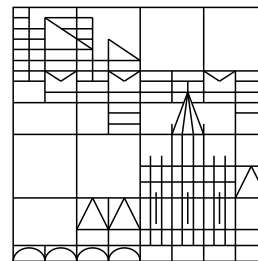


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Geometric Properties of Runge-Kutta Discretizations for Index 2 Differential Algebraic Systems

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Abstract

We analyze Runge-Kutta discretizations applied to index 2 differential algebraic equations (DAE's). We compare the asymptotic features of the numerical and the exact solutions. It is shown that Runge-Kutta methods satisfying the first order constraint condition of the DAE exactly reproduce the geometric properties of the continuous system correctly. The proof combines reduction techniques of discretized index 2 differential algebraic equations to discretized ordinary differential equations with some invariant manifolds results of Nipp, Stoffer [12]. The results support the favourable behavior of these Runge-Kutta methods applied to index 2 DAE's for $t \geq 0$.

1 Introduction

Differential algebraic problems of index 2 frequently arise when modelling phenomena from scientific computations. An important class for such problems is, e.g, multibody systems with constraints on the velocity level. They also occur as auxiliary systems for minimization problems when searching for an evolution that approaches a local minimum of an objective function restricted by algebraic constraints (see, e.g., Schropp [14]).

Quite often analytic treatment of the system is impossible and, hence, numerical simulations become important to gain a deeper understanding of the global behavior. Here the question arises which qualitative properties of the continuous system are preserved by a numerical method.

In the present paper we analyze the behavior of some widely spreaded Runge-Kutta type discretizations applied to index 2 DAE's in Hessenberg form. To be more precise, we focus our interest onto two different aspects. It is well known that the solution flow of the DAE takes place in a submanifold of the state times control space. We characterize how that submanifold persists under discretization with projected and half-explicit Runge-Kutta methods. We show

that the discretized dynamics possesses a submanifold too which is situated nearby the original one. Moreover, we deal with the following subject. The index 0 formulation of the DAE is an ordinary differential equation (ODE) on the manifold defined by the first order constraint condition. Runge-Kutta schemes satisfying that condition can be regarded as discrete flows on that manifold. Hence, the question about the behavior of numerical methods near invariant sets like stationary points or periodic orbits on manifolds is of interest.

Our main tools are embedding and invariant manifold techniques. We embed the original DAE into a DAE of the same index such that the corresponding index 0 ODE admits a representation as dynamical system on an open subset of the euclidian space. Then, using discrete invariant manifold techniques of Nipp, Stoffer ([12]) we mimic that approach for the projected and half-explicit Runge-Kutta dynamics. This will allow us to use classical convergence tools on \mathbb{R}^N . Applying the results of Beyn ([2]) for one-step methods in \mathbb{R}^N , we can establish that the phase portrait near hyperbolic periodic orbits is reproduced correctly. Moreover, it underpins the use of projected or half explicit Runge-Kutta DAE methods when dealing with the longtime behavior of index 2 DAE's.

Our work was largely motivated by the discretization results of Beyn ([2]), ([3]), Garay ([5]) and Kloeden, Lorenz ([10]) for one-step methods near compact, invariant sets. Later we learnt the convergence theory for DAE's from the excellent book of Hairer, Lubich & Roche ([7]). After finishing our paper we were informed about a forthcoming paper of Nipp ([11]). In ([11]) a persistence result of the invariant manifold of an index 2 DAE under discretization is shown for the special class of stiffly accurate Runge-Kutta methods.

2 The main results

We consider the DAE

$$\begin{aligned} \dot{u} &= f(u, \lambda), \\ 0 &= g(u), \end{aligned} \tag{2.1}$$

$u \in \mathbb{R}^N$ and $\lambda \in \mathbb{R}^l$ in Hessenberg form. Let C_b^r denote the space of functions of class C^r with bounded derivatives up to order r . We make the following assumptions.

(A1) f and g are C_b^r -functions for r sufficiently big.

(A2) There is a C_b^r -function ψ_0 satisfying $Dg(u)f(u, \psi_0(u)) = 0$ for $u \in D_\tau := \{u \in \mathbb{R}^N \mid \|g(u)\|_2 < \tau\}$, $\tau > 0$.

(A3) $Dg(u)\frac{\partial f}{\partial \lambda}(u, \psi_0(u))$ is invertible for $u \in D_\tau$ and the inverse has bounded norm.

In particular, problem (2.1) is of index 2. Additionally, condition (A3) says that $Dg(u)$ is of full rank so that the second equation of (2.1) defines the submanifold $M := \{u \in \mathbb{R}^N \mid g(u) = 0\}$ of \mathbb{R}^N and the underlying index 0 ODE reads

$$\dot{u} = f(u, \psi_0(u)), u \in M. \tag{2.2}$$

We denote the solution flow of (2.2) with $\bar{u}(t, u_0)$, $u_0 \in M$. Here, (A2) implies the solution flow $(\bar{u}(t, u_0), \bar{\lambda}(t, u_0))$, $\bar{\lambda}(t, u_0) = \psi_0(\bar{u}(t, u_0))$ for equation (2.1). This means that the manifold

$$M_0 = \{(u, \lambda) \in D_\tau \times \mathbb{R}^l \mid g(u) = 0, \lambda = \psi_0(u)\}$$

is invariant under the solution flow of (2.1). Moreover, the dynamics of the u -component can be interpreted as a dynamical system on the manifold $g(u) = 0$.

We are interested in the qualitative, geometric features of s -stage Runge-Kutta type methods with Butcher tableau

$$\frac{c}{b^T} \mid \begin{array}{c} A \\ b^T \end{array}, \quad A = (a_{ij})_{1 \leq i, j \leq s} \in \mathbb{R}^{s, s}, \quad b, c \in \mathbb{R}^s \quad (2.3)$$

and constant step size h when applied to (2.1). The Runge-Kutta method possesses stage order q , if

$$\sum_{j=1}^s a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \quad k = 1, \dots, q, \quad i = 1, \dots, s.$$

To avoid drift problems in the discrete long time run we have to focus our interest to Runge-Kutta type methods which retain the first order constraint $g(u) = 0$. This leads us to the widely spreaded projected Runge-Kutta methods introduced by Ascher & Petzold [1] or to the half-explicit Runge-Kutta methods due to Hairer, Lubich and Roche [7]. For the Butcher tableau of the projected Runge-Kutta method we impose the conditions:

(B1) The Runge-Kutta matrix A is invertible.

(B2) $R(\infty) = 1 - b^T A^{-1} \mathbb{I}$, $\mathbb{I} = (1, \dots, 1)$ satisfies $|R(\infty)| < 1$.

(B3) The method is of classical order p and possesses stage order q with $p \geq q \geq 1$.

For the half-explicit method, that is, $a_{i,j} = 0$ for $i \leq j$ we assume

(B1') $a_{i+1,i} \neq 0$ for $i = 1, \dots, s-1$ and $b_s \neq 0$.

(B2') The method is of order p .

Applied to equation (2.1) the projected Runge-Kutta method has the form

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + h(b^T \otimes I) \bar{f}(U^n, \Lambda^n), \\ \lambda_{n+1} &= (1 - b^T A^{-1} \mathbb{I}) \lambda_n + (b^T A^{-1} \otimes I) \Lambda^n \end{aligned} \quad (2.4)$$

where $U^n = (U_1^n, \dots, U_s^n) \in \mathbb{R}^{Ns}$, $\Lambda^n = (\Lambda_1^n, \dots, \Lambda_s^n) \in \mathbb{R}^{ls}$ denote the solution of the algebraic system

$$\begin{aligned} U - (\mathbb{I} \otimes u_n) &= h(A \otimes I) \bar{f}(U, \Lambda), \\ 0 &= \bar{g}(U) \end{aligned} \quad (2.5)$$

and \bar{f}, \bar{g} stand for $\bar{f}(U^n, \Lambda^n) = (f(U_1^n, \Lambda_1^n), \dots, f(U_s^n, \Lambda_s^n))$, $\bar{g}(U^n) = (g(U_1^n), \dots, g(U_s^n))$. Finally, the projection step

$$\begin{aligned} u_{n+1} &= \tilde{u}_{n+1} + \frac{\partial}{\partial \lambda} f(u_{n+1}, \lambda_{n+1}) \gamma, \\ 0 &= g(u_{n+1}) \end{aligned} \quad (2.6)$$

determines u_{n+1} .

