

Gaussian collocation via defect correction

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Summary. For the numerical integration of boundary value problems for first order ordinary differential systems, collocation on Gaussian points is known to provide a powerful method. In this paper we introduce a defect correction method for the iterative solution of such high order collocation equations. The method uses the trapezoidal scheme as the 'basic discretization' and an adapted form of the collocation equations for defect evaluation. The error analysis is based on estimates of the contractive power of the defect correction iteration. It is shown that the iteration produces $O(h^2)$ convergence rates for smooth starting vectors. A new result is that the iteration damps all kind of errors, so that it can also handle non-smooth starting vectors successfully.

Subject classifications: AMS(MOS): 65L10; CR: GI.7.

1 Introduction

We consider boundary value problems for first order systems of ordinary differential equations

(1.1) $y'(x) = f(x, y(x)), \quad x \in [0, 1],$ $b(y(0), y(1))=0$

where $f: [0, 1] \times \mathbb{R}^n \to \mathbb{R}^n$ and $b: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ are smooth functions. For these problems collocation schemes based on continuous piecewise polynomials have been extensively investigated in the numerical literature (e.g. deBoor and Swartz [71, Weiss [14], Ascher et al. [11, Ascher et al. [2]). A favourable feature of these schemes is the superconvergence property which is obtained if special classes of collocation nodes, such as Gaussian or Lobatto points, are used.

Since the effort required for the computation of the collocation spline grows rapidly with the order of the scheme, techniques for an efficient solution of high order collocation equations are of interest. One approach in this direction was described by Frank and Überhuber [9]. They observed that the fixed points of certain iterated defect correction methods permit a characterization as collocation splines. This result suggested the application of defect corrections for the iterative solution of the collocation equations. However, as it turned out, the method of Frank and Überhuber $[9]$ produced satisfactory convergence rates only in the special case of a collocation scheme with equidistant collocation nodes. In other cases, in particular for superconvergent schemes, the method worked rather poorly.

In this paper we present a defect correction method which overcomes this drawback. The main idea is to use two different grids, one consisting of the collocation points, the other consisting of equidistant points within each collocation subinterval. The collocation equations can be reformulated in terms of the values on the (piecewise) equidistant grid. This form of the collocation equations is used for defect evaluation. The trapezoidal scheme on the piecewise equidistant grid is employed as the 'basic discretization'. Our method becomes most attractive if either the order of the collocation scheme or the dimension of the differential system is large. In these cases the amount of computational work required for the solution of the collocation equations is considerably reduced. As with other iterative methods, the application of our method also increases the flexibility of the numerical solution process. The difference from other defect correction methods becomes most striking if Gaussian collocation points are used for defect evaluation. In that case we can achieve a final order of accuracy twice as high as standard defect correction methods with a comparable amount of work for each iteration step.

An outline of the paper follows. In Sect. 2 we recall some known properties of collocation schemes. Section 3 contains the description of our method and a brief demonstration of its efficiency. An error analysis of the method is given in Sects. 4 and 5. For the sake of simplicity we confine ourselves in these sections to linear boundary value problems

(1.2)
$$
Ly := y' - Ay = g, \quad By := B_0 \ y(0) + B_1 \ y(1) = \beta
$$

where $A(x)$, B_0 , $B_1 \in \mathbb{R}^{n \times n}$, $g(x)$, $\beta \in \mathbb{R}^n$. Using standard linearization techniques, the results can, however, be generalized to the nonlinear case. In Sect. 6 we present some numerical results obtained for nonlinear problems. An important topic not discussed in this paper is 'defect updating', i.e. the use of varying defect operators, the orders of which are increased during the iteration. It should also be mentioned that our method is not suited for extremely stiff problems.

The error analysis given in Sects. 4 and 5 is based on estimates of the contractive power of the defect correction iteration using Sobolev norms of various orders. To obtain realistic results, in particular for smooth starting vectors, a lower order Sobolev norm of the current iteration error must be estimated by a higher order norm of the previous error. Thus Sobolev norms of higher and higher orders have to be introduced during the iteration. An interesting effect occurs when the Sobolev order exceeds the order of the collocation scheme. Due to a saturation property of these norms, a global $O(h^2)$ -bound on the contractivity can be established for symmetric collocation schemes. Thus we can ensure that high order Sobolev norms of the iteration errors are decreased by an $O(h^2)$ -contraction factor per step, independently of the starting vector. Hence the success of the iteration does not depend on special properties of the starting vector, showing a certain robustness and flexibility of the method.

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We stress that this paper has gained from the ideas presented in Stetter [13], Frank and Oberhuber [9], B6hmer [4] and B6hmer et al. [5]. Contractivity results have also been obtained by Christiansen and Russell [8] and Skeel [12] for variants of the deferred correction procedure of Lentini and Pereyra [10] and by Auzinger and Monnet [3] for a defect correction method for second order boundary value problems. However, to our knowledge no attempt has been made so far to take advantage of particular properties of the 'target method' as we do by exploiting superconvergence.

2 Collocation schemes

Throughout the paper we assume that problem (1.1) possesses a (locally) unique solution z and that the functions f and b are sufficiently smooth.

Let

$$
\Delta_h = \{0 = x_0 < x_1 < \dots < x_N = 1\}
$$

be a grid in $[0, 1]$ with stepsizes

$$
h_i = x_{i+1} - x_i
$$
, $h = \max_{i=0,...,N-1} h_i$.

Further let, for some $k > 0$, a fixed set of points

$$
0 \le \xi_1 < \xi_2 < \ldots < \xi_k \le 1
$$

be given and set the collocation points as

$$
x_{i,j} := x_i + h_i \cdot \xi_j
$$
, $i = 0, ..., N-1, j = 1, ..., k$.

The $C⁰$ -collocation scheme is defined as follows: Find a continuous function p: $[0, 1] \rightarrow \mathbb{R}^n$ which (componentwise) reduces to a polynomial of degree $\leq k$ on each subinterval $[x_i, x_{i+1}]$ and satisfies

(2.1)
$$
p'(x_{i,j}) = f(x_{i,j}, p(x_{i,j})) \text{ for } i = 0, ..., N-1, j = 1, ..., k,
$$

$$
b(p(0), p(1)) = 0.
$$

We call a collocation scheme symmetric, if the collocation nodes ξ_i are symmetrically distributed in [0, 1] (i.e. if $\xi_i = 1 - \xi_{k-i+1}$).

