−02
6.6613E−15	1.6468E−09	1.92E+00	5.71E−01

puted using three consecutive values, and ‘const’ is the associated error constant. Here, ‘err’ denotes the distance between the respective Newton iterates and the exact solution. Again as in the regular case, we observe a convergence order of (approximately) 2. All calculations were carried out in MATLAB 5.3 using IEEE double precision arithmetic.

3. Classical Zadunaisky estimate

The method for the estimation of the global error described in detail later on in this section is based on an idea due to Zadunaisky. In the original version discussed in [13,35], the error estimate for the high-order method is obtained by applying this method twice: to the analytical problem (1.1) first, and to a properly defined ‘neighboring problem’ next. In [15,33], this procedure was modified in order to reduce the amount of computational work: instead of applying the high-order method twice, it is applied only to solve the original problem. Additionally, a computationally cheap low-order method is used to solve the original and the neighboring problem.

This classical version of the error estimate is now described in full detail: we consider the collocation scheme as a one-step method on the mesh Δ. We assume that $N = kN_1$ for a fixed positive integer k and $N_1 \in \mathbb{N}$. Moreover, we require the mesh to be piecewise equidistant. This means that for $j = 0, \ldots, N_1 - 1$, we choose the k step-sizes

$$h_{kj} = h_{kj+1} = \cdots = h_{k(j+1)-1} =: \bar{h}_j. \tag{3.1}$$

The numerical solution $R_\Delta(p)$ obtained by collocation is now interpolated by a continuous piecewise polynomial function $q(t)$, the so-called Zadunaisky polynomial, of degree $\leqslant k$. Using this interpolating function, we construct a neighboring problem,[3]

$$y'(t) = F\big(t, y(t)\big) + d(t), \quad t \in (0, 1], \tag{3.2a}$$

$$B_0 y(0) + B_1 y(1) = \beta, \tag{3.2b}$$

where $d(t)$ is the defect of $q(t)$ with respect to the given problem, i.e.,

$$d(t) := q'(t) - F\big(t, q(t)\big). \tag{3.3}$$

By construction, $q(t)$ is the exact solution of (3.2). If we assume the error in $R_\Delta(p)$ to be small, then we may expect the problems (1.1) and (3.2) and their solutions to be closely related and use the information available from (3.2) to estimate the error of $R_\Delta(p)$. For this purpose, we solve both (1.1) and (3.2) by an auxiliary low-order method to yield ξ_Δ and π_Δ. In our case, we used the backward Euler scheme, i.e.,

$$\frac{\xi_i - \xi_{i-1}}{h_{i-1}} = F(\tau_i, \xi_i), \quad \text{and} \tag{3.4a}$$

$$\frac{\pi_i - \pi_{i-1}}{h_{i-1}} = F(\tau_i, \pi_i) + d(\tau_i) \tag{3.4b}$$

(for $i = 1, \dots, N$, plus boundary conditions). In the following identity, we now substitute the unknown error of ξ_Δ for (1.1) by the known error of π_Δ for (3.2),

$$\begin{aligned} R_\Delta(p) - R_\Delta(z) &= R_\Delta(p) - \xi_\Delta + \big(\xi_\Delta - R_\Delta(z)\big) \\ &\approx R_\Delta(p) - \xi_\Delta + \big(\pi_\Delta - R_\Delta(p)\big) \\ &= \pi_\Delta - \xi_\Delta. \end{aligned} \tag{3.5}$$

This heuristic argument suggests that $\pi_\Delta - \xi_\Delta$ is a reasonable estimate for the global error of the high-order solution $R_\Delta(p)$. For regular problems, this indeed is an asymptotically correct error estimate if the degree[4] k of the polynomial $q(t)$ is chosen as $k = m + 1$. The same holds if $k > m + 1$, but no unnecessarily high degree of the polynomials is used, since the error bound cannot be improved by such a choice. More precisely, for the error in the error estimate the following bound holds:

$$\big\| \big(R_\Delta(p) - R_\Delta(z)\big) - (\pi_\Delta - \xi_\Delta) \big\|_\Delta = \mathrm{O}\big(\mathbf{h}^{m+1}\big). \tag{3.6}$$

This result follows immediately from [15] and standard results for collocation methods and the backward Euler scheme. The crucial tool in the proof is the asymptotic expansion of the global error which exists for both methods if the solution of (1.1) is sufficiently smooth, see [32, pp. 153–157].

[3] Here and in the sequel we use y as a generic variable in the problem setting.

[4] Recall that we assumed m to be even.