A Runge-Kutta method satisfying $a_{sj} = b_j$, $j = 1, \dots, s$ is called stiffly accurate. Stiffly accurate Runge-Kutta solutions satisfy the first order constraint $g(u) = 0$ and, hence, the projection step (2.6) is superfluous.

The application of a half-explicit Runge-Kutta method to (2.1) reads as follows. Solve (2.5) in the case $a_{i,j} = 0$ for $j \geq i$ and obtain U^n and Λ_i^n , $i = 1, \dots, s-1$. Then Λ_s^n and u_{n+1} are computed by

$$\begin{aligned} u_{n+1} &= u_n + h(b^T \otimes I) \bar{f}(U^n, \Lambda^n), \\ 0 &= g(u_{n+1}). \end{aligned} \quad (2.7)$$

In order to compute the λ -component one has several possibilities. The most accurate is the computation of λ from the index 2 condition, that is $\lambda_n = \psi_0(u_n)$. Here we follow the more efficient approach of Hairer, Lubich, Roche [8]. They propose to require $c_s = 1$ and take

$$\lambda_{n+1} = \Lambda_s^n. \quad (2.8)$$

Moreover, we assume

(B3') $\Lambda_s^n - \bar{\lambda}(h, u_n) = O(h^r)$, $r \leq p$ (see, e.g., Hairer, Brasey [6] for sufficient conditions on A, b, c).

The qualitative properties of the discrete schemes are characterized in

Theorem 2.1 *Consider the DAE (2.1) and assume (A1)-(A3). Let (u_n, λ_n) denote the sequences generated with a projected [half-explicit] Runge-Kutta method satisfying (B1)-(B3) [(B1')-(B3')], when applied to (2.1) with consistent initial values (u_0, λ_0) .*

Then for $0 < h < h_0$, $h_0 > 0$ sufficiently small there is a C_b^r -function $\psi_{0,h} : M \rightarrow \mathbb{R}^l$, $M = \{u \in \mathbb{R}^N \mid g(u) = 0\}$ such that the following assertions hold.

- i) The set $M_{0,h} = \{(u, \lambda) \in D_\gamma \times \mathbb{R}^l \mid g(u) = 0, \lambda = \psi_{0,h}(u)\}$ is invariant for the projected [half-explicit] Runge-Kutta map (2.4)-(2.6) [(2.7)-(2.8)].*
- ii) The manifold $M_{0,h}$ is uniformly attractive with attractivity constant $\chi_h = |R(\infty)| + O(h^{q+1})$ [$\chi_h = 0$].*
- iii) For every initial value (u_0, λ_0) with $\|\lambda_0 - \psi_0(u_0)\|$ sufficiently small there is $(\tilde{u}_0, \tilde{\lambda}_0) \in M_{0,h}$ and $c, \hat{c} > 0$ such that the corresponding evolutions (u_n, λ_n) and $(\tilde{u}_n, \tilde{\lambda}_n)$ satisfy*

$$\begin{aligned} \|u_i - \tilde{u}_i\| &\leq c \chi_h^i \|\lambda_0 - \psi_0(u_0)\|, \quad i = 0, 1, 2, \dots, \\ \|\lambda_i - \tilde{\lambda}_i\| &\leq \hat{c} \chi_h^i \|\lambda_0 - \psi_0(u_0)\| \quad i = 0, 1, 2, \dots \end{aligned}$$

iv) $\| \psi_0(u) - \psi_{0,h}(u) \| \leq Ch^q [Ch^r]$ for $u \in M$.

Remark: The invariant manifold $M_{0,h}$ in the projected Runge-Kutta case is highly attractive, if $R(\infty) = 0$. The manifold is infinite attractive, that is, $(u_1, \lambda_1) \in M_{0,h}$ for every (u_0, λ_0) , if $\chi_h = 0$. This is valid for half-explicit and stiffly accurate Runge-Kutta methods.

Next we characterize the behavior of the projected and half-explicit Runge-Kutta methods for index 2 DAE's (2.1) in a neighborhood of hyperbolic periodic orbits. Here, we call $(\bar{u}(t, u_0), \bar{\lambda}(t, u_0))$, $\bar{\lambda}(t, u_0) = \psi_0(\bar{u}(t, u_0))$, $\bar{u}(t, u_0) = \bar{u}(t+T, u_0)$ a hyperbolic T -periodic orbit of (2.1), if $\bar{u}(t, u_0)$ is a hyperbolic T -periodic solution of (2.2).

Theorem 2.2 *Let the assumptions of Theorem 2.1 hold and let $(\bar{u}(t, u_0), \bar{\lambda}(t, u_0))$, $\bar{\lambda}(t, u_0) = \psi_0(\bar{u}(t, u_0))$ be a hyperbolic T -periodic orbit of the DAE (2.1). Additionally, let (u_n, λ_n) be generated by applying the projected Runge-Kutta scheme (2.4)-(2.6) [half-explicit Runge-Kutta method (2.7)-(2.8)] onto the DAE (2.1).*

Then, the u -component of the discrete dynamics possesses an invariant curve $\gamma^h = u^h(\mathbb{R})$, $u^h(t) = u^h(t+T)$ satisfying

$$\max\{\| \bar{u}(t, u_0) - u^h(t) \| \mid t \in \mathbb{R}\} \leq Ch^q [Ch^r].$$

As a direct consequence of Theorem 2.1 and Theorem 2.2 we obtain

Corollary 2.3 *Under the hypotheses of Theorem 2.1 and Theorem 2.2 there is an invariant curve $S^h(\mathbb{R}) = (u^h(\mathbb{R}), \psi_{0,h}(u^h(\mathbb{R})))$, $S^h(t) = S^h(t+T)$ for the projected [half-explicit] Runge-Kutta map such that*

$$\max\{\| (\bar{u}(t, u_0), \bar{\lambda}(t, u_0)) - S^h(t) \| \mid t \in \mathbb{R}\} \leq Ch^q [Ch^r]$$

is valid.

Theorem 2.2 shows that half-explicit or projected Runge-Kutta methods reproduce the original phase portrait in a neighborhood of a periodic orbit correctly. Moreover, this result can be regarded as the analogue of Theorem 2.1 of Beyn ([2]) for ODE's on manifolds of the form $g(u) = 0$. Using the results of Beyn ([3]) and Garay ([5]) a similar result for the phase portrait projected or half-explicit Runge-Kutta methods near equilibria will be presented in a forthcoming paper.

3 Embedding techniques for index 2 DAE's

We have seen in the previous section that the corresponding index 0 version (2.2) to an index 2 DAE (2.1) is a dynamical system on a manifold. For technical reasons it might be useful to embed (2.2) into an ODE on an open neighborhood of M in \mathbb{R}^N . Assuming (A1)-(A3), a

smooth embedding of (2.2) into D_γ , $\gamma \in]0, \tau]$ sufficiently small can be established as follows. Consider the DAE

$$\begin{aligned} \dot{u} &= f(u, \lambda), \\ \dot{v} &= -B(u)v, \quad B(u) \in \mathbb{R}^{l,l}, \quad \mu_2(-B(u)) \leq -\eta, \quad \eta > 0 \text{ for } u \in D_\tau, \\ 0 &= g(u) - v \end{aligned} \tag{3.1}$$

with a C_b^r -function $B(\cdot)$ in D_τ (e.g. choose $B \equiv I$). Our aim here to show is that (A1)-(A3) hold analogously for (3.1). In particular, to guarantee a smooth function $\psi = \psi(u, v)$ satisfying $Dg(u)f(u, \psi(u, v)) + B(u)v = 0$, we need the following version of Banachs fixed point theorem in a ball which is for later purposes formulated in the more general concept of vectornorms.