It is well-known (see e.g. deBoor and Swartz [7]) that the collocation scheme (2.1) is globally convergent of order k:

(2.2)
$$
p(x) - z(x) = O(h^{k}) \quad \text{for all } x \in [0, 1], \quad h \to 0.
$$

For special classes of collocation nodes ξ_j a superconvergence effect is achieved at the breakpoints $x_i \in A_h$: If, for some $l > 0$, the polynomial

$$
N(\xi) = (\xi - \xi_1) \cdot \ldots \cdot (\xi - \xi_k)
$$

satisfies the orthogonality relations

$$
\int\limits_0^1 N(\xi) \cdot P(\xi) d\xi = 0
$$

for all polynomials P of degree $\lt l$, then

(2.3)
$$
p(x_i) - z(x_i) = O(h^{k+1}).
$$

In particular, the schemes based on Gaussian points are superconvergent of order 2k, those based on Lobatto points of order $2(k-1)$. These schemes are also symmetric.

It will be convenient to use the formulation of collocation schemes as projection methods, as presented in deBoor and Swartz [7]. We introduce the spaces

$$
C^{m}(\Lambda_{h}) := C^{m}[x_{0}, x_{1}] \times ... \times C^{m}[x_{N-1}, x_{N}]
$$

$$
P^{m}(\Lambda_{h}) := P^{m}[x_{0}, x_{1}] \times ... \times P^{m}[x_{N-1}, x_{N}]
$$

where $C^m(I)$ denotes the space of *m*-times continuously differentiable functions from the interval I into \mathbb{R}^n , $P^m(I)$ the space of (componentwise) polynomials of degree not exceeding *m* on *I*. If ϕ is an element of $C^m(A_h)$ or $P^m(A_h)$, then $\phi = (\phi_0, \dots, \phi_{N-1})$ where each piece ϕ_i is an element of $C^m[x_i, x_{i+1}]$ or $P^m[x_i, x_{i+1}]$. Operations on $C^m(A_h)$ or $P^m(A_h)$, such as addition, multiplication or differentiation, are defined by applying the operation to each piece. For example, the differentiation operator $\phi \rightarrow \phi'$ maps $C^m(\Lambda_h)$ onto $C^{m-1}(\Lambda_h)$ and $P^m(\Lambda_h)$ onto $P^{m-1}(\Lambda_h)$.

We also introduce the space

$$
P^{k,0}(\Lambda_h) := P^k(\Lambda_h) \cap C[0,1] := \{ p \in P^k(\Lambda_h) : p_i(x_i) = p_{i-1}(x_i), i = 1, ..., N-1 \}
$$

and the interpolation operator

$$
Q_h: C^0(\Lambda_h) \to P^{k-1}(\Lambda_h)
$$

 $(Q_h \phi)_i$ = interpolation polynomial of ϕ_i with respect to $x_{i,1}, \ldots, x_{i,k}$.

Obviously the collocation problem can now be formulated in the equivalent form: Find $p \in P^{k,0}(\Lambda_h)$ such that

(2.5)
$$
Q_h(p'-f(\cdot,p))\equiv 0, \qquad b(p(0), p(1))=0.
$$

We equip $C^m(\Lambda_h)$ with the Sobolev norm

(2.6)
$$
\|\phi\|_{m} := \sum_{\mu=0}^{m} \max_{i=0,\dots,N-1} \max_{x \in [x_{i},x_{i+1}]} |\phi_{i}^{(\mu)}(x)|
$$

where $|\cdot|$ denotes a fixed norm on \mathbb{R}^n . The norms (2.6) will also be used on the spaces $P^{k-1}(\Lambda_k)$ and $P^{k,0}(\Lambda_k)$.

The following estimates are easy to prove:

(2.7)
$$
\|Q_h \phi\|_m \leq C \|\phi\|_m, \qquad 0 \leq m \leq k-1,
$$

(2.8) *II(Qh-l)~H~Chm-tll~llm, l<m<k, O<l<m*

for all $\phi \in C^m(A_h)$, where C is independent of ϕ and A_h . Furthermore, *if* $p \in P^k(A_h)$ then

(2.9)
$$
\max_{x \in [x_1, x_{i+1}]} |p_i^{(l)}(x)| \leq \frac{C}{h_i^{l-m}} ||p||_m, \quad 0 \leq m \leq k, \ m < l \leq k.
$$

3 Defect corrections for the solution of the collocation problem

We introduce a further grid

(3.1)
$$
\Gamma_{h} := \left\{ t_{i,j} := x_{i} + h_{i} \cdot \frac{j}{k} : j = 0, ..., k, i = 0, ..., N - 1 \right\},
$$

i.e. Γ_h is derived from Δ_h by inserting $k+1$ equidistant points into each subinterval $[x_i, x_{i+1}]$. The stepsizes of Γ_h will be denoted by $\overline{h}_i := h_i/k$.

For gridfunctions y_h : $\overrightarrow{L}_h \rightarrow \mathbb{R}^n$ we write $y_{i,j}$ instead of $y_h(t_{i,j})$. Since $t_{i,0}$ $=t_{i-1,k}=x_i$, the gridfunctions are assumed to satisfy

$$
y_{i,0} = y_{i-1,k}, \quad i = 1, ..., N-1.
$$

Note that we now deal with two different grids, the 'x-grid' consisting of the collocation points and the piecewise equidistant 't-grid' Γ_h .