For singular problems, numerical experiments indicate a similar behavior of the Zadunaisky estimate. For even m, an asymptotic behavior analogous to (3.6) has been observed except for the case where $M(0)$ has a multiple eigenvalue 0 whose algebraic and geometric multiplicity do not coincide. In this (atypical) case, an order reduction may occur.

We now consider the following linear problem, where $M(0)$ has one positive and one negative eigenvalue:

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 1+\alpha^2 t^2 & 0 \end{pmatrix} z(t) + \begin{pmatrix} 0 \\ ct^{k-1}\mathrm{e}^{-\alpha t}\big(k^2 - 1 - \alpha t(1+2k)\big) \end{pmatrix}, \tag{3.7a}$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ c\mathrm{e}^{-\alpha} \end{pmatrix}, \tag{3.7b}$$

where $\alpha = 40,\ k = 36$ and $c = (\alpha/k)^k \mathrm{e}^k$. The exact solution of (3.7) is given by

$$z(t) = \big(ct^k \mathrm{e}^{-\alpha t}, ct^k \mathrm{e}^{-\alpha t}(k - \alpha t)\big)^{\mathrm{T}}.$$

This serves as an example of our experimental evidence for singular problems which suggests that the classical error estimation procedure described above is asymptotically correct. The empirical rate ‘ord’ of the convergence of the error estimate $\pi_\Delta - \xi_\Delta$ towards the true error $R_\Delta(p) - R_\Delta(z)$ of the numerical solution for this problem is shown in table 5.

At this point, it appears that we have provided an error estimate which can serve as a reliable basis for mesh selection. However, we have completely neglected the information computed at the collocation points. Certainly, it would be more reasonable to integrate these additional abscissae and the corresponding numerical solution values into the error estimation procedure and mesh selection algorithm. Moreover, applying the backward Euler scheme on a finer grid would certainly improve its quality and robustness. We will demonstrate this obvious advantage in section 5.

Table 5
Error of classical Zadunaisky estimate on Δ for (3.7), $m = 4$.

h	err	ord	const
1.0000E−01	7.6792E+03		
5.0000E−02	1.1599E−01	1.60E+01	7.94E+19
2.5000E−02	1.2146E−03	6.57E+00	4.18E+07
1.2500E−02	1.8854E−05	6.00E+00	5.15E+06
6.2500E−03	3.8823E−07	5.60E+00	8.63E+05
3.1250E−03	9.8104E−09	5.30E+00	1.92E+05
1.5625E−03	2.8520E−10	5.10E+00	6.00E+04
7.8125E−04	8.9659E−12	4.99E+00	2.89E+04

The most obvious way to apply the algorithm described above on the grid Δ^m is to carry out the auxiliary scheme in the following form:

$$\frac{\xi_{i,j} - \xi_{i,j-1}}{\delta_i} = F(t_{i,j}, \xi_{i,j}), \quad \text{and} \tag{3.8a}$$

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{\delta_i} = F(t_{i,j}, \pi_{i,j}) + d(t_{i,j}), \tag{3.8b}$$

with $d(t)$ defined as before (cf. (3.3)), for $i = 0, \ldots, N-1$, $j = 1, \ldots, m+1$ (plus boundary conditions). Such a procedure would yield, on the fine grid, an error estimate analogous to (3.5),

$$\pi_{\Delta^m} - \xi_{\Delta^m} \approx R_{\Delta^m}(p) - R_{\Delta^m}(z). \tag{3.9}$$

For given m, we again set $k := m + 1$, and in each subinterval J_i we interpolate the solution values at the m collocation points $t_{i,j}$, $j = 1, \ldots, m$, and at the endpoints τ_i, τ_{i+1}, in order to define $q(t)$.

Unfortunately, this straightforward modification of the scheme fails to provide an asymptotically correct error estimate. Indeed, an order reduction is clearly visible in table 6. Such order reductions are not caused by the singularity but can be observed for regular problems as well.

Two observations indicate why this method fails. In this setting, we have $q(t) \equiv p(t)$ and therefore, it is clear from the definition of $d(t)$ in (3.3) that $d(t)$ vanishes at the collocation points, and so the nontrivial information is transported *only via the mesh points* τ_i, $i = 0, \ldots, N$. Moreover, the proof of the asymptotic correctness of the error estimate (3.6) in Δ relies heavily on the existence of an asymptotic error expansion for the solution of the collocation scheme. It is clear from the estimate (2.2c) however, that such an error expansion can only hold in the mesh points τ_i.

In the procedure described in section 4, the whole grid Δ^m is involved in the interpolation process, and $q(t) \equiv p(t)$. Therefore we use $p(t)$ to denote both, the collocation and the Zadunaisky polynomial.