A functional $|\cdot| : W \rightarrow \mathbb{R}^k$ on a vector space W is called a generalized norm, if

$$\begin{aligned} |v| \geq 0, \quad |v| = 0 &\iff v = 0, \\ |v_1 + v_2| &\leq |v_1| + |v_2| \end{aligned} \tag{3.2}$$

holds with the natural ordering “ \leq ” on \mathbb{R}^k . Every norm $\|\cdot\|_*$ in \mathbb{R}^k defines a norm $\|\cdot\|$ in W via $\|v\| = \| |v| \|_*$.

Lemma 3.1 *Let $(W, |\cdot|)$ be a Banach space with generalized norm $|\cdot|$ and let $B := \{v \in W \mid |v - v_0| \leq r\}$ for $r > 0$. Let the map $F : B \mapsto W$ be continuously differentiable with invertible $DF(v_0)$. Moreover, for some nonnegative matrices $P, K \in \mathbb{R}^{k,k}$ we assume*

$$\begin{aligned} |DF(v_0)^{-1}z| &\leq P|z|, \quad z \in W, \\ |(DF(v_0) - DF(v))z| &\leq K|z|, \quad z \in W, \quad v \in B, \\ P|F(v_0)| &< (I - PK)r. \end{aligned}$$

Then, the equation $F(v) = 0$ has a unique solution in B . In addition, the matrix $I - PK$ is nonsingular and we have the stability inequality

$$|v - w| \leq (I - PK)^{-1}P|F(v) - F(w)| \quad \forall v, w \in B.$$

A proof of Lemma 3.1 can be found in Beyn, Schropp [4].

We construct ψ by applying Lemma 3.1 onto the equation

$$F_{u,v}(\zeta) := Dg(u)f(u, \psi_0(u) + \zeta) + B(u)v = 0. \tag{3.3}$$

For $\zeta_0 = 0$ we can compute with $\rho := \sup\{\|B(u)\|_2 \mid u \in D_\tau\} < \infty$ the inequalities

$$\begin{aligned} \|F_{u,v}(0)\| &\leq \rho \|v\|, \\ \|DF_{u,v}(0)^{-1}\| &\leq C \end{aligned}$$

as well as $DF_{u,v}(0) - DF_{u,v}(\zeta) = Dg(u)(\frac{\partial f}{\partial \lambda}(u, \psi_0(u)) - \frac{\partial f}{\partial \lambda}(u, \psi_0(u) + \zeta))$. Hence, we obtain

$$\| DF_{u,v}(0) - DF_{u,v}(\zeta) \| \leq \hat{C}r_0 \quad \text{for } \|\zeta\| \leq r_0.$$

Obviously, the inequality

$$C \| F_{u,v}(0) \| \leq C\rho \| v \| < (1 - C\hat{C}r_0)r_0$$

holds for $\|v\|, r_0 > 0$ sufficiently small. Then Lemma 3.1 guarantees that the equation (3.3) possesses exactly one solution $\hat{\zeta}_{u,v}$ in $K_{r_0}(0)$, that is, $\psi(u, v) = \psi_0(u) + \hat{\zeta}_{u,v}$ satisfies $Dg(u)f(u, \psi(u, v)) + B(u)v = 0$ for $u \in D_\gamma$, $\|v\|_2 \leq \gamma$ and an implicit function argument ensures the smoothness of ψ .

Moreover, an application of the banach lemma with $Dg(u)\frac{\partial f}{\partial \lambda}(u, \psi_0(u))$ and the perturbation $Dg(u)\frac{\partial f}{\partial \lambda}(u, \psi(u, v))$ shows that $Dg(u)\frac{\partial f}{\partial \lambda}(u, \psi(u, v))$, $\|v\| < \gamma$ is invertible and the inverse possesses a bounded norm.

Here the reader may notice that we have $\psi_0(u) = \psi(u, 0)$ by uniqueness. Using the theory of logarithmic norms (see, e.g., Strehmel & Weiner [15], Theorem 5.1.3) we obtain that

$$\|v(t)\|_2 \leq \|v(0)\|_2 \exp(-\eta t) \quad (3.4)$$

is valid for the v -component of every solution of (3.1). In particular, with $v(0) = 0$ problem (3.1) reduces to (2.1). After eliminating the v -variables the underlying index 0 ODE of (3.1) reads

$$\dot{u} = f(u, \psi(u, g(u))) =: k(u), \quad u \in D_\gamma \subset \mathbb{R}^N \text{ open.} \quad (3.5)$$

Next we summarize the qualitative properties of the solutions of (3.1).

Lemma 3.2 *Consider equation (3.1) on the phase space D_γ , $\gamma \in]0, \tau]$ and let (A1)-(A3) hold.*

Then every solution of (3.1) with initial value $u_0 \in D_\gamma$, $v_0 = g(u_0)$ and $\lambda_0 = \psi(u_0, v_0)$ exists for all $t \geq 0$. Moreover, $g^{-1}(0)$ is an invariant and globally attractive subset of the phase space.

The proof of Lemma 3.2 is a direct consequence of (3.4) and the fact that f, g, B are C_b^r -functions.

We are interested in the behavior of s -stage projected and half-explicit Runge-Kutta type methods of order p with Butcher tableau (2.3) and constant step size h when applied to (3.1). The projected Runge-Kutta method has the form

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + h(b^T \otimes I)\bar{f}(U^n, \Lambda^n), \\ v_{n+1} &= v_n - h(b^T \otimes I)\bar{B}(U^n)V^n, \\ \lambda_{n+1} &= (1 - b^T A^{-1}\mathbb{I})\lambda_n + (b^T A^{-1} \otimes I)\Lambda^n \end{aligned} \quad (3.6)$$

where $U^n = (U_1^n, \dots, U_s^n) \in \mathbb{R}^{Ns}$, $V^n = (V_1^n, \dots, V_s^n) \in \mathbb{R}^{ls}$, $\Lambda^n = (\Lambda_1^n, \dots, \Lambda_s^n) \in \mathbb{R}^{ls}$ denote the solution of the algebraic system

$$\begin{aligned} U - (\mathbb{I} \otimes u_n) &= h(A \otimes I) \bar{f}(U, \Lambda), \\ V - (\mathbb{I} \otimes v_n) &= -h(A \otimes I) \bar{B}(U) V, \\ 0 &= \bar{g}(U) - V \end{aligned} \quad (3.7)$$

and \bar{B} stands for $\bar{B}(U^n) = \text{diag}(B(U_1^n), \dots, B(U_s^n))$. Finally, the projection step

$$\begin{aligned} u_{n+1} &= \tilde{u}_{n+1} + \frac{\partial}{\partial \lambda} f(u_{n+1}, \lambda_{n+1}) \gamma, \\ 0 &= g(u_{n+1}) - v_{n+1} \end{aligned} \quad (3.8)$$

is used to compute u_{n+1} .

The application of half-explicit Runge-Kutta methods to (3.1) reads as follows. Solving (3.7) in the case $a_{i,j} = 0$ for $j \geq i$ gives us U^n , V^n and Λ_i^n , $i = 1, \dots, s-1$. Then Λ_s^n and u_{n+1} , v_{n+1} are obtained by

$$\begin{aligned} u_{n+1} &= u_n + h(b^T \otimes I) \bar{f}(U^n, \Lambda^n), \\ v_{n+1} &= v_n - h(b^T \otimes I) \bar{B}(U^n) V^n, \\ 0 &= g(u_{n+1}) - v_{n+1}. \end{aligned} \quad (3.9)$$

The reader may notice that (3.6)-(3.8) and (3.9) reduce to (2.4)-(2.6) and (2.7), respectively, when initialized with $v_n = 0$.

