

# Collocation methods for differential-algebraic equations of index 3

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**Summary.** This article gives sharp convergence results for stiffly accurate collocation methods as applied to differential-algebraic equations (DAE's) of index 3 in Hessenberg form, proving partially a conjecture of Hairer, Lubich, and Roche.

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## 1. Introduction

Index 3 problems often appear when modelling mechanical systems with constraints (for further details see [1, Sect. 6.2], [3, pp. 6–7] or [5, pp. 483–486 and pp. 539–540]). A usual way for solving such problems is by index reduction (see [1, Subsects. 2.5.3 and 5.4.1]). However, for multibody systems containing rigid springs with a Hooke's constant  $1/\epsilon^2$  ( $\epsilon$  very small), the numerical solution behaves as that for the limit problem ( $\epsilon \rightarrow 0$ ) which is of index 3 (see [3, pp. 10–12] or [6]). In this situation, an index reduction is not possible and one is compelled to study the convergence behaviour for the index 3 case. This remark also holds for very stiff mechanical systems in which a large potential forces the motion to be close to a manifold.

Convergence of BDF-methods is stated in [1, Subsect. 3.2.4]. Preliminary theoretical convergence results for general implicit Runge-Kutta (IRK) methods have been obtained in [3, Sect. 6], but numerical experiments have shown that they are not optimal and sharper orders of convergence have been hypothesized [3, pp. 18–19 and p. 86]. For solvable linear constant coefficients systems of arbitrary index, necessary and sufficient conditions to ensure that the local and global errors of an IRK method attain a given order of accuracy have already been derived in [2].

The main result of this paper (Theorem 2.2 below) will be a partial proof of the conjecture of [3, p. 86], giving sharp convergence bounds for stiffly accurate collocation methods, such as the Radau IIA processes. The necessary tools for this proof (Sect. 5), which relate on the ideas of [3, Sect. 6], and of [5, Sect. VI.7] (devoted to index 2 systems), are collected in Sect. 3 (existence, uniqueness, and study of perturbations in the initial values) and in Sect. 4 (local error).

#### 2. Collocation methods for index 3 DAE's

Let

(2.1) 
$$y' = f(y, z), \qquad y(x_0) = y_0 \in \mathbb{R}^n,$$
  
 $z' = k(y, z, u), \qquad z(x_0) = z_0 \in \mathbb{R}^m,$   
 $0 = g(y), \qquad u(x_0) = u_0 \in \mathbb{R}^p$ 

be a system of differential-algebraic equations given in an autonomous and semi-explicit formulation (or Hessenberg form). The initial values  $(y_0, z_0, u_0)$  are assumed to be *consistent*, i.e., to satisfy

$$(2.2a) 0 = g(y)$$

(2.2b) 
$$0 = (g_y f)(y, z)$$

(2.2c) 
$$0 = (g_{yy}(f,f) + g_y f_y f + g_y f_z k)(y, z, u).$$

Let us suppose that f, g, and k are sufficiently differentiable functions and that

(2.3) 
$$g_y f_z k_u$$
 is invertible

in a neighbourhood of the exact solution (*index* 3). If (2.2c) and (2.3) are satisfied for some  $(y^*, z^*, u^*)$ , then, in a vicinity of these values, (2.2c) defines an implicit function u = G(y, z).

One step of a collocation method applied to (2.1) is defined as follows:

**Definition 2.1.** Let  $c_1, \ldots, c_s$  be s distinct real numbers and let (Y(x), Z(x), U(x)) denote the collocation polynomials of degree s which satisfy

(2.4a)  $Y(x_0) = y_0, \quad Z(x_0) = z_0, \quad U(x_0) = u_0,$ 

(2.4b) 
$$Y'(x_0 + c_i h) = f(Y(x_0 + c_i h), Z(x_0 + c_i h)) Z'(x_0 + c_i h) = k(Y(x_0 + c_i h), Z(x_0 + c_i h), U(x_0 + c_i h)) 0 = g(Y(x_0 + c_i h))$$
  $i = 1, ..., s.$ 

Then the numerical solution is given by

(2.4c) 
$$y_1 = Y(x_0 + h), \quad z_1 = Z(x_0 + h), \quad u_1 = U(x_0 + h).$$

*Remark.* The condition  $U(x_0) = u_0$  in (2.4a) can be omitted if we require U(x) to be a polynomial of degree s-1 only, and  $U(x_0)$  to be close to  $u_0$ , i.e.,  $U(x_0) - u_0 = o(1)$ . This modification does not alter the polynomials Y(x) and Z(x), and will apply throughout this paper. Consequently the three collocation polynomials become independent of  $u_0$ .

In this article we turn our interest to collocation methods with  $s \ge 2$  and coefficients satisfying the hypotheses

H1:  $c_i \neq 0$  for i = 1, ..., s; H2:  $c_s = 1$ , i.e., the method is stiffly accurate.

It can be noticed that from H2 we get  $g(y_1)=0$  in (2.4). The following theorem gives the optimal orders of convergence for collocation methods satisfying these hypotheses, proving the conjecture stated in [3, p. 86] for such methods:

**Theorem 2.2.** Let us consider the differential-algebraic system (2.1) of index 3 with consistent initial values and the collocation method (2.4) satisfying  $s \ge 2$ , H1, and H2. Then, for  $x_n - x_0 = nh \le Const$ , the global error satisfies

(2.5) 
$$y_n - y(x_n) = O(h^{\min(p, 2s-2)}), \quad P_z(x_n)(z_n - z(x_n)) = O(h^{\min(p, 2s-2)}),$$
  
 $z_n - z(x_n) = O(h^s), \quad u_n - u(x_n) = O(h^{s-1})$ 

where  $P_z(x) = (I - k_u(g_y f_z k_u)^{-1} g_y f_z)(y(x), z(x), u(x))$  and p is the order of the underlying quadrature formula. If in addition the function k of (2.1) is linear in u then we get

(2.5')  $y_n - y(x_n) = O(h^p), \quad P_z(x_n)(z_n - z(x_n)) = O(h^p).$ 

The *proof* will be presented in Sect. 5, and it makes use of preliminary results contained in Sects. 3 and 4.