Table 6
Error of classical Zadunaisky estimate on Δ^m for (3.7), $m = 4$.

h	err	ord	const
5.0000E−01	1.5219E+04		
2.5000E−01	2.0719E−01	1.61E+01	1.11E+09
1.2500E−01	1.1541E−02	4.16E+00	6.67E+01
6.2500E−02	3.7040E−04	4.96E+00	3.49E+02
3.1250E−02	1.5881E−05	4.54E+00	1.09E+02
1.5625E−02	7.0352E−07	4.49E+00	9.30E+01
7.8125E−03	3.4065E−08	4.36E+00	5.45E+01
3.9062E−03	1.8069E−09	4.23E+00	2.88E+01
1.9531E−03	1.0174E−10	4.15E+00	1.78E+01

4. Modified Zadunaisky estimate

We now demonstrate how to overcome the difficulties encountered when using the classical Zadunaisky estimate in the collocation points. A modified defect definition is proposed which is proven to yield an asymptotically correct error estimate for the fine grid Δ^m (including the collocation points, cf. (3.8)) for regular problems. Experimental evidence suggests that this is also the case in presence of a singularity, see, for example, table 7.

We first note that the defect values $d(t_{i,j})$ occurring in the auxiliary equations (3.8b) are simply the residuals of the piecewise polynomial function $p(t)$ with respect to collocation equations of the form

$$y'(t_{i,j}) = F\big(t_{i,j}, y(t_{i,j})\big), \quad i = 0, \dots, N-1, \; j = 1, \dots, m+1, \tag{4.1}$$

where (in contrast to (2.1a)) the set of collocation nodes $t_{i,j}$ includes the right endpoints $\tau_{i+1} = t_{i,m+1}$ of the subintervals J_i. But this way to compute the defect is, in a sense, arbitrary: any collocation scheme of the form (4.1) can be written in different ways, for instance as a Runge–Kutta scheme with $m+1$ stages. Another equivalent formulation of (4.1) closely related to the Runge–Kutta formalism reads (here $y(t_{i,j})$ is denoted by $y_{i,j}$):

$$\frac{y_{i,j} - y_{i,j-1}}{\delta_i} = \sum_{k=1}^{m+1} \alpha_{j,k} F(t_{i,k}, y_{i,k}), \quad j = 1, \dots, m+1 \tag{4.2}$$

for each subinterval J_i, $i = 0, \dots, N-1$. The coefficients $\alpha_{j,k}$ are given by

$$\alpha_{j,k} = \begin{cases} (m+1)a_{1,k}, & j = 1, \\ (m+1)(a_{j,k} - a_{j-1,k}), & j = 2, \dots, m+1, \end{cases} \tag{4.3}$$

where $a_{j,k}$ are the entries of the corresponding Butcher array A, cf. [3, p. 69]. Note that the way that the first derivative y' is discretized is exactly the same in (4.2) and in the auxiliary scheme (3.8a).

Table 7
Error of modified Zadunaisky estimate for (3.7), $m = 4$.

h	err	ord	const
5.0000E−01	4.6855E+03		
2.5000E−01	2.1014E−01	1.44E+01	1.04E+08
1.2500E−01	3.5597E−03	5.88E+00	7.32E+02
6.2500E−02	8.9340E−05	5.31E+00	2.25E+02
3.1250E−02	1.8280E−06	5.61E+00	5.09E+02
1.5625E−02	4.1862E−08	5.44E+00	2.90E+02
7.8125E−03	1.1476E−09	5.18E+00	9.86E+01
3.9062E−03	3.7286E−11	4.94E+00	3.00E+01
1.9531E−03	1.1600E−12	5.00E+00	4.24E+01

Now, as an alternative to the classical approach, we compute the defect with respect to (4.2), which means that (3.8b) is replaced by

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{\delta_i} = F(t_{i,j}, \pi_{i,j}) + \bar{d}_{i,j}, \tag{4.4}$$

with the modified defect

$$\bar{d}_{i,j} := \frac{p(t_{i,j}) - p(t_{i,j-1})}{\delta_i} - \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, p(t_{i,k})\big). \tag{4.5}$$

All other algorithmic details remain unchanged.

We now prove the asymptotic correctness of the modified error estimate $\pi_{\Delta^m} - \xi_{\Delta^m}$, where π_{Δ^m} is defined by (4.4) and ξ_{Δ^m} by (3.8a), for the regular case where $M \equiv 0$ in (1.1), that is

$$z'(t) = f\big(t, z(t)\big), \quad t \in [0, 1], \tag{4.6a}$$

$$B_0 z(0) + B_1 z(1) = \beta, \tag{4.6b}$$

with f sufficiently smooth.