There is a one-to-one relation between the gridfunction space

$$
E_h := \{ y_h : \Gamma_h \to \mathbb{R}^n \}
$$

and the spline function space $P^{k,0}(\Lambda_k)$, given by

$$
(3.2) \t\t\t P_h: E_h \to P^{k,0}(\Lambda_h)
$$

 $(P_h y_h)_{i}$:=interpolation polynomial of $(t_{i,0}, y_{i,0}), \ldots, (t_{i,k}, y_{i,k}).$

This suggests that the collocation scheme possesses an equivalent formulation in terms of a discretization method on Γ_h . In fact, if $p \in P^{k,0}(\Lambda_h)$, then $y_h := p_{\Gamma_h}$ satisfies

$$
\frac{y_{i,j} - y_{i,j-1}}{\overline{h_i}} = \frac{1}{\overline{h_i}} \cdot \int_{t_{i,j-1}}^{t_{i,j}} p'(t) dt = \sum_{i=1}^{k} w_{j,i} \cdot p'(x_{i,i})
$$

where the $w_{i,t}$ are interpolatory quadrature weights, formally defined by

$$
(3.3) w_{j,l} := k \int_{(j-1)/k}^{j/k} L_l(\xi) d\xi, \qquad L_l := l \text{-th Lagrange polynomial w.r.t. } \xi_1, \ldots, \xi_k.
$$

Hence, if p solves the collocation equations (2.1), then y_h satisfies

$$
(3.4) \quad \frac{y_{i,j} - y_{i,j-1}}{h_i} = \sum_{l=1}^{k} w_{j,l} \cdot f(x_{i,l}, (P_h y_h)(x_{i,l})), \qquad i = 0, \ldots, N-1, \ j = 1, \ldots, k.
$$

Conversely, if y_h is a solution of these equations and $p:=P_h y_h$, then we may go back through the above transformation to arrive at

$$
\sum_{l=1}^{k} w_{j,l}(p'(x_{i,l}) - f(x_{i,l}, p(x_{i,l}))) = 0, \quad i = 0, ..., N-1, j = 1, ..., k.
$$

Now it is elementary to verify that the matrix $W := (w_{i,t})_{i,t \in \{1,\ldots,k\}}$ is nonsingular. Hence *must solve the collocation equations. Thus we have proved*

Theorem 1. $p \in P^{k,0}(\Lambda_h)$ is a solution of the collocation problem (2.1) if and only *if* $y_h := p_{1r}$ satisfies the Eqs. (3.4) and the boundary condition $b(y_h(0), y_h(1)) = 0$.

Remark. If we allow P_h to be *any* linear operator from E_h into $P^k(\Lambda_h)$ (i.e. if we drop the interpolation condition on P_n), then starting from (3.4) we arrive at a scheme of the form

$$
p'(x_{i,j}) - f(x_{i,j}, (P_h p)(x_{i,j})) = 0, \quad i = 0, \ldots, N-1, j = 1, \ldots, k.
$$

It has been proved by Norsett and Wanner [11] that these 'perturbed collocation schemes' comprise all (interpolatory) Runge Kutta schemes. This would suggest some generalizations of the following analysis which, however, will not be discussed in this paper.

Theorem 1 shows that the collocation spline can be identified with the solution y^* of the equation

(3.5) where (3.6) $F^*_{k}v^*_{k}=0$ F^* : $E_{h} \rightarrow \hat{E}_{h}$ $(F_{h}^{*} y_{h})_{0} := b(y_{h}(0), y_{h}(1))$ $(F_h^* y_h)_{i,j} = \frac{y_{i,j} - y_{i,j-1}}{h_i} - \sum_{l=1}^k w_{j,l} \cdot f(x_{i,l}, (P_h y_h)(x_{i,l}))$

 $(i=0, \ldots, N-1, j=1, \ldots, k)$

with $\hat{E}_h = \{ \hat{e}_h = (\hat{e}_0; \hat{e}_{0,1}, \dots, \hat{e}_{0,k}, \dots, \hat{e}_{N-1,1}, \dots, \hat{e}_{N-1,k}) : \hat{e}_0, \hat{e}_{i,j} \in \mathbb{R}^n \}.$ (The component \hat{e}_0 corresponds to the boundary condition.)

By construction, the operator F_h^* has a form very similar to the discretization operator of the trapezoidal rule on Γ_h :

(3.7)
\n
$$
F_h: E_h \to \hat{E}_h
$$
\n
$$
(F_h y_h)_{0} := b(y_h(0), y_h(1))
$$
\n
$$
(F_h y_h)_{i,j} := \frac{y_{i,j} - y_{i,j-1}}{\overline{h}_i} - \frac{1}{2} (f(t_{i,j}, y_{i,j}) + f(t_{i,j-1}, y_{i,j-1}))
$$
\n
$$
(i = 0, ..., N - 1, j = 1, ..., k).
$$

This suggests considering the iterative solution of (3.5) by means of the defect correction process (Stetter [13], Böhmer [4])

$$
(3.8) \tLh(yhm - yhm-1) = -Fh* yhm-1, \t m = 1, 2, ...
$$

where

$$
L_h = F'_h(y_h^0)
$$

is the derivative of F_h at y_h^0 . The starting vector y_h^0 may be chosen as the solution of

$$
(3.9) \t\t\t F_h y_h^0 = 0
$$

however our analysis will, to a certain degree, be independent of this choice.

If we assume that L_h^{-1} exists, then (3.8) is well-defined and its fixed points coincide with the solutions of (3.5). Hence, if (3.8) is convergent, the iterates will tend to a vector representing the values of the collocation spline on the grid Γ_h .

Remark. The process (3.8) is an application of the general defect correction principle, as explained e.g. in Böhmer et al. [5]. This version of defect corrections, also known as the 'linearized version of defect corrections' or the 'discrete Newton method', is due to Böhmer [4]. We might take other versions into consideration, for example 'version B' of Stetter [13]

$$
(3.10) \tF_h y_h^m = F_h y_h^{m-1} - F_h^* y_h^{m-1}
$$

which differs from (3.8) mainly in the treatment of nonlinearities. In our case the linearized version (3.8) has the advantage, that it requires evaluations of the right hand side f on the 'x-grid' only, whereas (3.10) would require function evaluations both on the 'x-grid' and the 't-grid'. Since our numerical experiments indicate no significant difference between the behaviour of (3.8) and (3.10), we shall deal only with (3.8) in this paper.