The result (2.5) shows that if in a last step the numerical solution is projected onto the manifold  $(g_y f)(y, z) = 0$ , the accuracy of the z-component can be improved. This projection can be done as follows:  $\hat{z}_n$  and  $\mu_n$  are the solution of

(2.6) 
$$\hat{z}_n = z_n + k_u(y_n, z_n, u_n) \mu_n$$
$$0 = (g_v f) (y_n, \hat{z}_n)$$

where  $(y_n, z_n, u_n)$  is the numerical solution of (2.4) at  $x_n$ . In this case we get

(2.7) 
$$\hat{z}_n - z(x_n) = \begin{cases} O(h^p) & \text{if } k \text{ is linear in } u, \\ O(h^{\min(p, 2s-2)}) & \text{else.} \end{cases}$$

Furthermore, if we define  $\hat{u}_n$  as the solution together with  $y_n$  and  $\hat{z}_n$  of (2.2c), we have

(2.8) 
$$\hat{u}_n - u(x_n) = \begin{cases} O(h^p) & \text{if } k \text{ is linear in } u, \\ O(h^{\min(p, 2s-2)}) & \text{else.} \end{cases}$$

The application of the above results to the Radau IIA processes leads to:

**Corollary 2.3.** For the s-stage  $(s \ge 2)$  Radau IIA method applied to the index 3 system (2.1), the global error satisfies

(2.9) 
$$y_n - y(x_n) = O(h^{2s-2}), \quad P_z(x_n)(z_n - z(x_n)) = O(h^{2s-2}),$$
  
 $z_n - z(x_n) = O(h^s), \quad \hat{z}_n - z(x_n) = O(h^{2s-2}),$   
 $u_n - u(x_n) = O(h^{s-1}), \quad \hat{u}_n - u(x_n) = O(h^{2s-2})$ 

and if k is linear in u we have

(2.9') 
$$y_n - y(x_n) = O(h^{2s-1}), \quad P_z(x_n)(z_n - z(x_n)) = O(h^{2s-1}),$$
  
 $\hat{z}_n - z(x_n) = O(h^{2s-1}), \quad \hat{u}_n - u(x_n) = O(h^{2s-1}).$ 

*Proof.* The proof is obtained by putting p=2s-1 in (2.5)–(2.5'), (2.7), and (2.8).

#### 3. Existence, uniqueness, and influence of perturbations

In this section,  $(y_0, z_0, u_0)$  in Definition 2.1 are replaced by approximate *h*-dependent starting values  $(\eta, \zeta, \nu)$ . We will first investigate the existence and uniqueness of the collocation polynomials.

**Theorem 3.1.** Let us suppose that  $s \ge 2$ , H1 is satisfied, (2.3) holds in a neighbourhood of  $(\eta, \zeta, \nu)$ , and that

$$(3.1a) g(\eta) = O(h^{\tau}), \quad \tau \ge 3,$$

(3.1 b) 
$$(g_y f)(\eta, \zeta) = O(h^{\kappa}), \quad \kappa \ge 2,$$

(3.1c) 
$$(g_{yy}(f,f) + g_y f_y f + g_y f_z k)(\eta, \zeta, v) = O(h).$$

Then for  $h \leq h_0$  the collocation polynomials (Y(x), Z(x), U(x)) of (2.4) with  $Y(x_0) = \eta$  and  $Z(x_0) = \zeta$  exist and are locally unique.

**Proof.** A straightforward extension of [4, Theorems II.7.6 and II.7.7] to index 3 problems shows the equivalence of (2.4) with an s-stage IRK method. More precisely, the values  $Y(x_0 + c_i h)$ ,  $Z(x_0 + c_i h)$ , and  $U(x_0 + c_i h)$  can be interpreted as the internal stages of a RK method whose coefficients, depending on the  $c_i$ , are defined by the simplifying assumptions B(s) and C(s) (see [3, pp. 15–16] or [5, Sect. IV.5]). H1 ensures that the corresponding RK matrix is invertible. By defining  $c_0 := 0$ , the collocation polynomials are uniquely determined by

(3.2a) 
$$Y(x_0 + th) = \sum_{i=0}^{s} l_i(t) Y(x_0 + c_i h) = l_0(t) \eta + \sum_{i=1}^{s} l_i(t) Y(x_0 + c_i h)$$

(3.2b) 
$$Z(x_0 + th) = \sum_{i=0}^{s} l_i(t) Z(x_0 + c_i h) = l_0(t) \zeta + \sum_{i=1}^{s} l_i(t) Z(x_0 + c_i h)$$

(3.2c) 
$$U(x_0 + th) = \sum_{i=1}^{s} L_i(t) U(x_0 + c_i h)$$

where the  $l_i(t)$  and  $L_i(t)$  are the Lagrange polynomials of degree s and s-1 respectively, given by

(3.3) 
$$l_i(t) = \prod_{\substack{j=0\\j\neq i}}^s \left(\frac{t-c_j}{c_i-c_j}\right), \quad L_i(t) = \prod_{\substack{j=1\\j\neq i}}^s \left(\frac{t-c_j}{c_i-c_j}\right).$$

The result is now an immediate consequence of the existence and uniqueness of the RK solution stated in [3, Theorem 6.1].  $\Box$ 

We will study next the influence of perturbations in the initial values on the collocation solution.

**Theorem 3.2.** In addition to the assumptions of Theorem 3.1, let us suppose that H2 holds and that

(3.4) 
$$\hat{\eta} = \eta + O(h^3), \quad \hat{\zeta} = \zeta + O(h^2).$$

Let us consider  $(\hat{Y}(x), \hat{Z}(x), \hat{U}(x))$  the collocation polynomials satisfying  $\hat{Y}(x_0) = \hat{\eta}$ and  $\hat{Z}(x_0) = \hat{\zeta}$ . Then we have

(3.5a) 
$$\Delta Y(x_{0} + h) = P_{y} \Delta \eta + h f_{z} P_{z} \Delta \zeta + O(h \|\Delta \eta\| + h^{2} \|P_{z} \Delta \zeta\| + h^{m+2} \|Q_{z} \Delta \zeta\| + \|Q_{z} \Delta \zeta\|^{2})$$
  
(3.5b) 
$$P_{z}(x_{0} + h) \Delta Z(x_{0} + h) = P_{z} \Delta \zeta + O\left(\|Q_{y} \Delta \eta\| + h \|P_{y} \Delta \eta\| + h \|P_{z} \Delta \zeta\| + h^{n+1} \cdot \|Q_{z} \Delta \zeta\| + \frac{1}{h} \|Q_{z} \Delta \zeta\|^{2}\right)$$
  