In this section we will guarantee the existence and uniqueness of the discrete iterates generated by a projected or a half-explicit Runge-Kutta method for all $n \in \mathbb{N}$. If one identifies the two state variables (u, v) the solubility of the discrete systems (3.6)-(3.9) for $n \in \mathbb{N}$ with $0 \leq nh \leq t_{end}$ is guaranteed by the standard theory, see e.g., Hairer and Wanner [9], Ch. VII.3 and VII.4. But in the process of proving Theorem 2.1 a refined stability inequality which distinguishes the two variables u and v is needed. To establish inequalities of that type we work with the concept of vector norms (see (3.2)).

Lemma 3.3 *Let the assumptions of Theorem 2.1 hold and let $u_0 \in D_\gamma$, $v_0 = g(u_0)$, $\lambda_0 = \psi(u_0, v_0)$ be a consistent initial value for the DAE (3.1).*

Then the projected and half-explicit Runge-Kutta iterates (u_n, v_n, λ_n) exist for $n \in \mathbb{N}$. For the stages (U, V, Λ) of the Runge-Kutta dynamics we have with $v_0(u) := (\mathbb{I} \otimes u, \mathbb{I} \otimes g(u), \mathbb{I} \otimes \psi(u, g(u)))$ the stability inequality

$$\|(U, V, \Lambda) - v_0(u)\| \leq O(h)(\|k(u)\| + \|g(u)\|) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \quad (3.10)$$

Moreover, the final projected Runge-Kutta iterates satisfy

$$(\|u_{n+1} - \tilde{u}_{n+1}\|, \|\gamma\|) = \min\{O(h^{q+1}), O(h^2)(\|k(u_n)\| + \|g(u_n)\|)\}.$$

Proof of Lemma 3.3: The first step of a projected Runge-Kutta method is a classical Runge-Kutta step. Following Hairer and Wanner [9], p.493 we replace (3.7) for $h > 0$ by the equivalent system

$$\begin{aligned} U - (\mathbb{I} \otimes u_n) &= h(A \otimes I)\bar{f}(U, \Lambda), \\ V - (\mathbb{I} \otimes v_n) &= -h(A \otimes I)\bar{B}(U)V, \\ 0 &= \int_0^1 \text{diag}(Dg(u_n + \tau(U_i^n - u_n)), i = 1, \dots, s)d\tau (A \otimes I)\bar{f}(U^n, \Lambda^n) \\ &\quad + (A \otimes I)\bar{B}(U)V + \frac{1}{h}(\bar{g}(\mathbb{I} \otimes u_n) - \mathbb{I} \otimes v_n). \end{aligned} \quad (3.11)$$

We use $v_n = g(u_n)$ and prove Lemma 3.3 by applying Lemma 3.1 onto the equation

$$\begin{aligned} T_1(h, u, U, V, \Lambda) &:= \begin{pmatrix} U - (\mathbb{I} \otimes u) - h(A \otimes I)\bar{f}(U, \Lambda) \\ V - (\mathbb{I} \otimes g(u)) + h(A \otimes I)\bar{B}(U)V \\ \int_0^1 \text{diag}(Dg(u + \tau(U_i - u)), i = 1, \dots, s)d\tau (A \otimes I)\bar{f}(U, \Lambda) \\ + (A \otimes I)\bar{B}(U)V \end{pmatrix} \\ &= 0, \quad 0 < h < h_0, \quad u \in D_\gamma. \end{aligned} \quad (3.12)$$

Introducing the generalized norm $|(U, V, \Lambda)| = (\|U\|, \|V\|, \|\Lambda\|) \in \mathbb{R}^3$ and the central point $v_0(u) := (\mathbb{I} \otimes u, \mathbb{I} \otimes g(u), \mathbb{I} \otimes \psi(u, g(u)))$, we calculate

$$T_1(h, u, v_0(u)) = (O(h), O(h), 0). \quad (3.13)$$

For the derivative of T_1 with respect to (U, V, Λ) we find with $\gamma(u) = (u, \psi(u, g(u)))$ the representation

$$\frac{\partial}{\partial(U, V, \Lambda)} T_1(h, u, v_0(u)) = \begin{pmatrix} I + O(h) & 0 & O(h) \\ O(h) & I + O(h) & 0 \\ O(1) & O(1) & A \otimes Dg(u) \frac{\partial f}{\partial \lambda}(\gamma(u)) \end{pmatrix}.$$

Now the analogue of (A3) for (3.1) and (B1) imply that $(A \otimes Dg(u) \frac{\partial f}{\partial \lambda}(\gamma(u)))$ is nonsingular. Hence, $\frac{\partial}{\partial(U, V, \Lambda)} T_1(h, u, v_0(u))$ is invertible for $0 < h \leq h_0$, $h_0 > 0$ sufficiently small and the inverse is of the form

$$\frac{\partial}{\partial(U, V, \Lambda)} T_1(h, u, v_0(u))^{-1} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ O(1) & O(1) & (A \otimes (Dg(u) \frac{\partial f}{\partial \lambda}(\gamma(u))))^{-1} \end{pmatrix} + O(h).$$

In terms of vector norms this leads to $|\frac{\partial}{\partial(U, V, \Lambda)} T_1(h, u, v_0(u))^{-1}| \leq P_h$ with

$$P_h := \begin{pmatrix} 1 + O(h) & O(h) & O(h) \\ O(h) & 1 + O(h) & O(h) \\ O(1) & O(1) & O(1) \end{pmatrix} \in \mathbb{R}^{3,3}.$$

Then, following the lines of the proof of Lemma 4.1 in Beyn, Schropp [4] we obtain the unique solubility of (3.12) in $B_r(v_0) := \{(U, V, \Lambda) \in \mathbb{R}^{(N+l+l)s} \mid \|(U, V, \Lambda) - (\mathbb{I} \otimes u, \mathbb{I} \otimes g(u), \mathbb{I} \otimes \psi(u, g(u)))\| \leq r\}$, $r = (r_1, r_2, r_3) > 0$. We remark that an application of the implicit function theorem ensures the smooth dependency of the solution (U, V, Λ) from (h, u) . In addition, the claimed stability inequality holds.

The second step is the projection of the classical Runge-Kutta iterates onto the constrained manifold $g(u) - v = 0$. We consider the equation

$$T_2(h, u, \lambda, u_p, v_p, \gamma) = \begin{pmatrix} u_p - u - h(b^T \otimes I)\bar{f}(U(h, u), \Lambda(h, u)) \\ -\frac{\partial}{\partial \lambda} f(u_p, R(\infty)\lambda + (b^T A^{-1} \otimes I)\Lambda(h, u))\gamma \\ v_p - g(u) + h(b^T \otimes I)\bar{B}(U(h, u))V(h, u) \\ g(u_p) - v_p \end{pmatrix} = 0 \quad (3.14)$$

for $0 < h < h_0$, $u \in D_\gamma$, $\|\lambda - \psi(u, g(u))\| < \epsilon$, $\epsilon > 0$ sufficiently small. With the central point $v_0(u) = (v_0(u)_1, v_0(u)_2, v_0(u)_3)$,

$$\begin{aligned} v_0(u)_1 &= u + h(b^T \otimes I)\bar{f}(U(h, u), \Lambda(h, u)), \\ v_0(u)_2 &= g(u) - h(b^T \otimes I)\bar{B}(U(h, u))V(h, u), \\ v_0(u)_3 &= 0 \end{aligned}$$

we can compute

$$T_2(h, u, \lambda, v_0(u)) = \begin{pmatrix} 0 \\ 0 \\ g(v_0(u)_1) - v_0(u)_2 \end{pmatrix} =: \begin{pmatrix} 0 \\ 0 \\ r(h, u) \end{pmatrix}.$$

Obviously, $r(h, u) = O(h^{q+1})$ holds from the local error of the underlying classical Runge-Kutta map (see, e.g., Lemma 4.4 in [9]).

