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New a posteriori error estimates for singular boundary value problems *

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In this paper, we discuss the asymptotic properties and efficiency of several a posteriori estimates for the global error of collocation methods. Proofs of the asymptotic correctness are given for regular problems and for problems with a singularity of the first kind. We were also strongly interested in finding out which of our error estimates can be applied for the efficient solution of boundary value problems in ordinary differential equations with an essential singularity. Particularly, we compare estimates based on the defect correction principle with a strategy based on mesh halving.

Keywords: collocation, essential singularity, boundary value problems, ordinary differential equations, a posteriori error estimation, defect correction

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1. Introduction

In this work we discuss the efficient numerical solution of boundary value problems for singular ODEs,

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

$$g\big(z(0), z(1)\big) = 0, \tag{1b}$$

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

which occur in various applications of current interest. Here, the unknown z is a vector-valued function of dimension n and the right-hand side f is a smooth function on a suitable domain in $[0, 1] \times \mathbb{R}^n$, and g is typically a smooth function of dimension $p < n$. The smoothness requirement (1c) implicitly defines $n - p$ relations posed at $t = 0$ that guarantee the well-posedness of the problem. For the numerical treatment, these relations need to be stated explicitly, see [15,17]. Note that $p = n$ implies that the

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smoothness requirement (1c) is trivially satisfied and does not enforce any additional boundary conditions. In (1a), the parameter α determines the type of singularity. While $\alpha = 0$ yields a regular problem, $\alpha = 1$ defines a singularity of the first kind, and for $\alpha > 1$ we are confronted with an essential singularity.[1] Analytical results like existence, uniqueness and smoothness of the solution of (1) are given in [15] for $\alpha = 1$ and in [18] for $\alpha > 1$.

Both kinds of singular problems are encountered in various applications. Numerous applications from physics, see [19], mechanics (buckling of spherical shells [13]), or ecology [21] feature a singularity of the first kind. Problems with an essential singularity are obtained for instance when a problem posed on an infinite interval is transformed to a finite interval. In applications from fluid mechanics [10,23], engineering [22] or nonlinear optics [12] models of this type arise, see also [9].

In the past years, the case of a singularity of the first kind was considered by several authors. In particular, collocation methods were analyzed in [16,26]. More recent results can be found in [5,7,20]. In these papers, not only the convergence of collocation methods was studied, but also an efficient and reliable method for the *a posteriori estimation* of the global error was developed and analyzed. Furthermore, the resulting numerical procedures were implemented in the MATLAB package `sbvp` designed for the efficient adaptive solution of problems with a singularity of the first kind, see [3].

The underlying global error estimate ('QDeC estimate', a defect correction approach based on *defect quadrature*), which is the basis for our adaptive grid strategy, is constructed as a nontrivial modification of the defect correction procedure originally proposed in [25,27]. In the QDeC estimate, a suitable *neighboring problem* is defined using a locally integrated defect of the collocation solution with respect to the differential equation. The estimate for the global error is determined from the solutions of the original and the neighboring problem by a computationally cheap auxiliary method, in this case the backward Euler method.

For problems with an essential singularity, theory and numerical software are less well developed. Our first attempts to tackle this class of problems using collocation and different methods for a posteriori error estimation are reported in [4,9]. These numerical results show that

- Collocation retains its favorable convergence properties: For the global error, at least the stage order was observed in all examples tested.
- The QDeC error estimate mentioned above, which was shown to be asymptotically correct for problems with a singularity of the first kind, cannot be applied to problems with an essential singularity. The backward Euler method which is used as an auxiliary scheme usually diverges rapidly when used for this problem class.

A possible remedy for this shortcoming of our error estimate is to replace the auxiliary method by a method which shows a more favorable convergence behavior in presence of an essential singularity. In [9] we proposed to use the box scheme instead

[1] Systems with mixed types of singularities are also covered in our discussion below.

of the backward Euler method. In this paper, we carry this idea further and discuss in detail the asymptotic properties of this error estimate using the box scheme as auxiliary method, and a variant where the neighboring problem is solved using the same collocation scheme as for the original problem. The results are compared with the performance of an estimate for the global error using mesh halving.

After introducing our notation in section 2, in section 3 we describe the error estimates to be compared in this paper. Particularly, two variants based on the defect correction principle are introduced and error estimation based on mesh halving is recapitulated. In section 4, we prove that the error estimates are asymptotically correct for regular problems. The analysis extends easily to problems with a singularity of the first kind if techniques from [5,20] are used. To prove analogous results for problems with an essential singularity, a comprehensive convergence theory for collocation applied to this problem class is necessary. So far, no general results have been published in the literature. Numerical evidence, however, is promising in that respect, see [9]. Therefore we examine the empirical asymptotic properties of our error estimates when applied to problems with an essential singularity in section 5. Finally, in section 6 we compare the efficiency of a collocation code using either of the available a posteriori estimates for the global error.

2. Preliminaries

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

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

to denote the maximum norm in $\mathbb{R}^n$. $C_n^p[0,1]$ is the space of real 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

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

$C_{n\times n}^p[0,1]$ is the space of real $n \times n$ matrices with columns in $C_n^p[0,1]$. For a matrix $A = (a_{ij})_{i,j=1}^n$, $A \in C_{n\times n}^0[0,1]$, $\|A\|$ is the induced norm,

$$\|A\| = \max_{0\leqslant t\leqslant 1} \left|A(t)\right| = \max_{0\leqslant t\leqslant 1} \left(\max_{1\leqslant i\leqslant n} \sum_{j=1}^{n} |a_{ij}(t)| \right).$$

Where there is no confusion, we will omit the subscripts n and $n \times n$ and denote $C[0,1] = C^0[0,1]$.