(3.5c) 
$$Q_{z}(x_{0} + h) \Delta Z(x_{0} + h) = -\frac{\sigma}{h} \cdot SQ_{y} \Delta \eta + O(\|\Delta \eta\| + h \|\Delta \zeta\|)$$

where  $\sigma$  is a constant depending on the coefficients of the method and is given in the proof,  $m = \min(\tau - 3, \kappa - 2, s - 2, \max(p - s - 1, 0))$ ,  $n = \min(\tau - 3, \kappa - 2, s - 2, p - s)$ . The projectors  $Q_y$ ,  $P_y$ ,  $Q_z$ , and  $P_z$  are defined under the hypothesis (2.3) by

(3.6)  $S := k_u (g_y f_z k_u)^{-1} g_y,$  $Q_y := f_z S, \quad P_y := I - Q_y, \quad Q_z := S f_z, \quad P_z := I - Q_z.$ 

In (3.5) they are evaluated at  $(\eta, \zeta, G(\eta, \zeta))$  with G described in Sect. 2 and the arguments of  $P_z(x_0+h)$  and  $Q_z(x_0+h)$  are  $(Y(x_0+h), Z(x_0+h), G(Y(x_0+h), Z(x_0+h)))$ .

*Remarks.* 1) The notation  $\Delta$  indicates a difference between a "non-hat value" with the corresponding "hat value", e.g., in (3.5a)  $\Delta Y(x_0 + h) = Y(x_0 + h) - \hat{Y}(x_0 + h)$  and  $\Delta \eta = \eta - \hat{\eta}$ .

2) The missing arguments for  $f_z$ , S,  $P_v$ , etc., are  $(\eta, \zeta, G(\eta, \zeta))$ .

3) The conditions (3.4) ensure the local existence and uniqueness of  $(\hat{Y}(x), \hat{Z}(x), \hat{U}(x))$ .

4) If  $g(\hat{\eta}) = 0 = g(\eta)$  then  $Q_y(\hat{\eta} - \eta) = O(||(\hat{\eta} - \eta)||^2)$ . Consequently this term may be neglected and the hypothesis  $\hat{\eta} = \eta + O(h^3)$  can be relaxed to  $\hat{\eta} = \eta + O(h^2)$ .

5) If the function  $\hat{k}$  of (2.1) is linear in u, then in (3.5a, b)  $m = \max(p-s-1, 0), n=p-s$ , and the terms  $||Q_z \Delta \zeta||^2$  are multiplied by one additional factor h.

6) It can be noticed that m and n satisfy  $0 \le m \le n \le m+1$ .

7) The important results consist in the splitting of  $\overline{\Delta \zeta}$  according to the projections  $P_z$  and  $Q_z$  and in the *h*-exponents in front of  $||Q_z \Delta \zeta||$  in (3.5a, b). 8) We point out that the constants entering in the  $O(\cdot)$  terms of (3.5) depend

8) We point out that the constants entering in the  $O(\cdot)$  terms of (3.5) depend on those implied by the  $O(\cdot)$  terms of (3.1a, b) and (3.4). Nevertheless this will not affect the proof of Theorem 2.2 (see Sect. 5) where Theorem 3.2 will be used.

*Proof.* A large number of the ideas contained in this proof are expressed in the demonstrations of [5, Theorem VI.7.9 and Lemma VI.7.10]. The proof is divided into four parts. Our first aim in a) is to show (3.15) with the help of the nonlinear variation-of-constants formula [4, Formula (I.14.20)]. In part b) we analyse in details the two terms entering in (3.15), leading to (3.22)-(3.23). Hence (3.15) can be rewritten as the sum (3.24) of several terms expressed in (3.25). Those are then estimated separately in the last part d) with the help of some technical results derived in c).

a) The defect of the collocation polynomials (Y(x), Z(x), U(x)) inserted into the differential-algebraic problem (2.1) is defined as follows

(3.7a) 
$$Y'(x) = f(Y(x), Z(x)) + \delta(x)$$

(3.7b) 
$$Z'(x) = k(Y(x), Z(x), U(x)) + \mu(x)$$

$$(3.7c) 0 = g(Y(x)) + \theta(x).$$

According to Definition 2.1  $\delta(x)$ ,  $\mu(x)$ , and  $\theta(x)$  vanish at the points  $x_0 + c_i h$ . By differentiating (3.7c) twice with respect to x and by taking (3.7a, b) into account, the collocation polynomials and the defect are seen to satisfy for all x

(3.7d) 
$$0 = g_{y}(Y)(f(Y, Z) + \delta) + \theta'$$
  
(3.7e) 
$$0 = g_{yy}(Y)(f(Y, Z) + \delta, f(Y, Z) + \delta) + g_{y}(Y)f_{y}(Y, Z)(f(Y, Z) + \delta) + g_{y}(Y)f_{z}(Y, Z)(k(Y, Z, U) + \mu) + g_{y}(Y)\delta' + \theta''.$$

Furthermore, these equations can be used in a vicinity of the solution of (2.1) for arbitrary (Y, Z, U) and sufficiently small "perturbations". In view of (2.3) U can be extracted from (3.7e), giving

(3.8) 
$$U = G(Y, Z, \delta, \delta', \mu, \theta'')$$

and it extends the definition of G(y, z) in Sect. 2 which simply corresponds to G(y, z, 0, 0, 0, 0). Thus, (3.7b) can be rewritten

$$(3.7b') \quad Z'(x) = k(Y(x), Z(x), G(Y(x), Z(x), \delta(x), \delta'(x), \mu(x), \theta''(x))) + \mu(x)$$

forming together with (3.7a) a differential system for Y(x) and Z(x). As it concerns  $(\hat{Y}(x), \hat{Z}(x), \hat{U}(x))$ , by straightforwardly following the above analysis with  $\delta(x)$ ,  $\hat{\mu}(x)$ , and  $\hat{\theta}(x)$  defined in the same way as in (3.7), we obtain

(3.9a) 
$$\hat{Y}'(x) = f(\hat{Y}(x), \hat{Z}(x)) + \hat{\delta}(x)$$

$$(3.9 b) \quad \hat{Z}'(x) = k(\hat{Y}(x), \hat{Z}(x), G(\hat{Y}(x), \hat{Z}(x), \hat{\delta}(x), \hat{\delta}'(x), \hat{\mu}(x), \hat{\theta}''(x))) + \hat{\mu}(x).$$