Remark. The analysis of the singular case is the subject of current investigations. In order to proceed in a similar way to extend theorem 4.1 to that case, special techniques have to be developed.

Theorem 4.1. Assume that the boundary value problem (4.6) has a unique (sufficiently smooth) solution. Then the following estimate holds:

$$\big\| \big(R_{\Delta^m}(p) - R_{\Delta^m}(z)\big) - (\pi_{\Delta^m} - \xi_{\Delta^m}) \big\|_{\Delta^m} = \mathrm{O}\big(\mathbf{h}^{m+1}\big). \tag{4.7}$$

Proof. Let

$$\varepsilon_{\Delta^m} := \xi_{\Delta^m} - R_{\Delta^m}(z), \qquad \bar{\varepsilon}_{\Delta^m} := \pi_{\Delta^m} - R_{\Delta^m}(p), \tag{4.8}$$

then the quantity to be estimated is

$$\big(R_{\Delta^m}(p) - R_{\Delta^m}(z)\big) - (\pi_{\Delta^m} - \xi_{\Delta^m}) = \varepsilon_{\Delta^m} - \bar{\varepsilon}_{\Delta^m}.$$

Here, ε_{Δ^m}, the error of the backward Euler scheme applied to the original problem, satisfies

$$\begin{aligned} \frac{\varepsilon_{i,j} - \varepsilon_{i,j-1}}{\delta_i} &= f(t_{i,j}, \xi_{i,j}) - \frac{z(t_{i,j}) - z(t_{i,j-1})}{\delta_i} \\ &= f(t_{i,j}, \xi_{i,j}) - \sum_{k=1}^{m+1} \alpha_{j,k} f\big(t_{i,k}, z(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big). \end{aligned} \tag{4.9}$$

This follows from (3.8a) and from the fact that the truncation error of the exact solution $z(t)$ with respect to the modified Runge–Kutta equations (4.2) is $\mathrm{O}(\mathbf{h}^{m+1})$. Moreover, $\bar{\varepsilon}_{\Delta^m}$ satisfies

$$\frac{\bar{\varepsilon}_{i,j} - \bar{\varepsilon}_{i,j-1}}{\delta_i} = f(t_{i,j}, \pi_{i,j}) + \bar{d}_{i,j} - \frac{p(t_{i,j}) - p(t_{i,j-1})}{\delta_i}$$
$$= f(t_{i,j}, \pi_{i,j}) - \sum_{k=1}^{m+1} \alpha_{j,k} f\big(t_{i,k}, p(t_{i,k})\big) \tag{4.10}$$

due to (4.4) and (4.5). Both (4.9) and (4.10) hold for $i = 0, \dots, N-1$, $j = 1, \dots, m+1$, and ε_{Δ^m} as well as $\bar{\varepsilon}_{\Delta^m}$ satisfies homogeneous boundary conditions.

In order to proceed, we use Taylor's theorem to conclude that

$$f(t_{i,j}, \xi_{i,j}) - f\big(t_{i,j}, z(t_{i,j})\big) = \int_0^1 \frac{\partial}{\partial y} f\big(t_{i,j}, z(t_{i,j}) + \tau\big(\xi_{i,j} - z(t_{i,j})\big)\big)\,\mathrm{d}\tau \cdot \varepsilon_{i,j}$$
$$=: A(t_{i,j})\varepsilon_{i,j}, \tag{4.11}$$

and analogously,

$$f(t_{i,j}, \pi_{i,j}) - f\big(t_{i,j}, p(t_{i,j})\big) =: \bar{A}(t_{i,j})\bar{\varepsilon}_{i,j}. \tag{4.12}$$

Here,

$$\bar{A}(t_{i,j})\bar{\varepsilon}_{i,j} = A(t_{i,j})\bar{\varepsilon}_{i,j} + \big(\bar{A}(t_{i,j}) - A(t_{i,j})\big)\bar{\varepsilon}_{i,j} = A(t_{i,j})\bar{\varepsilon}_{i,j} + \mathrm{O}\big(\mathbf{h}^{m+1}\big).$$

The latter representation follows from $p(t) - z(t) = \mathrm{O}(\mathbf{h}^m)$ and the facts that

$$\bar{d}_{i,j} = \mathrm{O}\big(\mathbf{h}^m\big) \Longrightarrow \xi_{i,j} - \pi_{i,j} = \mathrm{O}\big(\mathbf{h}^m\big)$$

and

$$\varepsilon_{i,j} = \mathrm{O}\big(\mathbf{h}\big), \qquad \bar{\varepsilon}_{i,j} = \mathrm{O}(\mathbf{h}).$$