For the numerical analysis, we define meshes

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

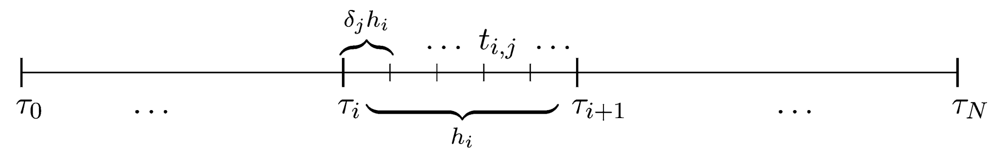

Figure 1. The computational grid.

and $h_i := \tau_{i+1} - \tau_i$, $i = 0, \dots, N-1$, $\tau_0 = 0$, $\tau_N = 1$. Moreover we denote $\mathbf{h} := \max_{i=0,\dots,N-1} h_i$. On Δ, we define corresponding grid vectors

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

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 $y \in C[0,1]$, we denote by R_Δ the pointwise projection onto the space of grid vectors,

$$R_\Delta(y) := \bigl(y(\tau_0), \dots, y(\tau_N)\bigr).$$

For collocation, m points $\tau_i + h_i\rho_j$, $j = 1, \dots, m$, are inserted in each subinterval $J_i := [\tau_i, \tau_{i+1}]$, where $0 < \rho_1 < \rho_2 < \cdots < \rho_m < 1$. This yields the (fine) grid[2]

$$\Delta^m := \{t_{i,j}\colon\ t_{i,j} = \tau_i + h_i\rho_j,\ i = 0, \dots, N-1,\ j = 0, \dots, m+1\}. \tag{2}$$

Since we focus on singular problems, we have assumed that $\rho_1 > 0$ in order to avoid a special treatment of the singular point. Since the definition of our error estimates based on defect correction requires evaluation of the differential equation at an additional point different from the collocation points in each interval J_i, we make the restriction $\rho_m < 1$ and use the endpoints of the collocation intervals as auxiliary evaluation points. For a grid Δ^m, u_{Δ^m}, $\|\cdot\|_{\Delta^m}$ and R_{Δ^m} are defined accordingly.

3. A posteriori error estimates

We introduce the numerical methods considered in this paper for regular problems to keep the notation short, and restrict ourselves to linear boundary conditions,

$$z'(t) = F\bigl(t, z(t)\bigr), \quad t \in [0,1], \tag{3a}$$

$$B_0 z(0) + B_1 z(1) = \beta. \tag{3b}$$

Formally, singular problems are included in this formulation if we set $F(t,z) = f(t,z)/t^\alpha$, cf. (1).

[2] For convenience, we denote τ_i by $t_{i,0} \equiv t_{i-1,m+1}$, $i = 1, \dots, N-1$. Moreover, we define $\rho_0 := 0$, $\rho_{m+1} := 1$.

3.1. Collocation methods

To compute the basic numerical solution, we use polynomial collocation. This means that on a grid (2) we require the collocating function $p(t) := p_i(t)$, $t \in J_i$, $i = 0, \ldots, N-1$, where p_i is a polynomial of degree $\leqslant m$, to satisfy

$$p_i'(t_{i,j}) = F\big(t_{i,j}, p_i(t_{i,j})\big), \quad i = 0, \ldots, N-1, \ j = 1, \ldots, m, \tag{4a}$$

$$p_i(\tau_i) = p_{i-1}(\tau_i), \qquad i = 1, \ldots, N-1, \tag{4b}$$

$$B_0 p_0(0) + B_1 p_{N-1}(1) = \beta. \tag{4c}$$

For regular problems, the following convergence result holds:

Theorem 1. Let $z(t)$ be an isolated, sufficiently smooth solution of (3) and let F be twice continuously differentiable in a neighborhood of z. Then for any collocation scheme of the form (4) there exist constants r, $\mathbf{h}_0 > 0$ such that the following statements hold for all meshes Δ with $\mathbf{h} \leqslant \mathbf{h}_0$:

- There exists a unique solution $p(t)$ of (4) in a tube of radius r 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:

$$\big\| R_\Delta(p) - R_\Delta(z) \big\|_\Delta = \mathrm{O}\big(\mathbf{h}^{m+\nu}\big), \tag{5a}$$

$$\| p - z \| = \mathrm{O}\big(\mathbf{h}^{m+\mu}\big), \tag{5b}$$

$$\big\| p^{(l)} - z^{(l)} \big\| = \mathrm{O}\big(\mathbf{h}^{m+1-l}\big), \quad l = 1, \ldots, m, \tag{5c}$$

provided that

$$\int_0^1 s^k \prod_{l=1}^m (s - \rho_l)\,\mathrm{d}s = 0, \quad k = 0, \ldots, \nu - 1. \tag{6}$$

In (5b), $\mu = 0$ for $\nu = 0$ and $\mu = 1$ otherwise.

For proofs see, for example, [1,11].

For problems with a singularity of the first kind, where $\alpha = 1$ in (1), similar existence and uniqueness results can be proven under appropriate assumptions which guarantee the well-posedness of the boundary value problem and the smoothness of its solution. The estimates (5a) and (5b) have to be replaced by

$$\big\| R_\Delta(p) - R_\Delta(z) \big\|_\Delta = \mathrm{O}\big(\mathbf{h}^{m+1} \big|\ln(\mathbf{h})\big|^{n_0 - 1}\big), \tag{7a}$$

$$\| p - z \| = \mathrm{O}\big(\mathbf{h}^{m+1} \big|\ln(\mathbf{h})\big|^{n_0 - 1}\big) \tag{7b}$$

if (6) holds with $\nu \geqslant 1$, see [5,20] for details. The positive integer n_0 is defined by the structure of the linearization of (1a), see, for example, [15]. The perturbation of the convergence order by the logarithmic terms is usually too small to be noticed experimentally.

For problems with an essential singularity, no theoretical results are known for general high-order collocation methods. However, we observed experimentally that the *stage order* $\mathrm{O}(\mathbf{h}^m)$ is retained for any choice of symmetric collocation points. The superconvergence orders for $\nu \geqslant 1$ in (6) are

$$\left\| R_\Delta(p) - R_\Delta(z) \right\|_\Delta = \mathrm{O}\big(\mathbf{h}^{m+\gamma}\big), \tag{8a}$$

$$\| p - z \| = \mathrm{O}\big(\mathbf{h}^{m+\gamma}\big), \tag{8b}$$

where $0 < \gamma = \gamma(\alpha) < 1$, and γ decreases with increasing α. For nonsymmetric collocation points, we observed rapid divergence of the numerical solution. Experimental evidence for these propositions is given in [4,9].

Remark. The analysis of the box scheme given in [17] implies that its order of convergence is $1 + \gamma$, where $0 < \gamma < 1$. Since the box scheme is equivalent to collocation at Gaussian points with $m = 1$, this is consistent with the above conjecture.

3.2. *QDeC error estimate based on the box scheme*

In this section we introduce our error estimate based on the defect correction principle, where the box scheme is used as auxiliary method. The construction of the estimate is similar to that using the backward Euler method, which was introduced and analyzed in [7]. Consequently, we keep the presentation close to [7] and refer the reader to that paper for additional details.