With the aim of expressing  $\Delta Y(x)$  and  $\Delta Z(x)$ , the nonlinear variation-of-constants formula of Gröbner-Alekseev [4, Corollary I.14.6] can be applied. The difference between Y', Z' and Y, Z formally inserted into (3.9) needs to be computed. We get

(3.10) 
$$d(x, Y, Z) = {Y' \choose Z'} - {f(Y, Z) + \delta(x) \choose k(Y, Z, G(Y, Z, \delta(x), \delta'(x), \hat{\mu}(x), \hat{\theta}''(x))) + \hat{\mu}(x)} = \Phi(x, Y, Z, 1) - \Phi(x, Y, Z, 0)$$

where, leaving out the x-argument in the "perturbations",

(3.11) 
$$\Phi(x, Y, Z, \tau) = \begin{pmatrix} \delta + (\tau - 1) \Delta \delta \\ \mu + (\tau - 1) \Delta \mu \end{pmatrix} + \begin{pmatrix} 0 \\ k(Y, Z, G(Y, Z, \delta + (\tau - 1) \Delta \delta, \delta' + (\tau - 1) \Delta \delta', \mu + (\tau - 1) \Delta \mu, \theta'' + (\tau - 1) \Delta \theta'') \end{pmatrix}.$$

With the shortened notation  $\Phi(x, \tau) = \Phi(x, Y(x), Z(x), \tau)$ , the formula  $\Phi(x, 1) - \Phi(x, 0) = \int_{0}^{1} \partial \Phi / \partial \tau(x, \tau) d\tau$  permits us to express the defect d(x, Y, Z) as

(3.12) 
$$d(x, Y,Z) = \begin{pmatrix} I \\ Q_1(x, Y,Z) \end{pmatrix} \Delta \delta(x) + \begin{pmatrix} 0 \\ Q_2(x, Y,Z) \end{pmatrix} \Delta \delta'(x) \\ + \begin{pmatrix} 0 \\ I + Q_3(x, Y,Z) \end{pmatrix} \Delta \mu(x) + \begin{pmatrix} 0 \\ Q_4(x, Y,Z) \end{pmatrix} \Delta \theta''(x).$$

We only give the expressions of  $Q_2$  and  $Q_4$ 

(3.13a) 
$$Q_2(x, Y,Z) = \int_0^1 k_u(Y,Z,G(\ldots)) \frac{\partial G}{\partial \delta'}(\ldots) d\tau$$

(3.13b) 
$$Q_4(x, Y, Z) = \int_0^1 k_u(Y, Z, G(...)) \frac{\partial G}{\partial \theta''}(...) d\tau$$

where the missing arguments (...) are identical to those of G in (3.11). A simple differentiation of (3.7e) with respect to  $\delta'$  and  $\theta''$  shows that

(3.14) 
$$\frac{\partial G}{\partial \delta'} = \frac{\partial U}{\partial \delta'} = -(g_y f_z k_u)^{-1} g_y, \quad \frac{\partial G}{\partial \theta''} = \frac{\partial U}{\partial \theta''} = -(g_y f_z k_u)^{-1},$$

hence we have

(3.13 a') 
$$Q_{2}(x, Y, Z) = -\int_{0}^{1} (k_{u}(g_{y}f_{z}k_{u})^{-1}g_{y})(Y, Z, G(...)) d\tau$$
$$= Q_{4}(x, Y, Z)g_{y}(Y)$$
(3.13 b') 
$$Q_{4}(x, Y, Z) = -\int_{0}^{1} (k_{u}(g_{y}f_{z}k_{u})^{-1})(Y, Z, G(...)) d\tau.$$

The application of [4, Formula (I.14.20)] leads to

(3.15) 
$$\begin{pmatrix} \Delta Y(x) \\ \Delta Z(x) \end{pmatrix} = \int_{x_0}^x R(x, t, Y(t), Z(t)) d(t, Y(t), Z(t)) dt + \int_0^1 R(x, x_0, \eta + (t-1) \Delta \eta, \zeta + (t-1) \Delta \zeta) dt \begin{pmatrix} \Delta \eta \\ \Delta \zeta \end{pmatrix}$$

where the resolvent R is given by

(3.16) 
$$R(x, t, y, z) = \frac{\partial(\hat{Y}, \hat{Z})}{\partial(y, z)}(x, t, y, z)$$

and  $(\hat{Y}, \hat{Z})(x, t, y, z)$  denotes the solution at x of (3.9) passing through (y, z) at t. R satisfies R(s, s, y, z) = I and is the solution of the variational equation associated with the system (3.9). In the sequel we will use the abbreviations

(3.17) 
$$R(x, t) = R(x, t, Y(t), Z(t)), \quad d(t) = d(t, Y(t), Z(t)),$$
$$Q_i(t) = Q_i(t, Y(t), Z(t)).$$

b) Let us now consider the first integral in (3.15). By the use of (3.12) we get, after some integrations by parts,

(3.18)  

$$\int_{x_0}^{x} R(x,t) d(t) dt = \int_{x_0}^{x} S_1(x,t) \Delta \delta(t) + S_2(x,t) \Delta \delta'(t) + S_3(x,t) \Delta \mu(t) + S_4(x,t) \Delta \theta''(t) dt$$

$$= S_2(x,t) \Delta \delta(t) - \frac{\partial S_4}{\partial t}(x,t) \Delta \theta(t) + S_4(x,t) \Delta \theta'(t) \Big|_{t=x_0}^{x} + \int_{x_0}^{x} \sigma(x,t) dt$$

where we have defined

$$(3.19) S_1(x,t) = R(x,t) \begin{pmatrix} I \\ Q_1(t) \end{pmatrix}, S_2(x,t) = R(x,t) \begin{pmatrix} 0 \\ Q_2(t) \end{pmatrix}, \\S_3(x,t) = R(x,t) \begin{pmatrix} 0 \\ I+Q_3(t) \end{pmatrix}, S_4(x,t) = R(x,t) \begin{pmatrix} 0 \\ Q_4(t) \end{pmatrix}, \\\sigma(x,t) = \left(S_1(x,t) - \frac{\partial S_2}{\partial t}(x,t)\right) \Delta \delta(t) + S_3(x,t) \Delta \mu(t) + \frac{\partial^2 S_4}{\partial t^2}(x,t) \Delta \theta(t).$$

An expression entering in (3.18) is

. . . . .