On the other hand, with (3.10), $k(u) = f(u, \psi(u, g(u)))$ and $\bar{k}(U) = \bar{f}(U, \bar{\psi}(U, \bar{g}(U)))$ we can calculate

$$\begin{aligned} \|r(h, u)\| &\leq \|g(u + h(b^T \otimes I)\bar{f}(U(h, u), \Lambda(h, u))) - g(u + h(b^T \otimes I)\bar{k}(\mathbb{I} \otimes u))\| \\ &\quad + \|g(u + hk(u)) - g(u) - hDg(u)k(u)\| \\ &\quad + h\|(b^T \otimes I)[D\bar{g}(\mathbb{I} \otimes u)\bar{k}(\mathbb{I} \otimes u) - D\bar{g}(U(h, u))\bar{k}(U(h, u))]\| \\ &= O(h^2)(\|k(u)\| + \|g(u)\|). \end{aligned}$$

Then, using $R(\infty)\lambda + (b^T A^{-1} \otimes I)\Lambda(h, u) = \psi(u, g(u)) + O(h) + O(\epsilon)$ and $v_0(u)_1 = u + O(h)$ we obtain

$$\frac{\partial}{\partial(u_p, v_p, \gamma)} T_2(h, u, \lambda, v_0(u)) = \begin{pmatrix} I & 0 & -\frac{\partial}{\partial \lambda} f(\gamma(u)) \\ 0 & I & 0 \\ Dg(u) & -I & 0 \end{pmatrix} + O(h) + O(\epsilon). \quad (3.15)$$

Thus, $\frac{\partial}{\partial(u_p, v_p, \gamma)} T_2(h, u, \lambda, v_0(u))$ is invertible for h and $\epsilon = \|\lambda - \psi(u, g(u))\|$ sufficiently small. Moreover, the equation $T_2(h, u, \lambda, \dots) = 0$ possesses a unique solution in $B_r(v_0)$ for $r > 0$ appropriate and according to our two estimations on $r(h, u)$ the two stability inequalities

$$(\|u_{n+1} - \tilde{u}_{n+1}\|, \|\gamma\|) = \min \{O(h^{q+1}), O(h^2)(\|k(u_n)\| + \|g(u_n)\|)\} \quad (3.16)$$

hold.

It remains to show that the sequence (u_n, v_n, λ_n) generated by a projected Runge-Kutta method with consistent initial value $u_0, v_0 = g(u_0), \lambda_0 = \psi(u_0, g(u_0))$ satisfies

$$\|\lambda_n - \psi(u_n, g(u_n))\| < \epsilon, \quad n \in \mathbb{N}. \quad (3.17)$$

To that purpose we define $\eta_n := \lambda_n - \psi(u_n, g(u_n))$. The iteration scheme of this sequence reads

$$\begin{aligned} \eta_{n+1} &= R(\infty)\eta_n + \psi(u_n, g(u_n)) - \psi(u_{n+1}, g(u_{n+1})) \\ &\quad + (b^T A^{-1} \otimes I)(\Lambda(h, u_n) - \mathbb{I} \otimes \psi(u_n, g(u_n))) \\ &=: R(\infty)\eta_n + \beta_n, \quad \eta_0 = 0 \end{aligned} \quad (3.18)$$

with $\beta_n = O(h)$. Using $|R(\infty)| < 1$, the theory of difference equations yields

$$\begin{aligned} \|\eta_n\| &\leq \|\eta_0\| + \frac{1}{1 - R(\infty)} \sup\{\|\beta_n\| \mid n \in \mathbb{N}\} \\ &= O(h) \quad \forall n \in \mathbb{N} \end{aligned} \quad (3.19)$$

and (3.17) is shown.

Next we prove the existence of the iterates (u_n, v_n, λ_n) for half-explicit Runge-Kutta methods. We define $\tilde{U} = (U_2, \dots, U_s, u_p)$, $\tilde{V} = (V_2, \dots, V_s, v_p)$, $\Lambda = (\Lambda_1, \dots, \Lambda_s)$ as well as $U_1 = u, V_1 = g(u)$ and apply Lemma 3.1 onto the equation

$$T(h, u, \tilde{U}, \tilde{V}, \Lambda) = \begin{pmatrix} U_i - u - h \sum_{j=1}^{i-1} a_{ij} f(U_j, \Lambda_j), \quad i = 2, \dots, s \\ u_p - u - h \sum_{j=1}^s b_j f(U_j, \Lambda_j) \\ V_i - g(u) + h \sum_{j=1}^{i-1} a_{ij} B(U_j) V_j, \quad i = 2, \dots, s \\ v_p - g(u) + h \sum_{j=1}^s b_j B(U_j) V_j \\ g(U_i) - V_i, \quad i = 2, \dots, s, \\ g(u_p) - v_p \end{pmatrix} = 0.$$

Now, we define

$$\tilde{A} = \begin{pmatrix} a_{21} & & & & & & & & \\ a_{31} & a_{32} & & & & & & & \\ \vdots & & \ddots & & & & & & \\ a_{s1} & \dots & \dots & a_{ss-1} & & & & & \\ b_1 & \dots & \dots & b_{s-1} & b_s & & & & \end{pmatrix}$$

which is invertible by (B1'). With \tilde{A} we can rewrite T in the form

$$T(h, u, \tilde{U}, \tilde{V}, \Lambda) = \begin{pmatrix} \tilde{U} - \mathbb{I} \otimes u - h(\tilde{A} \otimes I)\bar{f}((u, \tilde{U}_1, \dots, \tilde{U}_{s-1}), \Lambda) \\ \tilde{V} - \mathbb{I} \otimes g(u) + \\ + h(\tilde{A} \otimes I)\bar{B}((u, \tilde{U}_1, \dots, \tilde{U}_{s-1}))(g(u), \tilde{V}_1, \dots, \tilde{V}_{s-1}) \\ \bar{g}(\tilde{U}) - \tilde{V} \end{pmatrix}. \quad (3.20)$$

Except for the shift (U, V) to (\tilde{U}, \tilde{V}) this is equivalent to a classical Runge-Kutta step with invertible matrix \tilde{A} . Thus, we can adapt the first step of the projected Runge-Kutta proof with the central point $v_0(u) = (\mathbb{I} \otimes u, \mathbb{I} \otimes g(u), \mathbb{I} \otimes \psi(u, g(u)))$ to work for half explicit methods too. Moreover, the stability inequality

$$\begin{pmatrix} \|\tilde{U} - \mathbb{I} \otimes u\| \\ \|\tilde{V} - \mathbb{I} \otimes g(u)\| \\ \|\Lambda - \mathbb{I} \otimes \psi(u, g(u))\| \end{pmatrix} \leq Ch (\|k(u)\| + \|g(u)\|) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad (3.21)$$

is valid. We summarize our results for the projected and half-explicit Runge-Kutta methods in

Lemma 3.4 *Let the conditions of Lemma 3.2 hold for equation (3.1). By (u_n, v_n, λ_n) we denote the sequences generated with a projected Runge-Kutta method satisfying (B1)-(B3) or a half-explicit Runge-Kutta method fulfilling (B1')-(B3') when applied to (3.1) with initial values $u_0 \in D_\gamma$, $v_0 = g(u_0)$ and $\lambda_0 = \psi(u_0, v_0)$.*

Then $h_0 > 0$ exists such that the projected or half-explicit Runge-Kutta scheme is well defined for $0 < h < h_0$, $n \in \mathbb{N}$ and reproduces the phase portrait of (3.1) correctly, that is, $g^{-1}(0)$ is a positive invariant and globally attractive subset of the phase space.