The numerical solution p obtained by collocation is used to define a 'neighboring problem' to (3). The original and the neighboring problem are solved by the box scheme on the grid $t_{i,j}$, $i = 0, \ldots, N-1$, $j = 1, \ldots, m+1$, where the right-hand side is evaluated at the midpoints $t_{i,j-1/2} := (t_{i,j-1} + t_{i,j})/2$. This yields the grid vectors[3] $\xi_{i,j}$ and $\pi_{i,j}$ as the solutions of the following schemes, subject to boundary conditions (3b),

$$\frac{\xi_{i,j} - \xi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = F\left(t_{i,j-1/2}, \frac{\xi_{i,j-1} + \xi_{i,j}}{2}\right), \quad \text{and} \tag{9a}$$

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = F\left(t_{i,j-1/2}, \frac{\pi_{i,j-1} + \pi_{i,j}}{2}\right) + \bar{d}_{i,j}, \tag{9b}$$

where $\bar{d}_{i,j}$ is a defect term defined by

$$\bar{d}_{i,j} := \frac{p(t_{i,j}) - p(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, p(t_{i,k})\big). \tag{10}$$

[3] Here and in the subsequent discussion, we assume throughout $i = 0, \ldots, N-1$, $j = 1, \ldots, m+1$ unless otherwise stated.

Here, the coefficients $\alpha_{j,k}$ are chosen in such a way that the quadrature rules given by

$$\frac{1}{t_{i,j} - t_{i,j-1}} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(\tau)\,\mathrm{d}\tau \approx \sum_{k=1}^{m+1} \alpha_{j,k}\varphi(t_{i,k})$$

have precision $m + 1$. The quantities $\xi_{i,j} - \pi_{i,j}$ serve as our a posteriori estimates for the global error of the collocation solution at the grid points, which is $\mathrm{O}(h^m)$ in general.

3.3. *QDeC error estimate based on collocation*

Now, we introduce an error estimate based on defect correction, where the neighboring problem is solved using the same collocation method as for the original problem (3). In this setting, we only have to solve one additional problem instead of two problems, albeit with the expensive basic high-order method. Particularly, for linear problems, the additional effort is low since the LU-factorization from the original problem can be reused.

In order to define this error estimate, we require a reformulation of the underlying collocation method as a finite difference scheme. This representation is related to the Runge–Kutta formulation of the collocation scheme, but in contrast uses difference quotients at adjacent grid points. The scheme is introduced in the next lemma.

Lemma 1. The numerical solution values $p_{i,j} := p_i(t_{i,j})$, $i = 0, \dots, N-1$, $j = 0, \dots, m+1$ of (4) can equivalently be expressed as the solution of the finite difference scheme

$$\frac{p_{i,j} - p_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \sum_{k=1}^{m} \beta_{j,k} F(t_{i,k}, p_{i,k}), \quad i = 0, \dots, N-1, \ j = 1, \dots, m+1, \tag{11a}$$

$$B_0 p_{0,0} + B_1 p_{N-1,m+1} = \beta, \tag{11b}$$

where $\beta_{j,k}$ are the unique coefficients defining quadrature rules of precision m based on the abscissae $t_{i,j}$, $j = 1, \dots, m$,

$$\frac{1}{t_{i,j} - t_{i,j-1}} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(s)\,\mathrm{d}s = \sum_{k=1}^{m} \beta_{j,k}\varphi(t_{i,k}) + \mathrm{O}\big(h_i^m\big), \quad j = 1, \dots, m+1. \tag{12}$$

Proof. First, consider the solution of (4). Obviously,

$$\begin{aligned}
p_i(t_{i,j}) &= p_i(t_{i,j-1}) + \int_{t_{i,j-1}}^{t_{i,j}} p_i'(s)\,\mathrm{d}s \\
&= p_i(t_{i,j-1}) + (t_{i,j} - t_{i,j-1}) \sum_{k=1}^{m} \beta_{j,k} p_i'(t_{i,k}) \\
&= p_i(t_{i,j-1}) + (t_{i,j} - t_{i,j-1}) \sum_{k=1}^{m} \beta_{j,k} F\big(t_{i,k}, p_i(t_{i,k})\big), \quad j = 1, \dots, m+1,
\end{aligned}$$

since the quadrature formula (12) is precise for polynomials of degree $\leqslant m-1$. Consequently, (11a) is satisfied, because additionally $p_{i-1,m+1} = p_{i,0}$ due to (4b).

If conversely (11a) holds, we consider a piecewise polynomial function $p(t) = p_i(t)$, $i = 0, \dots, N-1$, interpolating $p_{i,j}$. Obviously, (11a) for $j = m+1$ implies the continuity condition (4b). For $j = 1, \dots, m$ we conclude analogously as above that

$$\frac{p_i(t_{i,j}) - p_i(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} = \sum_{k=1}^{m} \beta_{j,k} p_i'(t_{i,k}),$$

and consequently

$$\sum_{k=1}^{m} \beta_{j,k} \bigl(p_i'(t_{i,k}) - F\bigl(t_{i,k}, p_i(t_{i,k})\bigr)\bigr) = 0.$$

This implies (4a) if the matrix $B = (\beta_{j,k})_{j,k=1,\dots,m}$ is nonsingular. This fact is shown in lemma 2, which completes the proof of this lemma. □

Lemma 2. The matrix $B = (\beta_{j,k})_{j,k=1,\dots,m}$, where $\beta_{j,k}$ are defined in (12), is nonsingular.

Proof. The proposition is equivalent to the assertion that a polynomial $q(t)$ of degree $\leqslant m-1$ can uniquely be determined from

$$\frac{1}{\rho_j - \rho_{j-1}} \int_{\rho_{j-1}}^{\rho_j} q(s)\,\mathrm{d}s = c_j, \quad j = 1, \dots, m, \tag{13}$$

for every choice of c_j. To prove this, we choose a Newton representation for the integral of q,

$$\begin{aligned}\int q(t)\,\mathrm{d}t &= Q(t) \\ &= a_1(t-\rho_0) + a_2(t-\rho_1)(t-\rho_0) + \cdots + a_m(t-\rho_{m-1})\cdots(t-\rho_0),\end{aligned}$$

where without restriction of generality we have set the integration constant equal to zero, $Q(\rho_0) = Q(0) = a_0 = 0$. It is easily seen that we can compute the coefficients a_j recursively from (13),

$$\begin{aligned} a_1 &= c_1, \\ a_2 &= \frac{c_2 - a_1}{\rho_2 - \rho_0}, \\ &\vdots \end{aligned}$$

Thus B is nonsingular. □

Assume that the neighboring problem is solved by the same collocation method as the original problem. Then, using the representation (11) we define the QDeC error estimate based on defect correction as the difference $p_{i,j} - \pi_{i,j}$ between the two solutions of the finite difference schemes (11) and

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \sum_{k=1}^{m} \beta_{j,k} F(t_{i,k}, \pi_{i,k}) + \bar{d}_{i,j}, \quad i = 0, \ldots, N-1, \ j = 1, \ldots, m+1, \tag{14a}$$

$$B_0 \pi_{0,0,} + B_1 \pi_{N-1,m+1} = \beta, \tag{14b}$$

where $\bar{d}_{i,j}$ is the defect defined in (10).