(3.20) 
$$\frac{\partial S_4}{\partial t}(x,t) = \frac{\partial R}{\partial t}(x,t) \begin{pmatrix} 0\\ Q_4(t) \end{pmatrix} + R(x,t) \begin{pmatrix} 0\\ Q'_4(t) \end{pmatrix},$$

therefore  $\partial R/\partial t(x, t)$  remains to be computed. By using well-known properties of the resolvent, we arrive at

$$(3.21)$$

$$\frac{\partial R}{\partial t}(x,t) = -R(x,t) \begin{pmatrix} f_y(Y(t), Z(t)) & f_z(Y(t), Z(t)) \\ \left( k_y + k_u \frac{\partial G}{\partial y} \right) (Y(t), Z(t), H(t)) & \left( k_z + k_u \frac{\partial G}{\partial z} \right) (Y(t), Z(t), H(t)) \end{pmatrix}$$

$$+ \frac{\partial R}{\partial (y,z)} (x, t, Y(t), Z(t)) (d(t, Y(t), Z(t)), \cdot)$$

where  $H(t) := G(Y(t), Z(t), \hat{\delta}(t), \hat{\delta}'(t), \hat{\mu}(t), \hat{\theta}''(t))$  and we point out that  $\partial R/\partial(y, z)$ is a bilinear application. Now, we put  $x := x_0 + h$  in (3.15). The assumption  $c_s = 1$ implies that  $\delta(x), \delta(x), \theta(x)$ , and  $\hat{\theta}(x)$  vanish at this point. By replacing  $\theta'(x_0)$ and  $\hat{\theta}'(x_0)$  with the help of (3.7d) and by using the relation  $S_2(x, t)$  $= S_4(x, t) g_y(Y(t))$  which is a consequence of (3.13'), we deduce

$$(3.22) \int_{x_0+h}^{x_0+h} R(x_0+h,t) d(t) dt = S_4(x_0+h,x_0) ((\Delta g_y(\eta)) \cdot \delta(x_0) + \Delta (g_y f)(\eta,\zeta)) - \frac{\partial S_4}{\partial t} (x_0+h,x_0) \Delta g(\eta) + S_4(x_0+h,x_0+h) \Delta \theta'(x_0+h) + \int_{x_0}^{x_0+h} \sigma(x_0+h,t) dt.$$

Because of  $\partial R/\partial(y, z)(x_0+h, x_0, y, z) = O(h)$ , the second integral in (3.15) can be estimated by

(3.23) 
$$R(x_0+h,x_0)\binom{\Delta\eta}{\Delta\zeta}+O(h\|\Delta\eta\|^2+h\|\Delta\zeta\|^2).$$

By collecting the previous results and rearranging the terms, we obtain

(3.24) 
$$\begin{pmatrix} \Delta Y(x_0+h) \\ \Delta Z(x_0+h) \end{pmatrix} = (1) + (2) + (3) + (4) + O(h \|\Delta\eta\|^2 + h \|\Delta\zeta\|^2)$$

where

$$(3.25) \quad (1) = R(x_0 + h, x_0) \left[ \begin{pmatrix} \Delta \eta \\ \Delta \zeta \end{pmatrix} + \begin{pmatrix} 0 \\ Q_4(x_0)((\Delta g_y(\eta)) \cdot \delta(x_0) + \Delta(g_y f)(\eta, \zeta)) \end{pmatrix} \\ + \begin{pmatrix} f_z(\eta, \zeta) Q_4(x_0) \\ (k_z + k_u \frac{\partial G}{\partial z})(\eta, \zeta, H(x_0)) Q_4(x_0) - Q'_4(x_0) \end{pmatrix} \Delta g(\eta) \right], \\ (2) = -\frac{\partial R}{\partial (y, z)} (x_0 + h, x_0, \eta, \zeta) \left( d(x_0, \eta, \zeta), \begin{pmatrix} 0 \\ Q_4(x_0) \Delta g(\eta) \end{pmatrix} \right), \\ (3) = \begin{pmatrix} 0 \\ Q_4(x_0 + h) \Delta \theta'(x_0 + h) \end{pmatrix}, \quad (4) = \int_{x_0}^{x_0 + h} \sigma(x_0 + h, t) dt.$$

In order to estimate each of these terms, some intermediate results will be required.

c) First of all, by expanding the resolvent  $R(x_0 + h, x_0)$  at  $x_0$ , we obtain

$$(3.26) \quad R(x_0+h, x_0) = I + h \begin{pmatrix} f_y(\eta, \zeta) & f_z(\eta, \zeta) \\ \left(k_y + k_u \frac{\partial G}{\partial y}\right)(\ldots) & \left(k_z + k_u \frac{\partial G}{\partial z}\right)(\ldots) \end{pmatrix} + O(h^2)$$

with  $(\ldots) = (\eta, \zeta, H(x_0))$ . Secondly, by differentiating k times the difference of the two collocation polynomials, written in the form (3.2), we arrive at

(3.27 a) 
$$h^k \Delta Y^{(k)}(x_0 + th) = l_0^{(k)}(t) \Delta \eta + \sum_{i=1}^s l_i^{(k)}(t) \Delta Y(x_0 + c_i h), \quad k = 0, ..., s,$$

(3.27b) 
$$h^k \Delta Z^{(k)}(x_0 + th) = l_0^{(k)}(t) \Delta \zeta + \sum_{i=1}^s l_i^{(k)}(t) \Delta Z(x_0 + c_i h), \quad k = 0, ..., s,$$

(3.27c) 
$$h^k \Delta U^{(k)}(x_0 + th) = \sum_{i=1}^s L_i^{(k)}(t) \Delta U(x_0 + c_i h), \quad k = 0, \dots, s-1,$$

and the higher derivatives vanish identically. The proof of [3, Theorem 6.4] related to RK methods may be adapted in our situation, leading to

(3.28 a) 
$$\Delta Y(x_0 + c_i h) = P_y \Delta \eta + c_i h f_z P_z \Delta \zeta + O(h ||\Delta \eta|| + h^2 ||\Delta \zeta||)$$

(3.28 b) 
$$\Delta Z(x_0 + c_i h) = P_z \Delta \zeta + O\left(\frac{1}{h} \|Q_y \Delta \eta\| + \|P_y \Delta \eta\| + h \|\Delta \zeta\|\right)$$