Now we use (4.11), (4.12) to rewrite (4.9), (4.10) and obtain

$$\frac{\varepsilon_{i,j} - \varepsilon_{i,j-1}}{\delta_i} = A(t_{i,j})\varepsilon_{i,j} + f\big(t_{i,j}, z(t_{i,j})\big) - \sum_{k=1}^{m+1} \alpha_{j,k} f\big(t_{i,k}, z(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big), \tag{4.13}$$

and

$$\frac{\bar{\varepsilon}_{i,j} - \bar{\varepsilon}_{i,j-1}}{\delta_i} = A(t_{i,j})\bar{\varepsilon}_{i,j} + f\big(t_{i,j}, p(t_{i,j})\big) - \sum_{k=1}^{m+1} \alpha_{j,k} f\big(t_{i,k}, p(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big). \tag{4.14}$$

(4.13) and (4.14) are a pair of 'parallel' backward Euler schemes, with related inhomogeneous terms. The difference of these terms can be written as

$$\phi(t_{i,j}) - \sum_{k=1}^{m+1} \alpha_{j,k}\phi(t_{i,k}) + \mathrm{O}\big(\mathbf{h}^{m+1}\big), \tag{4.15}$$

where we use the shorthand notation $\phi(t) := f(t, p(t)) - f(t, z(t))$. It is clear from (4.2) that $\sum_{k=1}^{m+1} \alpha_{j,k} = 1$ for all j, and therefore the sum of the coefficients in the weighted sum $\phi(t_{i,j}) - \sum_{k=1}^{m+1} \alpha_{j,k}\phi(t_{i,k})$ is equal to zero. Taylor expansion of $\phi(t_{i,k})$ about $t_{i,j}$ now yields

$$\left|\phi(t_{i,j}) - \sum_{k=1}^{m+1} \alpha_{j,k}\phi(t_{i,k})\right| \leqslant \mathcal{C}\delta_i \max_{\tau_i \leqslant t \leqslant \tau_{i+1}} \left|\phi'(t)\right| \tag{4.16}$$

with a constant $\mathcal{C}$ (the data function $f(t, y)$ is assumed to be sufficiently smooth), and the total derivative

$$\begin{aligned}\phi'(t) &= \frac{\partial}{\partial t} f\big(t, p(t)\big) - \frac{\partial}{\partial t} f\big(t, z(t)\big) + \frac{\partial}{\partial y} f\big(t, p(t)\big)p'(t) - \frac{\partial}{\partial y} f\big(t, z(t)\big)z'(t) \\ &= \frac{\partial}{\partial t} f\big(t, p(t)\big) - \frac{\partial}{\partial t} f\big(t, z(t)\big) + \frac{\partial}{\partial y} f\big(t, p(t)\big)p'(t) - \frac{\partial}{\partial y} f\big(t, z(t)\big)p'(t) \\ &\quad + \frac{\partial}{\partial y} f\big(t, z(t)\big)p'(t) - \frac{\partial}{\partial y} f\big(t, z(t)\big)z'(t).\end{aligned} \tag{4.17}$$

Finally, the following bound for the expression from (4.15) follows:

$$\mathcal{C}\mathbf{h}\|p - z\|_\infty + \mathcal{C}\mathbf{h}\big(\|p - z\|_\infty + \|p' - z'\|_\infty\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big) = \mathrm{O}\big(\mathbf{h}^{m+1}\big), \tag{4.18}$$

since the error $p - z$ of the collocation polynomial p satisfies $\|p - z\|_\infty = \mathrm{O}(\mathbf{h}^m)$ and $\|p' - z'\|_\infty = \mathrm{O}(\mathbf{h}^m)$, cf. (2.2).

Stability of the backward Euler method (see [3, p. 201]) now yields

$$\|\bar{\varepsilon}_{\Delta^m} - \varepsilon_{\Delta^m}\|_{\Delta^m} = \mathrm{O}(\mathbf{h}^{m+1}), \tag{4.19}$$

and this completes the proof. □

Remarks.