Proof: It remains to show the last assertion. Therefore we consider the v -component of the discrete scheme (3.6)-(3.8) in more detail. We extract V from the second line in (3.7) explicitly, insert this representation into (3.6) and obtain

$$v_{n+1} = v_n - h(b^T \otimes I)\bar{B}(U(h, u_n))[I + h(A \otimes I)\bar{B}(U(h, u_n))]^{-1}(\mathbb{I} \otimes v_n). \quad (3.22)$$

Moreover, we know

$$\bar{B}(U(h, u_n)) = \bar{B}(\mathbb{I} \otimes u_n) + O(h) = (I \otimes B(u_n)) + O(h) \quad (3.23)$$

from Lemma 3.3. Combining (3.22) and (3.23) yields

$$\begin{aligned} v_{n+1} &= v_n - h(b^T \otimes I)(I \otimes B(u_n))(\mathbb{I} \otimes v_n) + O(h^2)v_n \\ &= (I - hB(u_n) + O(h^2))v_n \end{aligned} \quad (3.24)$$

Next, with $\mu_2(-B(u_n)) \leq -\eta$ we can compute

$$\begin{aligned} \|I - hB(u_n) + O(h^2)\|_2 &= \max\{\lambda \in \sigma(I - h/2(B(u_n) + B(u_n)^T) + O(h^2))\} \\ &\leq 1 - h\eta/4 + O(h^2) < 1 \text{ for } h > 0 \text{ sufficiently small} \end{aligned}$$

and the inequality

$$\|g(u_n)\|_2 \leq \|I - hB(u_n) + O(h^2)\|_2^n \|g(u_0)\|_2 \rightarrow 0 \text{ as } n \rightarrow \infty$$

follows. This shows our result.

The proof also works for half-explicit Runge-Kutta methods, since (3.22) holds for these methods too.

4 Embedded index 2 systems under discretization

In this section we give a proof of Theorem 2.1. First, let us analyze the projected Runge-Kutta methods. Using the structure of the operator T_2 (see (3.14)) and the scheme (3.6) the projected Runge-Kutta iteration can be written in the explicit form

$$\begin{aligned} u_{n+1} &= [I - \frac{\partial}{\partial \lambda} f(\cdot, R(\infty)\lambda_n + (b^T A^{-1} \otimes I)\Lambda(h, u_n))\gamma(h, u_n, \lambda_n)]^{-1}(u_n + \\ &\quad h(b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n))), \\ v_{n+1} &= g(u_n) - h(b^T \otimes I)\bar{B}(U(h, u_n))V(h, u_n), \\ \lambda_{n+1} &= R(\infty)\lambda_n + (b^T A^{-1} \otimes I)\Lambda(h, u_n). \end{aligned} \quad (4.1)$$

Moreover, the stability inequality of Lemma 3.3 implies $\gamma(h, u, \lambda) = O(h^{q+1})$. Then, using $(I - O(h^{q+1}))^{-1} = I + O(h^{q+1})$ and neglecting the v -component, the iteration (4.1) can be written in the form

$$\begin{aligned} u_{n+1} &= u_n + h((b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n)) + h^q \hat{f}(h, u_n, \lambda_n)) \\ \lambda_{n+1} &= R(\infty)\lambda_n + (b^T A^{-1} \otimes I)\Lambda(h, u_n) \end{aligned} \quad (4.2)$$

with a smooth and bounded function \hat{f} .

Introducing $\eta_n = \lambda_n - \psi(u_n, g(u_n))$ and rewriting (4.2) yields

$$\begin{aligned} u_{n+1} &= u_n + h((b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n)) + h^q \hat{f}(h, u_n, \eta_n + \psi(u_n, g(u_n)))) \\ &=: u_n + G_1(h, u_n, \eta_n), \\ \eta_{n+1} &= R(\infty)\eta_n + (b^T A^{-1} \otimes I)(\Lambda(h, u_n) - \mathbb{I} \otimes \psi(u_n, g(u_n))) \\ &\quad + \psi(u_n, g(u_n)) - \psi(u_n + G_1(h, u_n, \eta_n), g(u_n + G_1(h, u_n, \eta_n))) \\ &=: G_2(h, u_n, \eta_n). \end{aligned} \quad (4.3)$$

The functions G_1, G_2 are lipschitzian with the constants

$$\begin{aligned} L_{G_1, u} &= O(h), \quad L_{G_1, \eta} = O(h^{q+1}), \\ L_{G_2, u} &= O(1), \quad L_{G_2, \eta} = |R(\infty)| + O(h^{q+1}) < 1. \end{aligned} \quad (4.4)$$

Obviously, for $r \in \mathbb{N}$ fix the conditions

$$\begin{aligned} 2\sqrt{L_{G_1,\eta}L_{G_2,u}} &< 1 - L_{G_1,u} - L_{G_2,\eta}, \\ L_{G_2,\eta} + L_{G_1,\eta}\alpha &< (1 - L_{G_1,u} - L_{G_1,\eta}\alpha)^r \end{aligned}$$

with

$$\alpha := \frac{2L_{G_2,u}}{1 - L_{G_1,u} - L_{G_2,\eta} + \sqrt{(1 - L_{G_1,u} - L_{G_2,\eta})^2 - 4L_{G_1,\eta}L_{G_2,u}}}$$

are satisfied for $h > 0$ sufficiently small. Now, Theorem 5 of Nipp, Stoffer [12] guarantees the existence of a smooth function $\psi_h(\cdot, g(\cdot))$ which gives in (u, λ) -coordinates rise to an attractive invariant manifold

$$M_h := \{(u, \lambda) \in D_\gamma \times \mathbb{R}^l \mid \lambda = \psi_h(u, g(u))\}.$$

Additionally, the in phase property holds with the attraction coefficient $\chi_h = L_{G_2,\eta} + L_{G_1,\eta}\alpha = |R(\infty)| + O(h^{q+1})$.

Here the reader may notice that to apply Theorem 5 of Nipp, Stoffer [12]) formally we have to enlarge the domain of G_1, G_2 for $u \in \mathbb{R}^N$ as C_b^r -maps which satisfy the lipschitz conditions (4.4).

Reduced to the invariant manifold M_h the u -component of a projected Runge-Kutta method reads

$$u_{n+1} = u_n + h((b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n)) + h^q \hat{f}(h, u_n, \psi_h(u_n, g(u_n)))). \quad (4.5)$$

Obviously, the iteration scheme (4.5) can be regarded as a q th order one-step method applied to the initial value problem

$$\dot{u} = f(u, \psi(u, g(u))), \quad u(0) = u_0. \quad (4.6)$$

Next we estimate the distance between M_h and M_0 . Since $G_2(h, u, \eta)$ has the representation

$$G_2(h, u, \eta) = R(\infty)\eta + \beta(h, u, \eta)$$

with β from (3.18) we directly obtain $M_h - M_0 = O(h)$ from (3.19) and Theorem 5 in Nipp, Stoffer [12]. To complete the proof of Theorem 2.1 for the projected Runge-Kutta methods we have to show $\beta_n = \beta(h, u_n, \eta_n) = O(h^q)$. Due to formula (3.18) the representation

$$\begin{aligned} \beta_n &= (b^T A^{-1} \otimes I)(\Lambda(h, u_n) - \bar{\psi}(U(h, u_n), \bar{g}(U(h, u_n)))) \\ &\quad + (b^T A^{-1} \otimes I)(\bar{\psi}(U(h, u_n), \bar{g}(U(h, u_n))) - \mathbb{I} \otimes \psi(u_n, g(u_n))) \\ &\quad + \psi(u_n, g(u_n)) - \psi(u_{n+1}, g(u_{n+1})) \end{aligned} \quad (4.7)$$

is valid. Now, we analyze the first term on the right hand side of (4.7). With the solution flow $(\tilde{u}(t, u_0), \tilde{v}(t, u_0), \tilde{\lambda}(t, u_0))$, $u_0 \in D_\gamma$, $\tilde{v}(t, u_0) = g(\tilde{u}(t, u_0))$, $\tilde{\lambda}(t, u_0) = \psi(\tilde{u}(t, u_0), \tilde{v}(t, u_0))$ of (3.1) this gives

$$\begin{aligned} & \Lambda_i(h, u_n) + \psi(\tilde{u}(c_i h, u_n), g(\tilde{u}(c_i h, u_n))) \\ & - \tilde{\lambda}(c_i h, u_n) - \psi(U_i(h, u_n), g(U_i(h, u_n))) = O(h^q) \end{aligned}$$

since $U_i(h, u_n) - \tilde{u}(c_i h, u_n) = O(h^{q+1})$ and $\Lambda_i(h, u_n) - \tilde{\lambda}(c_i h, u_n) = O(h^q)$ hold for $i = 1, \dots, s$. To examine the second term on the right hand side of (4.7) appropriately we have to do some preparations. Let

$$\begin{aligned} \hat{u}_{n+1} &= \hat{u}_n + h(b^T \otimes I) \bar{f}(\hat{U}(h, \hat{u}_n), \hat{\Lambda}(h, \hat{u}_n)), \\ \hat{\lambda}_{n+1} &= R(\infty) \hat{\lambda}_n + (b^T A^{-1} \otimes I) \hat{\Lambda}(h, \hat{u}_n), \end{aligned} \quad (4.8)$$