(3.28 c) 
$$\Delta U(x_0 + c_i h) = O\left(\frac{1}{h^2} \|Q_y \Delta \eta\| + \frac{1}{h} \|P_y \Delta \eta\| + \frac{1}{h} \|Q_z \Delta \zeta\| + \|P_z \Delta \zeta\|\right).$$

By using  $\sum_{i=0}^{s} l_i(t) = 1$  and  $\sum_{i=0}^{s} l_i(t) c_i = t$ , these relations inserted into (3.27) yield for x in an O(h)-neighbourhood of  $x_0$ ,

$$(3.29 a) \quad h^{k} \Delta Y^{(k)}(x) = O\left( \|Q_{y} \Delta \eta\| + h^{1-s_{0k}} \|P_{y} \Delta \eta\| + h^{2} \|Q_{z} \Delta \zeta\| + h^{2-s_{1k}} \|P_{z} \Delta \zeta\| \right)$$

(3.29 b) 
$$h^k \Delta Z^{(k)}(x) = O\left(\frac{1}{h} \|Q_y \Delta \eta\| + \|P_y \Delta \eta\| + \|Q_z \Delta \zeta\| + h^{1-S_{0k}} \|P_z \Delta \zeta\|\right)$$

(3.29 c) 
$$h^k \Delta U^{(k)}(x) = O\left(\frac{1}{h^2} \|Q_y \Delta \eta\| + \frac{1}{h} \|P_y \Delta \eta\| + \frac{1}{h} \|Q_z \Delta \zeta\| + \|P_z \Delta \zeta\|\right)$$

where  $S_{jk} = 1$  if  $j \ge k$  else  $S_{jk} = 0$ . Since  $\Delta \delta(x) = \Delta Y'(x) - \Delta f(Y(x), Z(x)), \Delta \mu(x) = \Delta Z'(x) - \Delta k(Y(x), Z(x)), U(x))$ , and  $\Delta \theta(x) = -\Delta g(Y(x))$ , we have

$$(3.30) \qquad \Delta\delta(\mathbf{x}) = O\left(\frac{1}{h} \|Q_{\mathbf{y}} \Delta\eta\| + \|P_{\mathbf{y}} \Delta\eta\| + \|Q_{z} \Delta\zeta\| + \|P_{z} \Delta\zeta\|\right)$$
$$\Delta\delta'(\mathbf{x}) = O\left(\frac{1}{h^{2}} \|Q_{\mathbf{y}} \Delta\eta\| + \frac{1}{h} \|P_{\mathbf{y}} \Delta\eta\| + \frac{1}{h} \|Q_{z} \Delta\zeta\| + \|P_{z} \Delta\zeta\|\right)$$
$$\Delta\mu(\mathbf{x}) = O\left(\frac{1}{h^{2}} \|Q_{\mathbf{y}} \Delta\eta\| + \frac{1}{h} \|P_{\mathbf{y}} \Delta\eta\| + \frac{1}{h} \|Q_{z} \Delta\zeta\| + \|P_{z} \Delta\zeta\|\right)$$
$$\Delta\theta''(\mathbf{x}) = O\left(\frac{1}{h^{2}} \|Q_{\mathbf{y}} \Delta\eta\| + \frac{1}{h} \|P_{\mathbf{y}} \Delta\eta\| + \|Q_{z} \Delta\zeta\| + \|P_{z} \Delta\zeta\|\right).$$

Thirdly, we define  $(\tilde{\eta}, \tilde{\zeta}, \tilde{\nu})$  as consistent values close to  $(\eta, \zeta, \nu)$  uniquely determined by the equations (2.2),  $P_y(\eta - \tilde{\eta}) = 0$  and  $P_z(\zeta - \tilde{\zeta}) = 0$ . The hypothesis (3.1 a, b) shows that  $Q_y(\eta - \tilde{\eta}) = O(h^r)$  and  $Q_z(\zeta - \tilde{\zeta}) = O(h^{\min(r,\kappa)})$ . As in (3.7), we denote by  $\delta(x)$ ,  $\tilde{\mu}(x)$ , and  $\theta(x)$  the defects of the collocation polynomials passing through  $(\tilde{\eta}, \tilde{\zeta}, \tilde{\nu})$ . These defects vanish at the collocation points  $x_0 + c_i h$ , therefore we have  $\delta(x) = O(h^s)$ ,  $\delta'(x) = O(h^{s-1})$ ,  $\tilde{\mu}(x) = O(h^s)$ , and  $\tilde{\theta}(x) = O(h^{s+1})$ ,  $\tilde{\theta}'(x) = O(h^s)$ ,  $\tilde{\theta}''(x) = O(h^{s-1})$  by also taking into account the consistency of  $\tilde{\eta}$ , i.e.,  $\tilde{\theta}(x_0) = -g(\tilde{\eta}) = 0$ . These estimates and the application of (3.30) to  $\eta - \tilde{\eta}$  and  $\zeta - \tilde{\zeta}$  lead to

(3.31)  $\delta(x) = (\delta(x) - \tilde{\delta}(x)) + \tilde{\delta}(x) = O(h^{\min(\tau - 1, \kappa, s)}),$  $\delta'(x) = O(h^{\min(\tau - 2, \kappa - 1, s - 1)}),$  $\mu(x) = O(h^{\min(\tau - 2, \kappa - 1, s)}), \quad \theta''(x) = O(h^{\min(\tau - 2, \kappa, s - 1)}).$ 

d) With these preparations we are now able to treat each term of (3.25). From (3.30) and (3.31) we deduce that

(3.32) 
$$Q_{4}(x_{0}) g_{y} f_{z} Q_{z} \Delta \zeta = -Q_{z} \Delta \zeta + O\left( \|Q_{y} \Delta \eta\| + h \|P_{y} \Delta \eta\| + h^{\min(\tau-3,\kappa-2,s-2)+1} \|Q_{z} \Delta \zeta\| + \frac{1}{h} \|Q_{z} \Delta \zeta\|^{2} + h^{2} \|P_{z} \Delta \zeta\| \right)$$

and

(3.33a) 
$$Q_z(x_0+h)Q_4(x_0+h) = -k_u(g_yf_zk_u)^{-1}(\eta,\zeta,G(\eta,\zeta)) + O(h)$$

$$(3.350) P_{z}(x_{0}+h) Q_{4}(x_{0}+h) = O(h^{\min(\tau-2,\kappa-1,s-1)}) + O\left(\frac{1}{h^{2}} \|Q_{y}\Delta\zeta\| + \frac{1}{h} \|P_{y}\Delta\eta\| + \frac{1}{h} \|Q_{z}\Delta\zeta\| + \|P_{z}\Delta\zeta\|\right).$$