As the solution of (11) is in practice computed from the original collocation scheme (4), it would be favorable from a computational point of view if we could rewrite (14) as a scheme of collocation type. This is possible if we drop the continuity requirement (4b). We demonstrate this in the following lemma.

Lemma 3. The solution values $\pi_{i,j}$, $i = 0, \ldots, N-1$, $j = 0, \ldots, m+1$, of (14) can equivalently be computed as the values $\pi_{i,j} = \pi(t_{i,j})$ of the piecewise (in general, not continuous) polynomial function $\pi(t) = \pi_i(t)$, $t \in J_i$, $i = 0, \ldots, N-1$, of degree $\leqslant m$, which satisfies the relations

$$\pi_i'(t_{i,j}) = F\big(t_{i,j}, \pi_i(t_{i,j})\big) + \hat{d}_{i,j}, \quad i = 0, \ldots, N-1, \ j = 1, \ldots, m, \tag{15a}$$

$$\pi_i(\tau_i) = \pi_{i-1}(\tau_i) + (\tau_i - t_{i-1,m})\hat{d}_{i-1,m+1}, \quad i = 1, \ldots, N-1, \tag{15b}$$

$$B_0 \pi_0(0) + B_1 \pi_{N-1}(1) = \beta - B_1 \hat{d}_{N-1,m+1}, \tag{15c}$$

where

$$\big(\hat{d}_{i,1}, \ldots, \hat{d}_{i,m}\big)^{\mathrm{T}} = B^{-1}\big(\bar{d}_{i,1}, \ldots, \bar{d}_{i,m}\big)^{\mathrm{T}},$$
$$\hat{d}_{i,m+1} = \bar{d}_{i,m+1} - \sum_{k=1}^{m} \beta_{m+1,k} \hat{d}_{i,k}$$

with B defined as in lemma 2 and $\bar{d}_{i,j}$ from (10).

Proof. Obviously, (14a) for $j = 1, \ldots, m$ is equivalent to (15a), since

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \sum_{k=1}^{m} \beta_{j,k} \pi'(t_{i,k}), \quad j = 1, \ldots, m,$$

and lemma 2 holds. Furthermore, from extrapolation of the polynomial π_{i-1} to $t = \tau_i$ using the quadrature rule from (12) for $j = m+1$, we conclude

$$\frac{\pi_{i-1}(\tau_i) - \pi_{i-1}(t_{i-1,m})}{\tau_i - t_{i-1,m}} = \sum_{k=1}^{m} \beta_{m+1,k}\big(F\big(t_{i-1,k}, \pi_{i-1}(t_{i-1,k})\big) + \hat{d}_{i-1,k}\big).$$

Since instead of this relation we use (14a), the difference between $\pi_{i-1}(\tau_i)$ and $\pi_i(\tau_i)$ has to be taken into account in the transition condition (15b). To complete the proof, we only have to show that (15) has a unique solution. This is easy using the same arguments as for (4), see [1,20]. □

3.4. Error estimate based on mesh halving

Finally, we consider a classical error estimate based on mesh halving. In this approach, we compute the collocation solution at m points on a grid Δ with step sizes h_i and denote this approximation by $p_\Delta(t)$. Subsequently, we choose a second mesh Δ_2 where in every interval J_i of Δ we insert two subintervals of length $h_i/2$. On this mesh, we compute the numerical solution based on the same collocation scheme to obtain the collocating function $p_{\Delta_2}(t)$. Using these two quantities, we define

$$\mathcal{E}(t) := \frac{2^m}{1-2^m}\big(p_{\Delta_2}(t) - p_\Delta(t)\big) \tag{16}$$

as an error estimate for the approximation $p_\Delta(t)$. Assume that the global error $\delta(t) := p_\Delta(t) - z(t)$ of the collocation solution can be expressed in terms of the principal error function $e(t)$,

$$\delta(t) = e(t)h_i^m + \mathrm{O}\big(h_i^{m+1}\big), \quad t \in J_i, \tag{17}$$

where $e(t)$ is independent of Δ. Then obviously the quantity $\mathcal{E}(t)$ satisfies $\mathcal{E}(t) - \delta(t) = \mathrm{O}(\mathbf{h}^{m+1})$. The convergence results for collocation methods, see [9], suggest that this is a promising approach. However, numerical results reported in section 5 indicate that in case of an essential singularity (17) reads

$$\delta(t) = e(t)h_i^m + \mathrm{O}\big(h_i^{m+\gamma}\big), \quad t \in J_i, \tag{18}$$

with the same $\gamma < 1$ as in (8).

4. Asymptotical correctness for regular problems

In this section, we analyze the errors of the error estimates described in sections 3.2 and 3.3 with respect to the exact global errors of the underlying collocation solutions for regular problems. Moreover, we indicate how the proofs may be modified so as to apply to problems with a singularity of the first kind as well, using results from [5,20]. Numerical examples illustrating our theoretical results are given in [2]. The proofs are similar to the proof given in [7] for the error estimate based on defect correction using the backward Euler scheme as auxiliary method (see also [5,20]). Consequently, we focus on the points in the proofs where the analysis for the error estimates from sections 3.2 and 3.3 differs from [7] and refer to the latter reference for further details. First, we give the result for the estimate based on the box scheme.