- The definition of the defect via (4.5) is essential for the above proof: if we used the classical variant $d(t_{i,j})$ instead of $\bar{d}_{i,j}$, the right-hand side of (4.14) would contain the inhomogeneous term
$$p'(t_{i,j}) - \frac{p(t_{i,j}) - p(t_{i,j-1})}{\delta_i}.$$
Thus in the term corresponding to (4.15), the difference
$$(p' - z')(t_{i,j}) - \frac{(p - z)_{i,j} - (p - z)_{i,j-1}}{\delta_i}$$
would appear. In contrast to (4.18), however, this latter difference can only be estimated by $\mathcal{C}\mathbf{h}\|p'' - z''\|_\infty = \mathbf{h}\mathrm{O}(\mathbf{h}^{m-1}) = \mathrm{O}(\mathbf{h}^m)$, cf. (2.2c) for $l = 2$.
- A further remarkable advantage of the modified estimate is the fact that it can also be successfully applied in the case of non-equidistant collocation nodes. This is obvious from the above proof where the distribution of these nodes is of no relevance.

Consequently, the benefits of this method of error estimation could be utilized in the case of regular boundary value problems as well, when superconvergent collocation schemes are used.

- Due to theorem 4.1 it is easy to provide an asymptotically correct error estimate uniformly in t.
- There is strong experimental evidence that the result of theorem 4.1 also holds in the singular case if 0 is not a multiple eigenvalue of $M(0)$. We illustrate this behavior in table 7 by applying the modified error estimate for problem (3.7), see also table 6. In table 7, 'err' denotes the error of the error estimate, that is the quantity estimated in (4.7), and 'ord' and 'const' are the empirical convergence order and associated error constant computed from two successive values of 'err'.

5. Mesh selection

In this section, we show that the global error estimate from section 4 can serve as a reliable basis for a mesh selection algorithm, where the grid is adapted to approximately equidistribute the global error. Moreover, we demonstrate how the algorithm compares to the classical error estimate from section 3 in robustness, efficiency and flexibility. First, we will outline the main features of the mesh selection strategy and point out some measures we took to improve the reliability of the algorithm without going into details of the actual implementation. The main ideas are related to considerations from [31], where the equidistribution of the *global* error based on estimates for the *local* error is studied.

The basic steps of the algorithm are described in a general manner without distinguishing which of the possible error estimates, classical Zadunaisky from section 3 or modified Zadunaisky from section 4, is involved. The aim is to determine a mesh Δ_{TOL} (for the modified estimate it would be more consequent to write Δ^m_{TOL}, but for simplicity we use one notation throughout the section) on which the estimate of the error of the basic solution $R_{\Delta_{\mathrm{TOL}}}(p)$ is approximately equidistributed and satisfies a prescribed (mixed) tolerance[5] TOL.

Algorithm 5.1.

1. Choose the polynomial degree $m \in \{2, 4, 6, 8\}$ in dependence of the tolerance.
2. On a first mesh Δ_0, compute at every mesh point an estimate $\mathcal{E}_{\Delta_0}$ for the global error of the basic solution $R_{\Delta_0}(p)$. The default value for the step-size in the starting grid is $h_i \equiv h = \sqrt[m]{\mathrm{TOL}}$, cf. [17, p. 182]. At this point there are three possible situations.
   (a) The tolerance is satisfied. In this case, the solution is accepted and the algorithm stops.

[5] For a mixed tolerance two tolerance parameters, for the absolute and the relative error, are prescribed and the tolerance control also involves the values of the approximate solution. For simplicity, however, we only write TOL when checking against the tolerance.

(b) The relative error estimate is larger than 1. In this case, the error estimate is considered unreliable, a new refined grid is proposed and the algorithm restarts.

(c) The level of the error estimate is reasonable but the tolerance is not satisfied. In this case, the algorithm continues with step 3.

3. Using the error estimate $\mathcal{E}_{\Delta_0}$, define a *monitor function* Θ_{Δ_0} which measures the error in a way suitable for the equidistribution. We used $\Theta_i(\mathcal{E}_{\Delta_0}) = \sqrt[m]{|\mathcal{E}_i|}$, $i = 0, \dots, N$, when the basic solution was computed by a collocation method of (global) order m. The defect, some derivative of the solution, or the arclength may also be a reasonable choice for such a monitor function, cf. [31]. As a precaution to stabilize the algorithm, a locally smoothed version of the monitor function was used,

$$\widetilde{\Theta}_i := \max\{\Theta_i, \overline{\Theta}_i\}, \quad i = 0, \dots, N,$$

where

$$\overline{\Theta}_i := \frac{1}{\min\{N, i+s\} - \max\{0, i-s\} + 1} \sum_{l=\max\{0,i-s\}}^{\min\{N,i+s\}} \Theta_l$$

with $s \in \mathbb{N}$. Experiments suggested the choice $2 \leqslant s \leqslant N/20$.