To give a brief demonstration of the efficiency of (3.8), we consider a linear boundary value and compare the effort of a direct solution method for the collocation equations to that of the iterative method (3.8). Using the Runge-Kutta formulation of the collocation problem results in a linear system of dimension $\approx N k n$. When this system is solved by Gaussian elimination, the leading term in the operational count becomes

$$
\frac{1}{3}Nk^3n^3
$$

(el. Weiss [14]). Now consider the iterative solution of the collocation problem by means of (3.8), (3.9). The computation of y_h^0 from (3.9) requires roughly $\frac{1}{3}N k n^3$ operations. We shall prove below that $(k-1)$ iterations suffice to solve (3.5) up to an error of size $O(h^{2k})$. Straightforward implementation of the defects in the form (3.6) requires for each iteration the evaluation of $p:=P_hy_h^{m-1}$ at the collocation points $x_{i,j} (\approx N k^2 n$ operations), the computation of $(A p - g)(x_{i,j})$ ($N k n²$ operations) and the evaluation of the sums in (3.6) $(N k² n)$ operations). The effort for evaluating $A(x_{i,j})$, $g(x_{i,j})$ is not counted, since these values can, at least in principle, be saved. Once the defect $F_h^* y_h^{n-1}$ is available, the solution of (3.8) for y_{μ}^{m} takes roughly 2 N k n^{2} operations, assuming that the LU-factorization of L_b has been stored. The leading term in the operational count for solving (3.9) and performing $k-1$ iterations (3.8) thus becomes

$$
(3.12) \t\t N(\frac{1}{3}k n^3 + 2 k^3 n + 3 k^2 n^2).
$$

Since the exponents of k and n in (3.11) sum up to six, but those in (3.12) to four, the application of (3.8) will be advantageous if either k or n is large.

4 Convergence of the defect correction iteration

We consider the case of a linear boundary value problem of the form (1.2). In that case F_h and F_h^* become affine-linear operators and we denote their linear parts L_h and $L[*]_h$, respectively. The recursion for the iteration error is

 $y_h^m - y_h^* = M_h(y_h^{m-1} - y_h^*).$

where

(4.1) $M_h := (L_h)^{-1} (L_h - L_h^*)$.

Thus the convergence of the iteration (3.8) is determined by the 'contractivity' of M_h and our aim in this section is the derivation of norm bounds on M_h . These bounds will be given by means of Sobolev norms: For $m \in \mathbb{N}$, $e_h \in E_h$ let

(4.2) *]] eh* I[,, := [I Pa eh II re"

It is easy to verify that $\|\cdot\|_m$ is equivalent, uniformly in h, to the 'discrete' Sobolev norm

(4.3)
$$
\langle\!\langle e_h \rangle\!\rangle_m = \sum_{\mu=0}^m \max_{i=0,...,N-1} \max_{j=0,...,k-\mu} |e_h[t_{i,j},...,t_{i,j+\mu}]|
$$

where $[\cdot, ..., \cdot]$ denotes divided differences. Note that the divided differences in (4.3) involve only function values taken from the same subinterval $[x_i, x_{i+1}]$ (no 'overlapping'). Thus, our definition differs somewhat from the usual definition of discrete Sobolev norms.

The following saturation property of $\|\cdot\|_k$ is trivial, but worthy of mention: If $m > k$, then $||e_h||_m = ||e_h||_k$.

Theorem 2. For the 'error amplification operator' M_h of (3.8) the following esti*mates hold*

(4.4) $\|M_h e_h\|_m \leq C h \|e_h\|_m, \qquad 1 \leq m \leq k,$

and

(4.5) $\|M_{k}e_{k}\|_{m} \leq C h^{2} \|e_{k}\|_{m+1}, \quad 1 \leq m \leq k-1.$

If the collocation scheme is symmetric, then

(4.6)
$$
||M_h e_h||_k \leq C h^2 ||e_h||_k.
$$

Note that the estimates of this theorem are valid without any smoothness conditions imposed on the grids. The only restriction is that the grid Γ_h must be equidistant within each subinterval $[x_i, x_{i+1}]$.

Before we turn to the proof of Theorem 2 we give an immediate

Corollary 1. For the spectral radius $\rho(M_h)$ of M_h the estimate

$$
\rho(M_h) = O(h)
$$

holds. If the collocation scheme is symmetric, then

$$
\rho(M_h) = O(h^2).
$$

Proof. To obtain (4.7) we may choose any m in the range $1 \le m \le k$ and apply (4.4). The result for the symmetric case is a consequence of (4.6). \Box

Remark. Numerical experiments indicate that the $O(h^2)$ estimate for $\rho(M_h)$ is indeed valid only in the symmetric case. Furthermore, Sobolev norms of order less than k do not seem to reflect the $O(h^2)$ behaviour of $\rho(M_h)$.

For the proof of Theorem 2 we need two lemmas. The first one contains a stability estimate and will later be used to treat the L_h^{-1} factor in M_h . The second lemma, which contains the crucial and most laborious part of the proof, gives estimates for the $(L_h - L_h^*)$ factor involved in M_h . To formulate these lemmas we must extend the definition of Sobolev norms to the 'defect spaces' \hat{E}_h : If $\hat{e}_h \in \hat{E}_h$, then let r be the unique element of $P^{k-1}(A_h)$ which satisfies

$$
\sum_{l=1}^{k} w_{j,l} \cdot r(x_{i,l}) = \hat{e}_{i,j}, \quad i = 0, \dots, N-1, j = 1, \dots, k
$$

and set

(4.9) $\|\hat{e}_h\|_{m} := \|r\|_{m} + |\beta|$

where $\beta = \hat{e}_0$ is the boundary condition component of \hat{e}_h . Existence and uniqueness of r are immediately clear from the nonsingularity of the matrix W. We recall that

(4.10)
$$
\sum_{l=1}^{k} w_{j,l} \cdot r(x_{i,l}) = \frac{1}{\overline{h}_i} \int_{t_{i,j-1}}^{t_{i,j}} r(t) dt \quad \text{for all } r \in P^{k-1}(\Delta_h).
$$

Lemma 1. Let $1 \leq m \leq k$. There exists an $h_0 > 0$ and a bound S such that for *all* $h \leq h_0$

(4.11) *[1% I],, < S. ILL* ehllm- 1*

for all $e_h \in E_h$.