Theorem 2. Assume that the boundary value problem (3) has an isolated (sufficiently smooth)[4] solution z. Then, provided that $\mathbf{h}$ is sufficiently small, the following estimate holds for ξ_{Δ^m} and π_{Δ^m} defined by the finite difference schemes (9):

$$\big\| \big(R_{\Delta^m}(z) - R_{\Delta^m}(p)\big) - (\xi_{\Delta^m} - \pi_{\Delta^m}) \big\|_{\Delta^m} = \mathrm{O}\big(\mathbf{h}^{m+1}\big). \tag{19}$$

Proof. Let

$$\varepsilon_{\Delta^m} := \xi_{\Delta^m} - R_{\Delta^m}(z), \qquad \bar{\varepsilon}_{\Delta^m} := \pi_{\Delta^m} - R_{\Delta^m}(p), \tag{20}$$

then the quantity to be estimated is

$$\tilde{\varepsilon}_{\Delta^m} := \big(R_{\Delta^m}(p) - R_{\Delta^m}(z)\big) - (\pi_{\Delta^m} - \xi_{\Delta^m}) = \varepsilon_{\Delta^m} - \bar{\varepsilon}_{\Delta^m}. \tag{21}$$

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

$$\begin{aligned}\frac{\varepsilon_{i,j} - \varepsilon_{i,j-1}}{t_{i,j} - t_{i,j-1}} &= F\left(t_{i,j-1/2}, \frac{\xi_{i,j-1} + \xi_{i,j}}{2}\right) - \frac{z(t_{i,j}) - z(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} \\ &= F\left(t_{i,j-1/2}, \frac{\xi_{i,j-1} + \xi_{i,j}}{2}\right) - \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, z(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big),\end{aligned} \tag{22}$$

since the $\alpha_{j,k}$ define quadrature rules of precision $m+1$. Moreover, $\bar{\varepsilon}_{\Delta^m}$ satisfies

$$\begin{aligned}\frac{\bar{\varepsilon}_{i,j} - \bar{\varepsilon}_{i,j-1}}{t_{i,j} - t_{i,j-1}} &= F\left(t_{i,j-1/2}, \frac{\pi_{i,j-1} + \pi_{i,j}}{2}\right) + \bar{d}_{i,j} - \frac{p(t_{i,j}) - p(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} \\ &= F\left(t_{i,j-1/2}, \frac{\pi_{i,j-1} + \pi_{i,j}}{2}\right) - \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, p(t_{i,k})\big).\end{aligned} \tag{23}$$

Both (22) and (23) hold for $i = 0, \dots, N-1$, $j = 1, \dots, m+1$, and ε_{Δ^m} as well as $\bar{\varepsilon}_{\Delta^m}$ satisfy homogeneous boundary conditions.

Now, a Taylor expansion analogous to [7] yields the identities

$$\begin{aligned}\frac{\varepsilon_{i,j} - \varepsilon_{i,j-1}}{t_{i,j} - t_{i,j-1}} = A(t_{i,j-1/2})\frac{\varepsilon_{i,j-1} + \varepsilon_{i,j}}{2} + F\left(t_{i,j-1/2}, \frac{z(t_{i,j-1}) + z(t_{i,j})}{2}\right) \\ - \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, z(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big),\end{aligned} \tag{24}$$

and

$$\begin{aligned}\frac{\bar{\varepsilon}_{i,j} - \bar{\varepsilon}_{i,j-1}}{t_{i,j} - t_{i,j-1}} = A(t_{i,j-1/2})\frac{\bar{\varepsilon}_{i,j-1} + \bar{\varepsilon}_{i,j}}{2} + F\left(t_{i,j-1/2}, \frac{p(t_{i,j-1}) + p(t_{i,j})}{2}\right) \\ - \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, p(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+2}\big),\end{aligned} \tag{25}$$

[4] In fact, we require $z \in C^{m+2}[0, 1]$.

with a matrix $A(t)$ resulting from the linearization of F about a suitable function. In the derivation of the latter difference schemes, we used the relations $p(t) - z(t) = \mathrm{O}(\mathbf{h}^m)$ and the facts that

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

and

$$\varepsilon_{i,j} = \mathrm{O}(\mathbf{h}^2), \qquad \bar{\varepsilon}_{i,j} = \mathrm{O}(\mathbf{h}^2).$$

(24) and (25) are a pair of ‘parallel’ box schemes, with related inhomogeneous terms. The difference between these terms can be estimated in terms of[5] $\|p - z\|$, $\|p' - z'\|$ and $\|p'' - z''\|$, if we use Taylor expansion about $t_{i,j-1/2}$ similarly as in [7]. The convergence results from theorem 1, together with stability for the box scheme, now yield the assertion of the theorem. □

Remark. Note that alternatively to using the defect $\bar{d}_{i,j}$ from (10), for regular problems we could also use

$$\bar{d}_{i,j} := \frac{p(t_{i,j}) - p(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \sum_{k=0}^{m+1} \alpha_{j,k} F\big(t_{i,k}, p(t_{i,k})\big), \tag{26}$$

where in this case the coefficients $\alpha_{j,k}$ are chosen in such a way that the quadrature rules given by

$$\frac{1}{t_{i,j} - t_{i,j-1}} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(\tau)\,\mathrm{d}\tau \approx \sum_{k=0}^{m+1} \alpha_{j,k} \varphi(t_{i,k})$$

have precision $m+2$. By symmetry we might expect that this modification increases the order of the error of the error estimate to $m + 2$, which is equal to the sum of the orders of the basic method and the auxiliary scheme and also equals the order of the truncation error of the quadrature rule used in the defect definition. Moreover, estimates of the maximally attainable order for *Iterated Defect Correction* show that such an increase in the order can take place in certain situations [8,14]. When used for error estimation based on the box scheme according to section 3.2, the estimate (19) cannot be improved from order $m + 1$ to order $m + 2$ in general, however. Table 1 gives the numerical results for the following test problem demonstrating that (19) is sharp:

$$z'(t) = \begin{pmatrix} 0 & 1 \\ 4 & 0 \end{pmatrix} z(t) - 3 \begin{pmatrix} 0 \\ \exp(t) \end{pmatrix}, \tag{27a}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 1 \\ \mathrm{e} \end{pmatrix}. \tag{27b}$$

[5] If the backward Euler scheme serves as an auxiliary method, only $\|p - z\|$ and $\|p' - z'\|$ appear in the estimates. The asymptotic properties of the bounds are the same in both cases, however.

Table 1
Error of error estimate based on box scheme for (27), $m = 4$.