$(\hat{U}(h, \hat{u}_n), \hat{\Lambda}(h, \hat{u}_n))$ solution of

$$S(h, \hat{u}_n, \hat{U}, \hat{\Lambda}) = \begin{pmatrix} \hat{U} - \mathbb{I} \otimes \hat{u}_n - h(A \otimes I) \bar{f}(\hat{U}, \hat{\Lambda}) \\ D\bar{g}(\hat{U}) \bar{f}(\hat{U}, \hat{\Lambda}) + \bar{B}(\hat{U}) \bar{g}(\hat{U}) \end{pmatrix} = 0 \quad (4.9)$$

stand for the Runge-Kutta method with tableau (2.3) applied to the DAE

$$\begin{aligned} \dot{u} &= f(u, \lambda), \\ 0 &= Dg(u) f(u, \lambda) + B(u) g(u). \end{aligned} \quad (4.10)$$

(4.10) is the corresponding index 1 problem with eliminated v -variables to (3.1). From (4.9) we can conclude

$$S(h, \hat{u}_n, U(h, \hat{u}_n), \Lambda(h, \hat{u}_n)) = (0, O(h^q)).$$

Here, $(U, \Lambda) = (U(h, \hat{u}_n), \Lambda(h, \hat{u}_n))$ denote the solution of (3.12). Moreover, we have

$$\frac{\partial}{\partial(\hat{U}, \hat{\Lambda})} S(h, \hat{u}_n, \hat{U}(h, \hat{u}_n), \hat{\Lambda}(h, \hat{u}_n)) = \begin{pmatrix} I & 0 \\ O(1) & I \otimes Dg(\hat{u}_n) \frac{\partial f}{\partial \lambda}(\gamma(\hat{u}_n)) \end{pmatrix} + O(h).$$

Thus, for $h > 0$ sufficiently small $\frac{\partial}{\partial(\hat{U}, \hat{\Lambda})} S(h, \hat{u}_n, \hat{U}(h, \hat{u}_n), \hat{\Lambda}(h, \hat{u}_n))$ is invertible and the stability inequality shows

$$(U - \hat{U}, \Lambda - \hat{\Lambda})(h, \hat{u}_n) = O(h^q).$$

We insert this into formula (4.8) and obtain with $u_n = \hat{u}_n$ and (4.2) the relation

$$\hat{u}_{n+1} = u_{n+1} + O(h^{q+1}).$$

Then, we manipulate the second term on the right hand side of (4.7) as follows.

$$\begin{aligned}
& (b^T A^{-1} \otimes I) \cdot (\bar{\psi}(U(h, u_n), \bar{g}(U(h, u_n))) - \\
& \mathbb{I} \otimes \psi(u_n, g(u_n))) + \psi(u_n, g(u_n)) - \psi(u_{n+1}, g(u_{n+1})) \\
& = (b^T A^{-1} \otimes I) \cdot (\bar{\psi}(\hat{U}(h, \hat{u}_n), \bar{g}(\hat{U}(h, \hat{u}_n))) - \mathbb{I} \otimes \psi(\hat{u}_n, g(\hat{u}_n))) \\
& + \psi(\hat{u}_n, g(\hat{u}_n)) - \psi(\hat{u}_{n+1}, g(\hat{u}_{n+1})) + O(h^q).
\end{aligned}$$

Finally, we embed the index 1 problem (4.10) into the singular perturbed problem

$$\begin{aligned}
\dot{u} & = f(u, \lambda), \\
\epsilon \dot{\lambda} & = Dg(u)f(u, \lambda) + B(u)g(u)
\end{aligned} \tag{4.11}$$

Following Nipp, Stoffer [13] formulae (6), (7), we define the functions $E(\hat{u}_n, \hat{U}(h, \hat{u}_n))$ as well as $e(\hat{u}_n, \hat{u}_{n+1}, \hat{U}(h, \hat{u}_n))$. Then the relation

$$\begin{aligned}
& (b^T A^{-1} \otimes I)E(\hat{u}_n, \hat{U}(h, \hat{u}_n)) - e(\hat{u}_n, \hat{u}_{n+1}, \hat{U}(h, \hat{u}_n)) = \\
& (b^T A^{-1} \otimes I) \cdot (\bar{\psi}(\hat{U}(h, \hat{u}_n), \bar{g}(\hat{U}(h, \hat{u}_n))) - \mathbb{I} \otimes \psi(\hat{u}_n, g(\hat{u}_n))) \\
& + \psi(\hat{u}_n, g(\hat{u}_n)) - \psi(\hat{u}_{n+1}, g(\hat{u}_{n+1})) = O(h^{q+1}) + O(\epsilon)
\end{aligned} \tag{4.12}$$

is shown in Nipp, Stoffer [13]. We insert (4.12) into (4.7) and obtain with $\epsilon = 0$ the desired estimation.

Finally, to complete the proof of Theorem 2.1 for the projected Runge-Kutta methods we restrict (4.5) to the invariant set $g^{-1}(0)$, define $\psi_{0,h} := \psi_h|_{g^{-1}(0)}$ by $\psi_{0,h}(u) = \psi_h(u, 0)$ and $M_{0,h} = \{(u, \lambda) \in D_\gamma \times \mathbb{R}^l \mid \lambda = \psi_{0,h}(u)\}$.

In the case of half-explicit Runge-Kutta methods we obtain directly the iteration scheme

$$\begin{aligned}
u_{n+1} & = u_n + h(b^T \otimes I)\bar{f}((u_n, \tilde{U}_1(h, u_n), \dots, \tilde{U}_{s-1}(h, u_n)), \Lambda(h, u_n)), \\
\lambda_{n+1} & = \Lambda_s(h, u_n)
\end{aligned} \tag{4.13}$$

from (3.20) and (2.8). Again, introducing $\eta_n = \lambda_n - \psi(u_n, g(u_n))$ yields

$$\begin{aligned}
u_{n+1} & = u_n + h(b^T \otimes I)\bar{f}((u_n, \tilde{U}_1(h, u_n), \dots, \tilde{U}_{s-1}(h, u_n)), \Lambda(h, u_n)) \\
& = u_n + \tilde{G}_1(h, u_n, \eta_n), \\
\eta_{n+1} & = \Lambda_s(h, u_n) - \psi(u_n + \tilde{G}_1(h, u_n, \eta_n), g(u_n + \tilde{G}_1(h, u_n, \eta_n))) = \tilde{G}_2(h, u_n, \eta_n).
\end{aligned}$$

Then, we can adapt the proof of the projected Runge-Kutta method to the half-explicit Runge-Kutta scheme. With (B3') and $c_s = 1$ we can estimate

$$\begin{aligned}
\beta_n & = \Lambda_s(h, u_n) - \psi(u_{n+1}, g(u_{n+1})) \\
& = \Lambda_s(h, u_n) - \tilde{\lambda}(h, u_n) + \psi(\tilde{u}(h, u_n), g(\tilde{u}(h, u_n))) - \psi(u_{n+1}, g(u_{n+1})) = O(h^r).
\end{aligned}$$

Finally, the attraction constant $\chi_h = 0$ follows from the fact $L_{\tilde{G}_{1,\eta}} = L_{\tilde{G}_{2,\eta}} = 0$.

5 Discretization near periodic orbits

In the sections 2 and 3 we have seen that the DAE (2.1) can be embedded into the DAE (3.1). The corresponding index 0 equation of (2.1) is the ODE (2.2) with phase space $M := \{u \in \mathbb{R}^N \mid g(u) = 0\}$ and the index 0 equation of (3.1) with eliminated v -variables can be regarded as a dynamical system on the open subset D_γ of \mathbb{R}^n (see formula (3.5)).