Proof. The proof uses a similar technique as developed in deBoor et al. [6], relating the stability bound of the 'discrete' problem to that of the 'continuous' problem.

Let $e_h \in E_h$. Set $\hat{e}_h := L_h^* e_h$ and let $r \in P^{k-1}(\Lambda_h)$ and $\beta \in \mathbb{R}^n$ be defined as in (4.9). In view of our definition of the norms, we have to show that for $p_i = P_h e_h$ the estimate

$$
||p||_{m} \leq S \cdot (||r||_{m-1} + |\beta|)
$$

holds. Theorem 1 shows that p satisfies the collocation equations

$$
Q_h L p = r, \qquad B p = \beta.
$$

Since $Q_h p' = p'$, we see that p solves the boundary value problem

$$
Lp = r + (Q_h - I) A p, \qquad Bp = \beta.
$$

Let G be the Greens operator for (L, B) and Y the fundamental system of L that satisfies $BY = I$. Then

$$
(4.12) \t\t\t p = Y\beta + Gr + G(Q_h - I) A p.
$$

Since G is the inverse of a first order differential operator, we have

and, using **(2.8),**

$$
||G(Q_h - I) A p||_{m} \leq K_1 Ch ||A p||_{m}
$$

\n
$$
\leq h K_1 C ||A||_{m} \cdot ||p||_{m}
$$

 $||Gr||_{m} \leq K$, $||r||_{m-1}$

where $||A||_m$ denotes the norm of the multiplication operator $A: C^m(A_h) \to C^m(A_h)$, $\varphi \rightarrow A \varphi$. Furthermore

$$
||Y\beta||_{m} \leq K_2 |\beta|.
$$

The constants K_1, K_2 depend only on the given boundary value problem. Substituting these estimates into **(4.12),** we get

$$
||p||_{m} (1 - h K_1 C ||A||_{m}) \leq K_1 ||r||_{m-1} + K_2 |\beta|.
$$

This proves (4.11) for sufficiently small h_0 . \Box

Lemma 2. The *following estimates hold*

(4.13) *[[(Lh--L*)ehll,,_l<Chrleh[[,., l<m<_k,*

and

(4.14) *N(Lh--L~)ehH,n_I <=Ch 2 Ileh]l,,+l, l<_m<--k--l.*

If the target collocation scheme is symmetric, then also

(4.15) *H(Lh-- g*)ehllk-1 <= C h 2 IPehll~.*

The validity of (4.14) and (4.15) seems to be restricted to the case where the $t_{i,j}$, $j = 0, \ldots, k$ are equidistant (i.e. we may not allow that $t_{i,j} = x_i + h_i \tau_i$, $\tau_i \neq j/k$).

Proof. We shall prove only (4.14) and (4.15), since the verification of (4.13) is completely analogous. We have

$$
((L_h - L_h^*) e_h)_{i,j} = \sum_{l=1}^k w_{j,l} \cdot \varphi(x_{i,l}) - \frac{1}{2} \cdot (\varphi(t_{i,j}) + \varphi(t_{i,j-1}))
$$

where

$$
\varphi:=A\cdot (P_h\,e_h).
$$

Let $r \in P^{k-1}(\Lambda_h)$ be defined by

$$
\frac{1}{2}(\varphi(t_{i,j}) + \varphi(t_{i,j-1})) - \sum_{l=1}^{k} w_{j,l} \cdot \varphi(x_{i,l}) = \sum_{l=1}^{k} w_{j,l} \cdot r(x_{i,l})
$$

Then $||(L_h - L_h^*)e_h||_{m-1} = ||r||_{m-1}$ and to obtain (4.14), (4.15) it is sufficient to show that

(4.16) $||r||_{m-1} \leq C h^2 ||\varphi||_{m+1}$, $1 \leq m \leq \begin{cases} k-1 & \text{in the non-symmetric case} \\ k & \text{in the symmetric case} \end{cases}$,

since $\|\varphi\|_{m+1} \leq \|A\|_{m+1} \|e_h\|_{m+1}$ and by the saturation property, $\|e_h\|_{k+1} = \|e_h\|_{k+1}$

We first treat the case $\varphi \in P^{k,0}(\Lambda_h)$. An application of the Euler-MacLaurin formula then yields

$$
(4.17) \qquad \frac{1}{2}\left(\varphi(t_{i,j})+\varphi(t_{i,j-1})\right)=\frac{1}{\overline{h}_i}\int\limits_{t_{i,j-1}}^{t_{i,j}}\varphi(t)\,dt+\sum\limits_{\mu=2}^k c_\mu\overline{h}_i^\mu\,\frac{1}{\overline{h}_i}\int\limits_{t_{i,j-1}}^{t_{i,j}}\varphi^{(\mu)}(t)\,dt
$$

with appropriate constants c_u (c_u = 0 for odd μ). On the other hand

$$
(4.18) \qquad \sum_{l=1}^{k} w_{j,l} \cdot \varphi(x_{i,l}) = \frac{1}{h_i} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(t) \, dt + \frac{1}{h_i} \int_{t_{i,j-1}}^{t_{i,j}} (Q_h - I) \, \varphi(t) \, dt.
$$

Taking the difference of (4.17) and (4.18) we obtain

$$
(4.19) \frac{1}{2} (\varphi(t_{i,j}) + \varphi(t_{i,j-1})) - \sum_{l=1}^{k} w_{j,l} \cdot \varphi(x_{i,l}) = \frac{1}{h_i} \int_{t_{i,j-1}}^{t_{i,j}} q(t) dt + \frac{1}{h_i} \int_{t_{i,j-1}}^{t_{i,j}} s(t) dt
$$

where

$$
s := (I - Q_h) \varphi
$$

and $q=(q_0, \ldots, q_{N-1})$ is defined by

$$
q_i(t) := \sum_{\mu=2}^k c_{\mu} \overline{h_i^{\mu}} \varphi^{(\mu)}(t), \qquad t \in [x_i, x_{i+1}].
$$