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/2	3.023E−05		2.468E−06	
1/4	1.740E−06	4.12	6.574E−08	5.23
1/8	1.064E−07	4.03	1.916E−09	5.10
1/16	6.617E−09	4.01	5.803E−11	5.05
1/32	4.130E−10	4.00	1.750E−12	5.05

The exact solution of (27) reads $z(t) = (\mathrm{e}^t, \mathrm{e}^t)$. For each equidistant step size $h \equiv h_i$, we give the maximum norm of the exact global error $\mathrm{err}_{\mathrm{coll}}$ of the collocation solution computed using $m = 4$ equidistant collocation points, its empirical convergence order $\mathrm{ord}_{\mathrm{coll}}$ computed from two successive approximations and the error of the error estimate $\mathrm{err}_{\mathrm{est}}$ and its order $\mathrm{ord}_{\mathrm{est}}$. All the computations reported in this paper were performed using the collocation solver `sbvpcol` from our MATLAB solver `sbvp`, see [3]. We used double precision arithmetic with machine precision $\approx 1.11 \cdot 10^{-16}$. We find that the error of the error estimate has the empirical convergence order $m + 1 = 5$. Consequently, we conclude that the estimate (19) cannot be improved in general.

For problems with a singularity of the first kind, a similar argument can be used to analyze the error of the error estimate, if we take into account the modifications necessary for singular problems which are given in [5,20]. In this case, the estimate (19) has to be replaced by

$$\big\| \big(R_{\Delta^m}(z) - R_{\Delta^m}(p)\big) - (\xi_{\Delta^m} - \pi_{\Delta^m}) \big\|_{\Delta^m} = \mathrm{O}\big(\big|\ln(\mathbf{h})\big|^{n_0-1}\mathbf{h}^{m+1}\big), \tag{28}$$

with the same positive integer n_0 as in (7), see [5].

For the analysis of the QDeC estimate based on collocation introduced in section 3.3, we proceed in the same way as for the estimate based on the box scheme, see theorem 2. Now, the auxiliary quantities

$$\varepsilon_{\Delta^m} := R_{\Delta^m}(p) - R_{\Delta^m}(z), \qquad \bar{\varepsilon}_{\Delta^m} := \pi_{\Delta^m} - R_{\Delta^m}(p) \tag{29}$$

satisfy the difference schemes

$$\begin{aligned} \frac{\varepsilon_{i,j} - \varepsilon_{i,j-1}}{t_{i,j} - t_{i,j-1}} = &\sum_{k=1}^{m} \beta_{j,k} A(t_{i,k})\varepsilon_{i,k} + \sum_{k=1}^{m} \beta_{j,k} F\big(t_{i,k}, z(t_{i,k})\big) \\ &- \sum_{k=1}^{m+1} \alpha_{j,k} F\big(t_{i,k}, z(t_{i,k})\big) + \mathrm{O}\big(\mathbf{h}^{m+1}\big), \end{aligned} \tag{30}$$

and

$$\frac{\bar{\varepsilon}_{i,j} - \bar{\varepsilon}_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \sum_{k=1}^{m} \beta_{j,k} A(t_{i,k}) \bar{\varepsilon}_{i,k} + \sum_{k=1}^{m} \beta_{j,k} F\bigl(t_{i,k}, p(t_{i,k})\bigr) - \sum_{k=1}^{m+1} \alpha_{j,k} F\bigl(t_{i,k}, p(t_{i,k})\bigr) + \mathrm{O}\bigl(\mathbf{h}^{2m}\bigr). \tag{31}$$

Note that in this case,

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

The difference in the inhomogeneous terms appearing in (30) and (31) can be estimated as before, noting that

$$\sum_{k=1}^{m} \beta_{j,k} = \sum_{k=1}^{m+1} \alpha_{j,k} = 1, \quad j = 1, \ldots, m+1.$$

Thus, we can prove the following theorem.

Theorem 3. Assume that the boundary value problem (3) has an isolated (sufficiently smooth) solution z. Then, provided that $\mathbf{h}$ is sufficiently small, the following estimate holds for the error estimate $R_{\Delta^m}(p) - \pi_{\Delta^m}$ defined by the finite difference schemes (11) and (14) – or equivalently, by the collocation schemes (4) and (15):

$$\bigl\| \bigl(R_{\Delta^m}(z) - R_{\Delta^m}(p)\bigr) - \bigl(R_{\Delta^m}(p) - \pi_{\Delta^m}\bigr) \bigr\|_{\Delta^m} = \mathrm{O}\bigl(\mathbf{h}^{m+1}\bigr). \tag{32}$$

Proof. It only remains to show that the finite difference scheme for $\tilde{\varepsilon}_{\Delta^m} = \varepsilon_{\Delta^m} - \bar{\varepsilon}_{\Delta^m}$ is stable. For regular problems this is clear from classical theory. We use a different argument, however, which can be used without modifications for problems with a singularity of the first kind as well. To this end, we rewrite the finite difference scheme

$$\frac{\tilde{\varepsilon}_{i,j} - \tilde{\varepsilon}_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \sum_{k=1}^{m} \beta_{j,k} A(t_{i,k}) \tilde{\varepsilon}_{i,k} + \mathrm{O}\bigl(\mathbf{h}^{m+1}\bigr)$$

as a collocation scheme

$$\tilde{\varepsilon}_i'(t_{i,j}) = A(t_{i,j}) \tilde{\varepsilon}_i(t_{i,j}) + \mathrm{O}\bigl(\mathbf{h}^{m+1}\bigr), \quad i = 0, \ldots, N-1, \ j = 1, \ldots, m, \tag{33a}$$

$$\tilde{\varepsilon}_i(\tau_i) = \tilde{\varepsilon}_{i-1}(\tau_i) + \mathrm{O}\bigl(\mathbf{h}^{m+2}\bigr), \qquad i = 1, \ldots, N-1, \tag{33b}$$

$$B_0 \tilde{\varepsilon}_0(0) + B_1 \tilde{\varepsilon}_{N-1}(1) = \mathrm{O}\bigl(\mathbf{h}^{m+1}\bigr). \tag{33c}$$

Using a shooting argument, we conclude that

$$\|\tilde{\varepsilon}\| = \mathrm{O}\bigl(\mathbf{h}^{m+1}\bigr)$$

from the stability of collocation schemes [1], since the inhomogeneous terms in (33b) accumulate to

$$\sum_{i=0}^{k} \mathrm{O}\big(\mathbf{h}^{m+2}\big) = \mathrm{O}\big(\mathbf{h}^{m+1}\big), \quad k = 0, \ldots, N-1. \qquad \square$$

For problems with a singularity of the first kind, the same arguments as before, again taking into account [5,20], can be used to show a similar proposition, where the estimate (32) is replaced by

$$\big\| \big(R_{\Delta^m}(z) - R_{\Delta^m}(p)\big) - \big(R_{\Delta^m}(p) - \pi_{\Delta^m}\big) \big\|_{\Delta^m} = \mathrm{O}\big(\big|\ln(\mathbf{h})\big|^{n_0-1}\mathbf{h}^{m+1}\big).$$