4. Compute the integral of a piecewise linear function $\widetilde{\Theta}(t)$ interpolating $\widetilde{\Theta}_{\Delta_0}$ on the interval [0, 1],

$$I := \int_0^1 \widetilde{\Theta}(t)\,\mathrm{d}t = \sum_{l=0}^{N-1} \frac{\widetilde{\Theta}_{l+1} + \widetilde{\Theta}_l}{2} (\tau_{l+1} - \tau_l).$$

Note that this is equivalent to applying the trapezoidal rule for the approximation of the integral of any function interpolating $\widetilde{\Theta}_{\Delta_0}$. Using I, determine a new mesh $\bar{\Delta} = (\bar{\tau}_0, \dots, \bar{\tau}_{\overline{N}})$ such that the contribution to the integral of the monitor function is the same for each subinterval $\bar{J}_i := [\bar{\tau}_i, \bar{\tau}_{i+1}]$, that is

$$\int_{\bar{\tau}_i}^{\bar{\tau}_{i+1}} \widetilde{\Theta}(t)\,\mathrm{d}t = \frac{I}{\overline{N}}, \quad i = 0, \dots, \overline{N} - 1.$$

Since the tolerance TOL is to be satisfied, choose

$$\overline{N} \geqslant N \frac{I}{\sqrt[m]{\mathrm{TOL}}},$$

in such a way that the resulting mesh is suitable for interpolation by the Zadunaisky polynomial, i.e. $\overline{N} = (m+1)N_1$ for suitable $N_1 \in \mathbb{N}$.

5. Compute the numerical solution and the error estimate on the new mesh. For this step, a piecewise constant grid for interpolation with the Zadunaisky polynomial is required. Thus, we fix the points $\tau_{l(m+1)}$, $l = 0, \dots, N_1$, and insert m equidistant

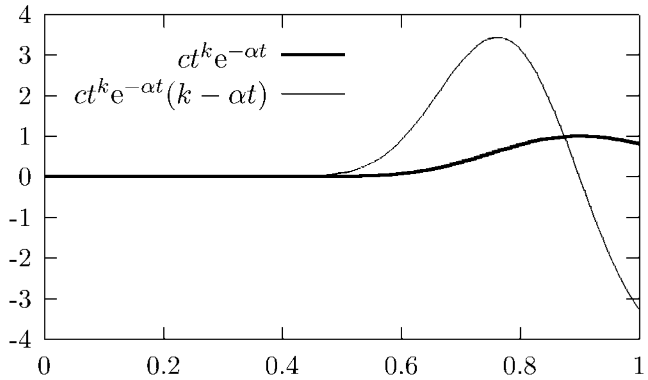

Figure 2. Exact solution of (3.7).

points in the resulting intervals.[6] Moreover, to enhance the stability on the new grid additional intervals are inserted whenever

$$\frac{\max_{0\leqslant i\leqslant \overline{N}-1} h_i}{\min_{0\leqslant i\leqslant \overline{N}-1} h_i}$$

becomes too large. We expect the tolerance on the new mesh to be satisfied, and if this is the case the algorithm stops.

6. Otherwise, a further refinement of the mesh is necessary. From the comparison of the computed error and the (mixed) tolerance, a factor for the step-size reduction is computed (cf. [17, pp. 166–167]). For practical reasons, this factor is rounded to a factor in the set $\{1.5, 2, 3, 4, 6, 8\}$. This last step is repeated until either the tolerance is satisfied or the code terminates the calculation with an 'emergency' stop.

To demonstrate how the above algorithm performs and to illustrate the difference between the two alternative methods of error estimation, we again consider the test example (3.7). To gain an impression of a mesh suitably adapted to the solution behavior, both components of the exact solution are shown in figure 2. Collocation with $m = 4$ is used to reach a mixed tolerance, with the absolute and relative tolerance parameters equal to $5 \cdot 10^{-4}$.

We now discuss the results of the most important steps of the algorithm based on the modified Zadunaisky estimate. For the equidistant starting mesh with $N = 5$, the exact and the estimated global error are shown in figure 3, marked by $\star$ and $\bullet$, respectively.

The number of grid points in the new mesh to satisfy the tolerance was estimated as $\overline{N} \geqslant 42$, and the corresponding new mesh already made suitable for the equidistant collocation and modified Zadunaisky estimate is shown in figure 4 (the collocation points are indicated by small dots between the mesh points). Note that mesh points are denser

[6] Note that this is a restriction on the possible meshes for the classical Zadunaisky estimate, whereas for the modified Zadunaisky estimate the mesh is still arbitrary. This means that the latter estimate improves the grid flexibility and better resolves the local variation of the error estimate over the grid.