Since $\varphi \in P^{k,0}(\Lambda_h)$, q is clearly an element of $P^{k-1}(\Lambda_h)$. If s were also in $P^{k-1}(\Lambda_h)$, then, by (4.10) and (4.19), r could be represented as $r = q + s$. However, s is given by

$$
s_i(t) = (t - x_{i,1}) \dots (t - x_{i,k}) \frac{\varphi_i^{(k)}}{k!}, \quad t \in [x_i, x_{i+1}]
$$

and thus has degree k in general. To circumvent this difficulty we define

$$
\bar{s}(t) := \frac{d}{dt} (P_h S)(t), \qquad S(t) := \int_a^t s(x) \, d\,x.
$$

Then $\bar{s} \in P^{k-1}(\Lambda_k)$ and the right hand side of (4.19) remains unchanged, if s is replaced by \bar{s} :

$$
\frac{1}{\overline{h}_i} \int_{t_{i,j-1}}^{t_{i,j}} \overline{s}(t) dt = \frac{S(t_{i,j}) - S(t_{i,j-1})}{\overline{h}_i} = \frac{1}{\overline{h}_i} \int_{t_{i,j-1}}^{t_{i,j}} s(t) dt.
$$

We conclude that $r = a + \bar{s}$.

To prove (4.16), we treat the two terms q and \bar{s} separately. Since $\varphi \in P^{k,0}(\Lambda_h)$, the estimate (2.9) can be used to obtain

$$
|q_i^{(v)}(t)| = \left| \sum_{\mu=2}^{k-v} c_{\mu} \bar{h}_i^{\mu} \varphi_i^{(\mu+v)}(t) \right|
$$

$$
\leq \sum_{\mu=2}^{k-v} |c_{\mu}| \bar{h}_i^{\mu} \frac{C}{\bar{h}_i^{\mu-2}} ||\varphi||_{v+2} \leq C h^2 ||\varphi||_{v+2}
$$

for $0 \leq v \leq k-2$. Hence

$$
(4.20) \t\t\t ||q||_{m-1} \leq C h^2 ||\varphi||_{m+1}, \t 1 \leq m \leq k-1.
$$

Formula (2.8) shows that the same estimate is valid for s:

$$
(4.21) \t\t\t ||s||_{m-1} \leq C h^2 ||\varphi||_{m+1}, \t 1 \leq m \leq k-1.
$$

This estimate carries over to \bar{s} , since the definition of \bar{s} immediately implies $\|\bar{s}\|_{m-1} \leq C \|s\|_{m-1}$, $1 \leq m \leq k$. Combining (4.20) and (4.21), we obtain the desired estimate (4.16) for $1 \le m \le k-1$.

Now consider the symmetric case. Since $q^{(k-1)} \equiv 0$, the estimate (4.20) trivially extends to the case $m=k$, independently of the symmetry. The validity of the corresponding estimate for \bar{s} is less evident. We claim that, due to the symmetry, $\bar{s} \in P^{k-2}(\Lambda_h)$. Since $s_i(t)$ is a multiple of $(t-x_{i,1}) \dots (t-x_{i,k})$, the symmetry of the collocation points implies that s_i is an even (odd) function with resp. to the midpoint $\frac{1}{2}(x_i+x_{i+1})$, whenever k is even (odd). From the definition of \bar{s} we conclude that the same holds for \bar{s}_i . Consequently, $\bar{s} \in P^{k-2}(\Lambda_k)$ and

$$
\|\bar{s}\|_{k-1}=\|\bar{s}\|_{k-2}\leqq C\,\|s\|_{k-2}\leqq C\,h^2\,\|\varphi\|_{k}.
$$

This completes the proof in case $\varphi \in P^{k,0}(\Lambda_h)$.

If $\varphi \notin P^{k,0}(\Lambda_h)$, then we perform the above considerations with φ replaced by $p := P_h \varphi$. Writing $R_h \varphi$ for the r corresponding to φ and $R_h p$ for the one corresponding to p, we then have $R_h(\varphi - p) = -Q_h(\varphi - p)$ (since $\frac{1}{2}[\varphi(t_{i,j})]$) $+ \varphi(t_{i,j-1}) = \frac{1}{2} [p(t_{i,j}) + p(t_{i,j-1})]$. The desired estimates now follow from

$$
R_h \varphi = R_h p + Q_h (p - \varphi). \quad \Box
$$

Proof of Theorem 2. The stability estimate of Lemma 1 for $L[*]_h$ carries over to L_{h} , i.e. there is an $h_0 > 0$ and a bound \overline{S} such that for $h \leq h_0$

(4.22) *II eh H., < ~. [(Lh eh H,.- 1, 1 <_ m <_ k*

for all $e_h \in E_h$. This is an immediate consequence of Lemma 1 and Lemma 2 (4.13):

$$
||e_h||_m \leq S \cdot ||L_h^* e_h||_{m-1} \leq S(||L_h e_h||_{m-1} + ||(L_h^* - L_h) e_h||_{m-1})
$$

$$
\leq S ||L_h e_h||_{m-1} + S Ch ||e_h||_m.
$$

For sufficiently small h_0 we obtain (4.22).

The estimates of Theorem 2 for $M_h = (L_h)^{-1} (L_h - L_h^*)$ now are easily derived from (4.22) and the corresponding estimates of Lemma 2. \square

Theorem 2 clearly ensures that, for sufficiently small h , the iterates will converge to $v_{\mathbf{k}}^*$. Corollary 1 would suggest that the iteration errors are decreased by constant contraction factors of size $O(h)$ in the nonsymmetric case and $O(h^2)$ in the symmetric case. However, this gives only a very crude description of the 'real' numerical behaviour of the process. A more realistic description is contained in the following theorem.