By collecting the results (3.26) and (3.32), we get

$$(3.34) (1) = \begin{pmatrix} P_{y} \Delta \eta + h f_{z} P_{z} \Delta \zeta \\ P_{z} \Delta \zeta \end{pmatrix} + \begin{pmatrix} O(h \| \Delta \eta \| + h^{\min(\tau - 3, \kappa - 2, s - 2) + 2} \| Q_{z} \Delta \zeta \| + \| Q_{z} \Delta \zeta \|^{2} + h^{2} \| P_{z} \Delta \zeta \|) \\ O(\| \Delta \eta \| + h^{\min(\tau - 3, \kappa - 2, s - 2) + 1} \| Q_{z} \Delta \zeta \| + \frac{1}{h} \| Q_{z} \Delta \zeta \|^{2} + h \| P_{z} \Delta \zeta \| \end{pmatrix} \end{pmatrix}.$$

Because of  $d(x_0, \eta, \zeta) = O(h)$  we have the rough estimate  $(2) = O(h ||\Delta \eta||)$ . By setting  $\sigma := \sum_{i=1}^{s} l_i^{(1)}(1) = -l_0^{(1)}(1)$ , a consequence of

(3.35) 
$$\Delta Y'(x_0+h) = -\frac{\sigma}{h}Q_y \Delta \eta + f_z P_z \Delta \zeta + O(\|\Delta \eta\| + h \|\Delta \zeta\|)$$

and  $\Delta \theta'(x) = -\Delta [g_y(Y(x)) Y'(x)]$  is

(3.36) 
$$\Delta \theta'(x_0+h) = \frac{\sigma}{h} g_y Q_y \Delta \eta + O(\|\Delta \eta\| + h \|\Delta \zeta\|).$$

Combined with (3.33) we obtain the following decomposition for  $Q_4(x_0 + h) \Delta \theta'(x_0 + h)$  entering in (3)

(3.37a) 
$$Q_z(x_0+h) Q_4(x_0+h) \Delta \theta'(x_0+h) = -\frac{\sigma}{h} SQ_y \Delta \eta + O(\|\Delta \eta + h\|\Delta \zeta\|)$$

(3.37b)  

$$P_{z}(x_{0}+h) Q_{4}(x_{0}+h) \Delta \theta'(x_{0}+h)$$

$$= O(||Q_{y} \Delta \eta|| + h ||P_{y} \Delta \eta|| + h^{\min(\tau-3,\kappa-2,s-2)+2} ||Q_{z} \Delta \zeta|| + ||Q_{z} \Delta \zeta||^{2} + h^{2} ||P_{z} \Delta \zeta||).$$

As in the proof of [5, Theorem VI.7.9],  $\sigma(x_0 + h, t)$  in (4) can be integrated by the use of the quadrature formula  $\{b_i, c_i\}_{i=1}^s$ , yielding

(3.38) 
$$(4) = \sum_{i=1}^{s} b_i \underbrace{\sigma(x_0 + h, x_0 + c_i h)}_{= 0} + err(\sigma).$$

The quadrature error is estimated by

(3.39) 
$$err(\sigma) = O\left(h^{p+1} \cdot \max_{t \in [x_0, x_0+h]} \left\| \frac{\partial^p}{\partial t^p} \sigma(x_0+h, t) \right\| \right).$$

From (3.29) it follows that

(3.40)  
(4) = 
$$O(h^{p-s} ||Q_y \Delta \eta|| + h^{p-s+1} ||P_y \Delta \eta|| + h^{p-s+1} ||Q_z \Delta \zeta|| + h^{p-s+2} ||P_z \Delta \zeta||).$$

Insertion of the expressions (1), (2), (3.37a, b), and (4) into (3.24) gives the desired result, except that if p = s, the term  $O(||Q_y \Delta \eta|| + h ||Q_z \Delta \zeta||)$  in  $\Delta Y(x_0 + h)$  coming from (4) has to be neglected in view of (3.28a) for i = s, and the term  $P_y \Delta \eta$  entering in  $P_z(x_0 + h) \Delta Z(x_0 + h)$  is  $O(h ||P_y \Delta \eta||)$ , because of

$$(3.41) \quad P_{z}(x_{0}+c_{i}h) \Delta Z(x_{0}+c_{i}h) = P_{z} \Delta \zeta + O(||Q_{y} \Delta \eta|| + h ||P_{y} \Delta \eta|| + h ||\Delta \zeta||)$$

which can be proven in the same way as (3.28).

#### 4. The local error

We consider one step of a collocation method (2.4) with consistent initial values  $(y_0, z_0, u_0)$ . The local error

(4.1) 
$$\delta y_h(x_0) = y_1 - y(x_0 + h), \quad \delta z_h(x_0) = z_1 - z(x_0 + h), \quad \delta u_h(x_0) = u_1 - u(x_0 + h)$$

can be estimated as follows:

**Theorem 4.1.** Let us assume that  $s \ge 2$  and that H 1 holds. Then we get

(4.2) 
$$\begin{aligned} \delta y_h(x_0) &= O(h^{s+1}), \quad P_y(x_0+h) \, \delta y_h(x_0) = O(h^{\min(p,s+1)+1}), \\ \delta z_h(x_0) &= O(h^s), \quad P_z(x_0+h) \, \delta z_h(x_0) = O(h^{s+1}), \\ \delta u_h(x_0) &= O(h^{s-1}) \end{aligned}$$

where p is the order of the underlying quadrature formula.  $P_y(x)$ ,  $P_z(x)$  are the projectors (3.6) evaluated at the exact solution of (2.1) at x. If in addition H2 is satisfied, we have

(4.3) 
$$\delta y_h(x_0) = O(h^{p+1}), \quad P_z(x_0+h) \,\delta z_h(x_0) = O(h^{\min(p, 2s-2)+1}).$$

*Remark.* If the function k of (2.1) is linear in u, then instead of (4.3) we get

(4.3') 
$$P_{z}(x_{0}+h)\,\delta z_{h}(x_{0}) = O(h^{p+1}).$$

*Proof.* The interpretation of the collocation solution in terms of one corresponding IRK method (see Theorem 3.1 for more details) allows us to apply [3, Lemma 6.3] which leads to (4.2).