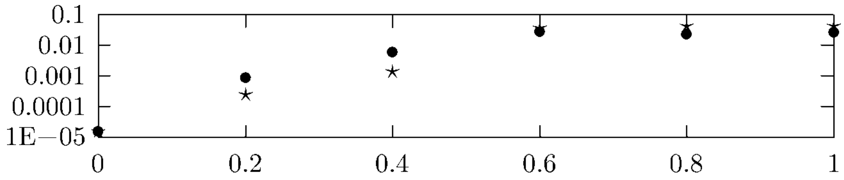

Figure 3. Evaluation on basic mesh for modified Zadunaisky.

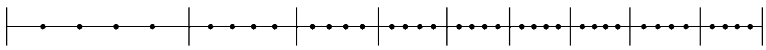

Figure 4. Final grid to reach TOL for modified Zadunaisky.

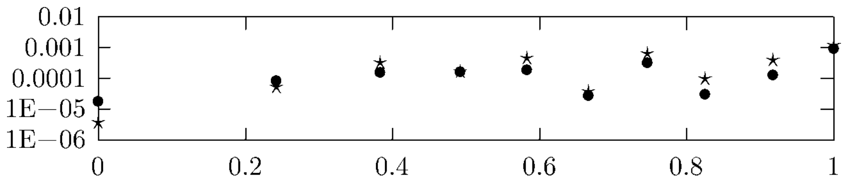

Figure 5. Evaluation on the final mesh for modified Zadunaisky.

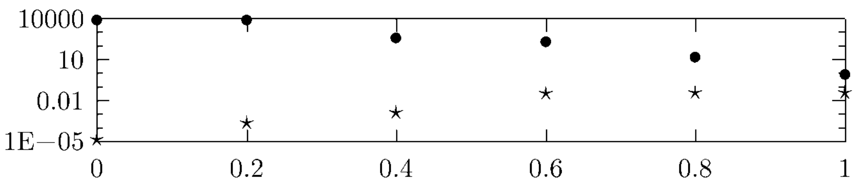

Figure 6. Evaluation on basic mesh for classical Zadunaisky.

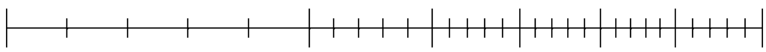

Figure 7. Mesh predicted to reach TOL for classical Zadunaisky.

in the region properly related to the behavior of the solution, see figure 2. As aimed for, the tolerance requirement on the new mesh is satisfied. For the exact and the estimated global error see figure 5.

We now briefly look at the corresponding results for the classical Zadunaisky estimate. For the same problem setting and parameter values, the estimate on the basic mesh with $N = 5$ is completely unreliable, see figure 6. Most probably this is due to the coarse step-size used for the backward Euler scheme in this case. The lack of accuracy is also reflected by the condition number of the associated system matrix approximately equal to $8 \cdot 10^7$.

A refined basic mesh with $N = 30$ provides an estimate suitable for the equidistribution step resulting in a mesh displayed in figure 7.

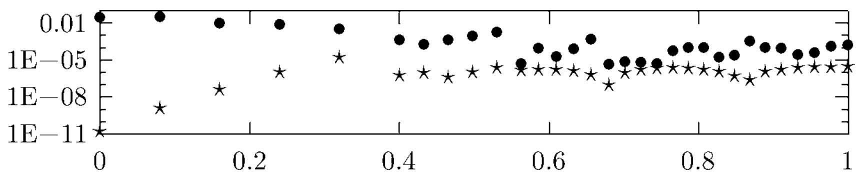

Figure 8. Evaluation on the predicted mesh for classical Zadunaisky.

According to figure 8, the estimate on this mesh is still quite unreliable and a further halving of the grid is predicted, although the true error is already smaller than in the comparable step of the modified version of the method. After this refinement, TOL is finally satisfied and the algorithm terminates after a computing time approximately six times longer than before.

6. Conclusions

In this paper a new error estimate (based on classical ideas due to Zadunaisky and Stetter) for the global error of collocation methods applied to solve two-point boundary value problems was presented. A proof of the asymptotic correctness of this estimate was given for regular problems. Experimental results suggest that the method can also be successfully applied to singular problems. This estimate was used as a basis for a reliable and efficient adaptive mesh selection procedure. Its most remarkable feature is the proper grid adjustment in the singular case, correctly reflecting the solution behavior and unaffected by the unsmoothness of the direction field.

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