Theorem 3. For the first $k-1$ iterations of (3.8) the estimates

$$
(4.23) \t\t\t ||y_n^m - y_h^*||_1 \leq C h^{2m} ||y_h^0 - y_h^*||_{m+1}, \t 1 \leq m \leq k-1,
$$

hold (independently of the symmetry). For subsequent iterations we have

$$
(4.24) \quad \|y_h^m - y_h^*\|_1 \leq \begin{cases} C \, h^{2m} \, \|y_h^0 - y_h^*\|_k & \text{in the symmetric case} \\ C \, h^{k+m-1} \, \|y_h^0 - y_h^*\|_k & \text{in the non-symmetric case} \end{cases}, \quad m \geq k.
$$

Proof. For the first $k-1$ iterations we get from (4.5)

$$
\|y_h^m - y_h^*\|_1 \leq C h^2 \|y_h^{m-1} - y_h^*\|_2 \leq \ldots \leq C h^{2m} \|y_h^0 - y_h^*\|_{m+1}.
$$

If $m \geq k$, the orders of the Sobolev norms on the right hand side exceed k and the results now depend on whether the collocation scheme is symmetric or not. In the symmetric case we obtain for $m \ge k$, using (4.6),

$$
||y_n^m - y_n^*||_1 \le \dots \le C h^{2(k-1)} ||y_n^{m-(k-1)} - y_n^*||_k
$$

\n
$$
\le C h^{2k} ||y_n^{m-k} - y_n^*||_k \le \dots \le C h^{2m} ||y_n^0 - y_n^*||_k
$$

and in the non-symmetric case, using (4.4) for $m = k$,

$$
||y_{h}^{m} - y_{h}^{*}||_{1} \leq \dots \leq C h^{2(k-1)} ||y_{h}^{m-(k-1)} - y_{h}^{*}||_{k}
$$

\n
$$
\leq C h^{2k-1} ||y_{h}^{m-k} - y_{h}^{*}||_{k} \leq \dots \leq C h^{k+m-1} ||y_{h}^{0} - y_{h}^{*}||_{k}.
$$

We stress that the estimates (4.23) and (4.24) give a rather precise prediction of the behaviour of the iteration observed in practice. Note that for $m < k$ a quite complicated situation may arise, since the Sobolev norms appearing on the right hand side of (4.23) depend on m. For example, if the starting vector is very smooth (say $||y_h^0 - y_h^*||_{m+1} = O(1)$ for all *m*) then two powers of h may be gained with each iteration step. However, if the starting vector is rough (say $||y_h^0 - y_h^*||_m = O(h^{-m})$), then each step may yield only one power of h. The situation gets clearer after the first $k-1$ iterations have been performed. Since the Sobolev order occuring on the right hand side of (4.24) remains constant, we now gain one or two powers of h per step, depending on the symmetry, but independent of the starting vector. Roughly speaking, after the first $k-1$ iterations have been performed, the error reduction proceeds as described by the estimates for $\rho(M_h)$ given in Corollary 1, while in the initial phase the behaviour is also determined by the smoothness of the starting vector.

5 Order results

In the previous section we were concerned with the convergence of the iterates y_k^m to the fixed point y_k^* . We now consider convergence to the exact solution z of the problem. The error of the *m*-th iterate can be decomposed into

(5.1)
$$
y_h^m - z_h = (y_h^m - y_h^*) + (y_h^* - z_h), \qquad z_h := z_{|F_h}.
$$

For small h, the effect of the iteration is to decrease the first term, the iteration error $y_{n}^{m}-y_{n}^{*}$, so that the accuracy of the iterates will increase until the level of the second term, the discretization error $y_i^* - z_h$ of the target collocation scheme, is reached.

We consider in more detail the case where the starting vector y_h^0 is obtained from (3.9) as the solution of the trapezoidal scheme. We shall prove below that in this case

$$
(5.2) \t\t\t\t ||y_h^0 - y_h^*||_m = O(h^2), \t 1 \le m \le k - 1
$$

and

(5.3) σ_0 \downarrow σ *(O(h²)* for symmetric collocation schemes \mathcal{V}^{h} \mathcal{V}^{h} ¹⁸ $\{O(h)$ for non-symmetric collocation schemes

Inserting these estimates into (4.23), we obtain

(5.4)
$$
|y_h^m(x_i) - z(x_i)| \leq |y_h^m(x_i) - y_h^*(x_i)| + |y_h^*(x_i) - z(x_i)|
$$

$$
\leq O(h^{2(m+1)}) + O(h^{k*}), \quad 1 \leq m \leq k - 2
$$

and

 $k = 1$ \cdots $\qquad \qquad$ $\qquad (O(h^{2k}) + O(h^{k})$ for symmetric collocation schemes $|y_h^* - (x_i) - z(x_i)| \geq 0(h^{2k-1}) + O(h^{k})$ for non-symmetric collocation schemes

where k_{\ast} is the order of (super-)convergence of the target collocation scheme. Since $k_* \le 2k$ and $k_* = 2k$ is achieved only for the (symmetric) Gaussian scheme, we get

Theorem 4. *If the defect correction iteration* (3.8) *is started from the solution* y_h^0 of the trapezoidal scheme (3.9), then for the error at the breakpoints $x_i \in A_h$ *the estimate*

(5.5)
$$
y_n^m(x_i) - z(x_i) = O(h^{\min(2(m+1),k_*)}), \quad m = 0, 1, ...
$$

holds, where k_{\ast} *is the order of (super-)convergence of the target collocation scheme. In particular, for the method based on Gaussian points*

(5.6)
$$
y_h^m(x_i) - z(x_i) = O(h^{2(m+1)}), \quad m = 0, ..., k-1.
$$

Proof. It remains to verify (5.2) and (5.3). Since $F_h y_h^0 = 0$, $F_h^* y_h^* = 0$, we have

$$
L_h(y_h^0 - y_h^*) = F_h y_h^0 - F_h y_h^* = F_h^* y_h^* - F_h y_h^*.
$$

Replacing $L_h - L_h^*$ by $F_h - F_h^*$ in the proof of Lemma 2, we obtain an estimate of the form

$$
||F_h^* y_h^* - F_h y_h^* ||_{m-1} \leq C h^2 ||A p + g||_{m+1}, \qquad 1 \leq m \leq k-1,
$$

where $p:=P_h y_h^*$ is the collocation spline. From the stability estimate (4.22) we conclude that

$$
||y_h^0 - y_h^*||_m \leq S C h^2 (||A||_{m+1} ||p||_{m+1} + ||g||_{m+1}).
$$

Using Lemma 1, it is easily verified that $||p||_{m+1}$ is bounded, independently of h. This proves (5.2). The verification of (5.3) is analogous. \Box

With a 'normal' collocation scheme no superconvergence effects occur and $k_* = k$ in (5.5). The $O(h^k)$ bound thus obtained for the last successful iterate $\overline{\text{is}}$ a typical result for defect correction procedures based on k -th order defect evaluations (see e.g. Frank and Überhuber [9], Böhmer [4]). However, with our method, a final order of accuracy twice as high can be achieved, if the defect evaluation is based on Gaussian points. To put it another way, our method allows for a reduction of the degree of the interpolating polynomials to half of that required by standard defect correction methods.