5. Asymptotics for essential singularities

In this section, we give numerical examples showing the order of accuracy of the error estimates described in section 3 when applied to problems with an essential singularity. We report our experimental observations for three numerical examples. In the first example we consider a simple linear scalar terminal value problem. The second example from [18] deals with a linear system. Finally, the third example from [24] is a nonlinear boundary value problem which arises from the transformation of an unbounded integration domain onto the bounded interval (0, 1]. Further numerical evidence supporting our conjecture on the orders of the errors of the respective error estimates is reported in [2]. To prove the observed convergence orders, an analysis of collocation methods for problems with an essential singularity would be required. Unfortunately, such a result is not available so far. However, numerical results in [4,9] suggest that the error has the structure (18). Consequently, a similar analysis as in section 4 should reveal that the error of the error estimates is $\mathrm{O}(\mathbf{h}^{m+\gamma})$. The arguments will have to be adapted especially for the singular case, similarly as the extension of the results from [7] for problems with a singularity of the first kind given in [5,20]. Experimental results to support this proposition are given in [2].

First, we show that the estimate based on defect correction using collocation (section 3.3) for the solution of the neighboring problems does not work efficiently when applied to problems with an essential singularity, cf. example 1.

Example 1. We consider the simple scalar terminal value problem

$$z'(t) = \frac{1}{t^\alpha} z(t) + \mathrm{e}^t - \frac{\mathrm{e}^t}{t^\alpha}, \qquad z(1) = \mathrm{e}, \tag{34}$$

for $\alpha = 3$. The exact solution is given by $z(t) = \mathrm{e}^t$. In table 2 we show the error of the collocation solution, the error of the error estimate, and associated empirical convergence rates for every (equidistant) step size h, where the basic numerical approximation for (34) is computed using collocation at $m = 4$ equidistant collocation points.

Table 2
Error of error estimate based on collocation for (34), $m = 4$.

h	$\mathrm{err_{coll}}$	$\mathrm{ord_{coll}}$	$\mathrm{err_{est}}$	$\mathrm{ord_{est}}$
1/16	1.824E−09		2.403E−08	
1/32	1.106E−10	4.04	5.357E−09	2.17
1/64	6.796E−12	4.03	1.075E−09	2.32
1/128	4.208E−13	4.01	2.460E−10	2.13
1/256	2.953E−14	3.83	3.292E−10	−0.42

Table 3
Error of error estimate based on box scheme for (34), $m = 4$.

h	$\mathrm{err_{coll}}$	$\mathrm{ord_{coll}}$	$\mathrm{err_{est}}$	$\mathrm{ord_{est}}$
1/16	1.824E−09		6.088E−10	
1/32	1.106E−10	4.04	2.814E−11	4.43
1/64	6.796E−12	4.03	1.203E−12	4.55
1/128	4.208E−13	4.01	4.266E−14	4.82
1/256	2.953E−14	3.83	1.442E−14	1.56

As expected, we observe an experimental convergence order 4 for the error. On the other hand, the error of the error estimate based on collocation suffers from a significant order reduction down to almost 2. The absolute value of the error estimate is generally much larger than the global error of the collocation solution. Consequently, this error estimation method cannot be used reliably for problems with an essential singularity. Further examples with massive order reductions can be found in [2].

The performance of the estimates based on the defect correction principle using the box scheme (section 3.2) and mesh halving (section 3.4) is more promising. The results are given in tables 3 and 4, respectively. For step sizes $h = 1/16$ down to $h = 1/128$, we observe an empirical convergence order of about 4.5 for the error of the error estimate which is therefore seen to be asymptotically correct. For smaller step sizes, the computations are dominated by roundoff error.

Both estimates show a similar asymptotic behavior. The error of the error estimate as compared with the exact global error is generally $\mathrm{O}(\mathbf{h}^{m+\gamma})$, where $0 < \gamma < 1$. We observed in [2,4,9] that γ decreases when the parameter α in (1) increases. This is consistent with our conjecture that the global error of the collocation solution has the form (18) rather than (17), see [9].

To underline the good performance of the error estimators based on defect correction using the box scheme and on mesh-halving, we consider two further examples from [18,24]. Since the exact solutions are unknown, we compute a reference solution by collocation at $m = 6$ equidistant collocation points on a mesh with step size $h = 1/1000$. This solution is used to determine the errors of the collocation solution and the errors of the error estimates.

Table 4
Error of error estimate based on mesh halving for (34), $m = 4$.

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/16	1.824E−09		1.610E−11	
1/32	1.106E−10	4.04	6.942E−13	4.54
1/64	6.796E−12	4.03	3.969E−14	4.13
1/128	4.208E−13	4.01	3.952E−15	3.33
1/256	2.953E−14	3.83	5.892E−15	−0.58

Table 5
Error of error estimate based on box scheme for (35), $m = 4$.

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/16	9.837E−05		5.574E−05	
1/32	4.473E−06	4.46	1.504E−06	5.21
1/64	2.962E−07	3.92	2.974E−08	5.66
1/128	1.820E−08	4.02	8.288E−10	5.17
1/256	1.091E−09	4.06	2.401E−11	5.11
1/512	6.628E−11	4.04	7.203E−13	5.06

Example 2. We consider the linear boundary value problem

$$z'(t) = \frac{1}{t^{\alpha+2}} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & \alpha t^{\alpha+1} & -1 & 0 \\ 0 & 0 & 2\alpha t^{\alpha+1} & -1 \\ 4 & 0 & 0 & 3\alpha t^{\alpha+1} \end{pmatrix} z(t), \tag{35a}$$

$$\begin{pmatrix} 4 & -2 & 0 & 1 \\ -2 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 4 & 2 & 0 & -1 \\ 2 & 2 & 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \tag{35b}$$

with $\alpha = 1$. The numerical results are shown in tables 5 and 6. In the same experimental setting as in example 1, the collocation method leads to an empirical convergence order 4 for the error. Defect correction based on the box scheme as well as mesh-halving lead to asymptotically correct error estimates. For both strategies, the error of the error estimation is of order 5 and therefore of higher order compared to the discretization error.

Example 3. Finally, the following nonlinear boundary value problem is taken from [24]:

$$z'(t) = \frac{1}{t^2} \begin{pmatrix} -z_2(t) \\ -z_3(t) \\ -z_4(t) \\ 1 - \mathrm{e}^{-z_1(t)/2} \end{pmatrix}, \tag{36a}$$

Table 6
Error of error estimate based on mesh halving for (35), $m = 4$.