The results (4.3) can be found quite easily with the same techniques used in the proof of Theorem 3.2. Instead of computing the difference between two collocation polynomials with distinct initial values, we must estimate the difference between a collocation polynomial and the exact solution of (2.1), here with identical initial values. The exact solution has no defect (see (3.7)). The defect of the collocation polynomials vanishes at the collocation points  $x_0 + c_i h$ , therefore for  $x \in [x_0, x_0 + h]$  we have  $\delta(x) = O(h^s)$ ,  $\delta'(x) = O(h^{s-1})$ ,  $\mu(x) = O(h^s)$ , and  $\theta(x) = O(h^{s+1})$ ,  $\theta'(x) = O(h^s)$ ,  $\theta''(x) = O(h^{s-1})$  by consistency of the initial value  $y_0$ , i.e.,  $\theta(x_0) = -g(y_0) = 0$ . It can be easily shown that the derivatives of the collocation polynomials are uniformly bounded (see [5, Theorem VI.7.8] for an equivalent result concerning index 2 systems). With similar formulas to (3.15) and (3.22) we finally arrive at

$$(4.4) \begin{pmatrix} y(x_0+h) - Y(x_0+h) \\ z(x_0+h) - Z(x_0+h) \end{pmatrix} = \int_{x_0}^{x_0+h} \sigma(x_0+h,t) dt - S_4(x_0+h, x_0+h) \theta'(x_0+h) \\ = O(h^{p+1}) + \begin{pmatrix} 0 \\ \int_0^1 k_u (g_y f_z k_u)^{-1} (y, z, G(y, z, \tau \delta, \tau \delta', \tau \mu, \tau \theta'')) d\tau \cdot \theta' \end{pmatrix}$$

where y, z,  $\delta$ ,  $\delta'$ ,  $\mu$ ,  $\theta''$ , and  $\theta'$  are evaluated at  $x_0 + h$  in the last expression.

#### 5. Proof of Theorem 2.2

We only outline the main points.

Following the proof given in [3, Theorem 6.4], we denote two neighbouring collocation solutions by  $\{\tilde{y}_n, \tilde{z}_n\}$ ,  $\{\hat{y}_n, \hat{z}_n\}$  and their difference by  $\Delta y_n = \tilde{y}_n - \hat{y}_n, \Delta z_n = \tilde{z}_n - \hat{z}_n$ . In a first step it can be shown that (see [3, Theorem 6.4] or apply the second step with m = n = 0)

(5.1) 
$$\|\Delta y_n\| \leq C_1 h^{s+1}, \quad \|\Delta z_n\| \leq C_2 h^{s+1}.$$

Therefore global convergence of order s for the y- and z-component occurs. We thus get

(5.2) 
$$||(g_y f)(\tilde{y}_n, \tilde{z}_n)|| \leq C_3 h^s, \quad ||(g_y f)(\hat{y}_n, \hat{z}_n)|| \leq C_3 h^s.$$

We insist on the fact that the constants  $C_1$ ,  $C_2$ , and  $C_3$  can be chosen independently of *n* if *h* is sufficiently small.

Secondly, because of  $g(\tilde{y}_n) = 0 = g(\tilde{y}_n)$  the fourth remark after Theorem 3.2 holds, implying that

(5.3a) 
$$(Q_{y})_{n} \Delta y_{n} = O(||\Delta y_{n}||^{2}) = O(h^{s+1} ||(P_{y})_{n} \Delta y_{n}||),$$

though this is not essential for the present demonstration. With the above results, Theorem 3.2 can be applied, yielding

(5.3 b)  $(P_y)_{n+1} \Delta y_{n+1} = (P_y)_n \Delta y_n + h(P_y)_n (f_z)_n \Delta z_n$  $+ O(h ||(P_y)_n \Delta y_n|| + h^2 ||(P_z)_n \Delta z_n|| + h^{m+2} ||(Q_z)_n \Delta z_n|| + ||(Q_z)_n \Delta z_n||^2 )$ 

(5.3c) 
$$h(P_z)_{n+1} \Delta z_{n+1} = h(P_z)_n \Delta z_n$$

(5.3 d)  

$$+ O(h^2 ||(P_y)_n \Delta y_n|| + h^2 ||(P_z)_n \Delta z_n|| + h^{n+2} ||(Q_z)_n \Delta z_n|| + ||(Q_z)_n \Delta z_n||^2)$$

$$h(Q_z)_{n+1} \Delta z_{n+1} = O(h ||(P_y)_n \Delta y_n|| + h^2 ||\Delta z_n||)$$

where  $m = \min(s-2, \max(p-s-1, 0))$ ,  $n = \min(s-2, p-s)$  and  $(P_y)_n$ ,  $(Q_y)_n$ ,  $(f_z)_n$ ,  $(P_z)_n$ ,  $(Q_z)_n$  are evaluated at  $(\hat{y}_n, \hat{z}_n, \hat{u}_n^*)$ . Here  $\hat{u}_n^* := G(\hat{y}_n, \hat{z}_n)$ , with G as defined in Sect. 2. This choice of  $\hat{u}_n^*$  does not influence the values  $(\hat{y}_n, \hat{z}_n)$  (see the remark after Definition 2.1) and simplifies the proof. Hence the estimates (5.3) lead to

(5.4a) 
$$\|\Delta y_n\| \leq C(\|(P_y)_0 \Delta y_0\| + \|(P_z)_0 \Delta z_0\| + h^{n+1}\|(Q_z)_0 \Delta z_0\|)$$

(5.4b)  $h \| (P_z)_n \Delta z_n \| \leq C (h \| (P_y)_0 \Delta y_0 \| + h \| (P_z)_0 \Delta z_0 \| + h^{n+2} \| (Q_z)_0 \Delta z_0 \|)$ 

$$(5.4c) heta \| (Q_z)_n \Delta z_n \| \leq C(h \| (P_y)_0 \Delta y_0 \| + h \| (P_z)_0 \Delta z_0 \| + h^2 \| (Q_z)_0 \Delta z_0 \|).$$

If the function k of (2.1) is linear in u then the fifth remark after Theorem 3.2 and the remark after Theorem 4.1 hold. The final convergence result follows now from standard techniques (see [3, Fig. 4.1] or [4, Fig. II.3.2]).  $\Box$ 

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