6 Numerical examples

To illustrate the numerical behaviour of our method, we consider the simple test problem

(6.1)
$$
y'_1 = y_2, \quad y'_2 = -y_2 - y_1^2 + e^{-2x},
$$

$$
y_1(0) = 1, \quad y_1(1) = e^{-1}
$$

with exact solution $z_1(x) = -z_2(x) = e^{-x}$.

We present the results obtained by using the defect operator (3.6) with $k = 6$ Gaussian points on uniform grids $A_h(h=h_i=1/N)$. The starting vector y_h^0 is chosen as the solution of the trapezoidal scheme and the iterates are computed from the linearized version (3.8) of the method. (The results are not qualitatively different for the more expensive version (3.10).) The entries in the following table show the maximal errors of the iterates at the points $x_i \in A_h$. Each column corresponds to a fixed iteration level, each line to a fixed grid. Behind each column we list estimates for the orders of accuracy, which are obtained by forming the quotients of the errors on two consecutive grids.

The statements of the previous sections are clearly confirmed. Each iterate vields an $O(h^2)$ improvement until the order of the target collocation scheme is reached. Of course, after that no error reduction is observed (while the iteration continues to converge to v^*). The figures may also be compared to those given in Christiansen and Russell [8] for the same example, using deferred corrections. It turns out that our method can obtain results with a sixth order defect evaluation equivalent to those of a standard method which uses, at least in the final stage, twelth order defect evaluations.

We now initiate the iteration with a rough starting vector, obtained by adding to the solution of the trapezoidal scheme a perturbation of absolute value 1, alternating in consecutive gridpoints. Since for this starting vector $||y_h^0||$ $-y_h^*$ $\|_m = O(h^{-m})(0 \le m \le k)$, the estimates (4.23), (4.24) predict that $y_h^m(x_i)$ $-z(x_i) = O(h^{2m-(m+1)}) = O(h^{m-1})$ for $1 \le m \le k-1$ and $y_k^m(x_i) - z(x_i) = O(h^{2m-k})$ for $m \ge k$, $2m - k \le k_*$. We obtained

Although the predicted orders for the second and fourth iterate are not very precisely attained (they would be more precise, if we would list the first order norms $||y_h^m - z_h||_1$ instead of max $|y_h(x_i) - z(x_i)|$, we note that proceeding $i=0,\ldots, N$

from the first to the fifth iteration yields four orders of accuracy, while proceeding from the fifth to the ninth iteration yields eight orders of accuracy. Thus the average convergence factor is $O(h)$ in the initial phase and $O(h^2)$ in the final phase. Note that this confirms the statement on the global $O(h^2)$ -contractivity of the iteration. Also note that our theory allows for a rather precise prediction of the number of successful iteration steps, given some information about the smoothness of the starting vector.

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To give a more realistic example, we consider the motion of a satellite in the earth-moon gravitational field. In a barycentric, rotating coordinate system the motion is described by

(6.2)
$$
\ddot{x} = x + 2 \dot{y} - \mu' \frac{y + \mu}{((x + \mu)^2 + y^2)^{3/2}} - \mu \frac{x - \mu'}{((x - \mu')^2 + y^2)^{3/2}}
$$

$$
\ddot{y} = y - 2 \dot{x} - \mu' \frac{y}{((x + \mu)^2 + y^2)^{3/2}} - \mu \frac{y}{((x - \mu')^2 + y^2)^{3/2}}
$$

where $\mu = 0.0123$, $\mu' = 1 - \mu$ and the position of the earth is near $(x, y) = (0, 0)$, that of the moon near $(x, y) = (1, 0)$. We want to find a solution subject to the 'free' boundary conditions

$$
x(0) = -0.1, \quad y(0) = 0
$$

$$
x(T) = 1.05, \quad y(T) = 0, \quad \dot{x}^{2}(T) + \dot{y}^{2}(T) = 1
$$

where T is unknown. We reduce (6.2) to a system of first order differential equations, introduce the new independent variable $\tau = t/T$, and add the trivial differential equation $\dot{T}=0$. This leads to a boundary value problem of the form (1.1) in $n=5$ dependent variables. We solved this problem with method (3.8), (3.9) using the collocation scheme with $k=7$ Gaussian points. The solution of the trapezoidal scheme was obtained by Newton's method. The starting vector for Newton's method and the initial grid were obtained by solving the initial value problem for (6.2) with some estimated values for $\dot{x}(0)$, $\dot{y}(0)$ and T. The numerical results indicate that the problem has several (isolated) solutions.

The following table lists the corrections $y_n^{m+1} - y_n^m$. Due to the rather rapid convergence of the iteration we may consider these numbers to be estimates for the errors $z_h - y_h^m$ as long as the order of the target collocation scheme has not been reached (i.e. for $m=0, \ldots, k-2$, cf. Theorem 4). Note that this procedure gives no error estimate for the last iterate y_k^{k-1} , although this iterate may still yield a gain in accuracy.

We now attempt to achieve a final accuracy of 10^{-8} by refining the grid. The new grid is determined by an error equidistributing procedure. The information on the error functions is obtained from the estimates (corrections) on the old grid.

Here again, the iteration was started from the solution of the trapezoidal scheme. Since the success of our method does not depend on special properties of the starting vector, we may as well initiate the iteration with a starting vector obtained by extending the final iterate on the old grid to the new grid. Using the interpolation operator P_h on the old grid for the extension, we obtained

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