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/16	9.837E−05		4.197E−06	
1/32	4.473E−06	4.46	1.635E−07	4.68
1/64	2.962E−07	3.92	4.724E−09	5.11
1/128	1.820E−08	4.02	1.446E−10	5.03
1/256	1.091E−09	4.06	4.400E−12	5.04
1/512	6.628E−11	4.04	1.358E−13	5.02

Table 7
Error of error estimate based on box scheme for (36).

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/16	4.172E−03		4.272E−03	
1/32	2.404E−04	4.12	2.014E−04	4.41
1/64	7.968E−06	4.92	3.667E−06	5.78
1/128	5.416E−07	3.88	9.741E−08	5.23
1/256	3.608E−08	3.91	2.427E−09	5.33
1/512	2.171E−09	4.05	1.997E−11	3.60

Table 8
Error of error estimate based on mesh halving for (36), $m = 4$.

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/16	4.172E−03		3.097E−04	
1/32	2.404E−04	4.12	1.874E−05	4.05
1/64	7.968E−06	4.92	4.084E−07	5.52
1/128	5.416E−07	3.88	1.335E−08	4.94
1/256	3.608E−08	3.91	3.805E−10	5.13
1/512	2.171E−09	4.05	1.170E−11	5.02

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{36b}$$

As before, we consider collocation at $m = 4$ equidistant collocation points. The numerical results for error estimation based on defect correction using the box scheme are shown in table 7. Table 8 provides the results for error estimation based on mesh halving. Again, we obtain the expected convergence order 4 for the discretization error and asymptotically correct error estimation for both strategies.

For the last examples (35) and (36), we even observe an order $m + 1 = 5$ for both error estimates. If we take a look at the order of magnitude of the errors of the two error estimates, however, we note that even though the estimates have the same asymptotic qualities, the error of the estimate based on mesh halving is smaller throughout our numerical experiments, see also [2]. Thus, we should expect the error based on mesh halving to work more reliably. However, this is also the computationally more expensive procedure. It is therefore not clear which of these two estimates is more favorable for the efficiency of the implementation of a collocation solver designed especially for the numerical solution of boundary value problems with an essential singularity. We attempt to answer this question in the next section.

6. Performance comparisons

In this section, we compare the performance of our MATLAB collocation solver for boundary value problems with an essential singularity, where alternatively we use the error estimates from sections 3.2 and 3.4 as the basis for adaptive mesh refinement, see [3,6].

Our mesh adaptation is based on the equidistribution of the global error of the numerical solution. Thus, we define a *monitor function* $\Theta(t) := \sqrt[m]{\mathcal{E}(t)}/h(t)$, where $\mathcal{E}(t)$ is any asymptotically correct a posteriori error estimate and $h(t) := h_i$ for $t \in J_i$. Now, the mesh selection strategy aims at the equidistribution of

$$\int_{\tilde{\tau}_i}^{\tilde{\tau}_{i+1}} \Theta(t)\,\mathrm{d}t$$

on the mesh consisting of the points $\tilde{\tau}_i$ to be determined accordingly, where at the same time measures are taken to ensure that the variation of the step sizes is restricted and tolerance requirements are satisfied with small computational effort. Details of the mesh selection algorithm and a proof that our strategy implies that the global error of the numerical solution is *asymptotically equidistributed* are given in [6].

Here, we compare the run times t_{run} of our code until a mixed stopping criterion, with absolute and relative tolerances both set to $TOL = 10^{-3}$, 10^{-6}, 10^{-9}, is satisfied. Additionally, in tables 9 and 10 we give the number of mesh points N in the final meshes and the number fcount of evaluations of the right-hand side of the differential equation occurring in the solution process for problems (35) and (36), respectively. Moreover, the maximal values of the error estimates and of the true errors (computed w.r.t. a reference solution) are displayed. All experiments were carried out on a common PC with Athlon XP 1800 CPU and 2 GB of RAM running under Linux.

We observe that the numbers N are comparable for both variants of error estimation. The values of the absolute errors and error estimates show that in all cases the tolerances are reliably satisfied, but mesh halving seems to produce meshes better suited to reduce the global error. However, since the run times and the values of fcount are favorable for the estimate based on the box scheme, this is the best choice for reaching a specified tolerance efficiently. This view is supported by more comprehensive comparisons reported in [2].

Table 9
Performance comparisons for (35), $m = 6$.

	TOL	t_{run}	N	fcount	estimate	error
box scheme	1E−03	0.09	10	330	5.54E−05	1.27E−04
mesh halving	1E−03	0.12	10	360	1.64E−04	2.64E−06
box scheme	1E−06	0.14	15	825	6.83E−07	8.04E−07
mesh halving	1E−06	0.21	15	900	5.30E−07	1.02E−08
box scheme	1E−09	0.33	47	1574	5.58E−10	1.86E−10
mesh halving	1E−09	0.64	47	2808	4.06E−10	4.33E−12

Table 10
Performance comparisons for (36), $m = 6$.

	TOL	t_{run}	N	fcount	estimate	error
box scheme	1E−03	1.34	16	16652	5.17E−04	1.50E−03
mesh halving	1E−03	1.55	15	16560	5.73E−04	3.47E−05
box scheme	1E−06	4.29	44	45399	8.25E−09	4.57E−09
mesh halving	1E−06	6.54	44	58896	1.83E−08	2.16E−10
box scheme	1E−09	9.71	102	89431	1.80E−10	6.84E−10
mesh halving	1E−09	16.69	104	135522	5.77E−10	8.60E−12

7. Conclusions

We have investigated the convergence properties and performance of three different a posteriori error estimates for the numerical approximations of the solution of boundary value problems computed by polynomial collocation methods. For two error estimation schemes based on the defect correction principle, we have shown the rapid convergence of the estimates towards the true errors of the collocation solutions for regular problems and for problems with a singularity of the first kind. For problems with an essential singularity, the error estimate based on defect correction using collocation as auxiliary method does not show satisfactory convergence properties. The same estimate using the box scheme instead shows the same favorable asymptotic properties as an error estimate based on mesh halving. The absolute value of the error of the latter, computationally more expensive, estimate is smaller, however. In the last section, we compared the performance of our MATLAB code `sbvp` when either of the estimates is used as the basis for mesh selection. It turned out that the estimate based on the box scheme serves to meet tolerance requirements more efficiently, while the estimate based on mesh halving produces more favorable meshes, where the absolute error of the numerical solution is generally smaller for a value of N not exceeding that for the alternative estimate.

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