Now, let $(\bar{u}(t, u_0), \psi_0(\bar{u}(t, u_0)))$ be a hyperbolic periodic orbit of (2.1). Obviously, (3.1) possesses the periodic orbit $(\bar{u}(t, u_0), 0, \psi_0(\bar{u}(t, u_0)))$.

Our first goal to show is that also the hyperbolicity of periodic orbits carries over from (2.1) to (3.1) and (3.5). For fixed t we have the linearization

$$\frac{\partial}{\partial u} \bar{u}(t, u_0) : N(Dg(u_0)) \rightarrow N(Dg(\bar{u}(t, u_0)))$$

of (2.1) and $\frac{\partial}{\partial u} \bar{u}(t, u_0)v$, $v \in N(Dg(u_0))$ solves the linearized system

$$\begin{aligned} \dot{z} &= \left[\frac{\partial f}{\partial u}(\Gamma(t, u_0)) + \frac{\partial f}{\partial \lambda}(\Gamma(t, u_0)) D\psi_0(\bar{u}(t, u_0)) \right] z, \\ z(0) &= v \in N(Dg(u_0)). \end{aligned}$$

Here $\Gamma(t, u_0)$ stands for $(\bar{u}(t, u_0), \psi_0(\bar{u}(t, u_0)))$.

Next we analyze the ODE (3.5) in more detail. A straightforward calculation with $\gamma(u) = (u, \psi(u, g(u)))$ shows

$$Dk(u) = \frac{\partial f}{\partial u}(\gamma(u)) + \frac{\partial f}{\partial \lambda}(\gamma(u)) \left(\frac{\partial \psi}{\partial u}(u, g(u)) + \frac{\partial \psi}{\partial v}(u, g(u)) Dg(u) \right). \quad (5.1)$$

Moreover, implicit differentiation of the relation $Dg(u)f(u, \psi(u, v)) + B(u)v = 0$ with respect to u and v yields

$$\begin{aligned} \frac{\partial \psi}{\partial u}(u, v) &= -(Dg(u) \frac{\partial f}{\partial \lambda}(u, \psi(u, v)))^{-1} [Dg(u) \frac{\partial f}{\partial u}(u, \psi(u, v)) \\ &\quad + DB(u)v + D^2g(u)f(u, \psi(u, v))], \\ \frac{\partial \psi}{\partial v}(u, v) &= -(Dg(u) \frac{\partial f}{\partial \lambda}(u, \psi(u, v)))^{-1} B(u). \end{aligned} \quad (5.2)$$

Thus, with $v = g(u)$ and $Q(u) = \frac{\partial f}{\partial \lambda}(\gamma(u))(Dg(u) \frac{\partial f}{\partial \lambda}(\gamma(u)))^{-1} Dg(u)$ we insert (5.2) into (5.1) and obtain

$$\begin{aligned} Dk(u) &= (I - Q(u)) \frac{\partial f}{\partial u}(\gamma(u)) - \frac{\partial f}{\partial \lambda}(\gamma(u)) (Dg(u) \frac{\partial f}{\partial \lambda}(\gamma(u)))^{-1} [B(u) Dg(u) \\ &\quad + DB(u)g(u) + D^2g(u)k(u)]. \end{aligned}$$

Using the relation

$$D^2g(u)k(u) + Dg(u)Dk(u) = -DB(u)g(u) - B(u)Dg(u) \quad (5.3)$$

which follows from the definition of ψ , we can compute

$$(I - Q(u))Dk(u) = (I - Q(u))\frac{\partial f}{\partial u}(\gamma(u)). \quad (5.4)$$

Lemma 5.1 *Let (A1)-(A3) hold and let $(\bar{u}(t, u_0), \psi_0(\bar{u}(t, u_0)))$, $\bar{u}(t, u_0) = \bar{u}(t+T, u_0)$ denote a hyperbolic T -periodic orbit of the DAE (2.1). Then $\bar{u}(t, u_0)$ is a hyperbolic T -periodic orbit of the ODE (3.5).*

Proof: Let $\tilde{u}(t, u_0)$ denote the solution flow of (3.5) and let $\bar{u}(t, u_0)$ stand for the solution flow of (2.2). The reader may recall $\tilde{u}(t, u_0) = \bar{u}(t, u_0)$ provided $g(u_0) = 0$ holds. Linearized at an orbit $\bar{u}(t, u_0)$ we obtain that $\frac{\partial}{\partial u}\tilde{u}(t, u_0)$ solves the variational equation

$$\dot{Y}(t) = Dk(\bar{u}(t, u_0))Y(t), \quad Y(0) = I.$$

In order to analyze $Y(t)$ in more detail we define $r(t) := Dg(\tilde{u}(t, u_0))\frac{\partial}{\partial u}\tilde{u}(t, u_0)$ for $u_0 \in D_\gamma$ with $g(u_0) = 0$. A straightforward calculation shows

$$\dot{r}(t) = -B(\bar{u}(t, u_0))r(t), \quad r(0) = Dg(u_0). \quad (5.5)$$

Now, let $V \in \mathbb{R}^{N, N-l}$ denote an orthonormal basis of $N(Dg(u_0))$ and let $W = \frac{\partial f}{\partial \lambda}(u_0, \psi_0(u_0))$. Using (5.5) we obtain $r(t)V \equiv 0$ and $\frac{\partial}{\partial u}\tilde{u}(t, u_0)V\alpha \in N(Dg(\bar{u}(t, u_0)))$, $\alpha \in \mathbb{R}^{N-l}$ follows.

Moreover, with (5.2)-(5.4) and $S(u) = Dg(u)\frac{\partial f}{\partial \lambda}(u, \psi_0(u))$ we can compute

$$\begin{aligned} \frac{\partial^2}{\partial t \partial u}\tilde{u}(t, u_0)V\alpha &= Dk(\tilde{u}(t, u_0))\frac{\partial}{\partial u}\tilde{u}(t, u_0)V\alpha \\ &= [(I - Q(\tilde{u}(t, u_0)))\frac{\partial f}{\partial u}(\Gamma(t, u_0)) \\ &\quad + Q(\tilde{u}(t, u_0))Dk(\tilde{u}(t, u_0))]\frac{\partial}{\partial u}\tilde{u}(t, u_0)V\alpha \\ &= [\frac{\partial f}{\partial u}(\Gamma(t, u_0)) - \frac{\partial f}{\partial \lambda}(\Gamma(t, u_0))S(\tilde{u}(t, u_0))^{-1}[Dg(\tilde{u}(t, u_0)) \\ &\quad \cdot \frac{\partial f}{\partial u}(\Gamma(t, u_0)) - D^2g(\tilde{u}(t, u_0))k(\tilde{u}(t, u_0))]]\frac{\partial}{\partial u}\tilde{u}(t, u_0)V\alpha \\ &= [\frac{\partial f}{\partial u}(\Gamma(t, u_0)) + \frac{\partial f}{\partial \lambda}(\Gamma(t, u_0))D\psi_0(\bar{u}(t, u_0))]\frac{\partial}{\partial u}\tilde{u}(t, u_0)V\alpha. \end{aligned} \quad (5.6)$$

Formula (5.6) shows that $\frac{\partial}{\partial u}\tilde{u}(t, u_0)$ restricted to $N(Dg(u_0))$ solves the linearized problem to equation (2.1) at $\bar{u}(t, u_0)$.

Let $X(t) \in \mathbb{R}^{N-l, N-l}$ denote the fundamental matrix of

$$\dot{w} = \left(\frac{\partial f}{\partial u}(\Gamma(t, u_0)) + \frac{\partial f}{\partial \lambda}(\Gamma(t, u_0))D\psi_0(\bar{u}(t, u_0))\right)w, \quad w(0) \in R(V) = N(Dg(u_0)).$$

Then $Y(t)V = VX(t)$ follows from (5.6).

Moreover, let $Z(t) := Dg(\bar{u}(t, u_0))Y(t)\frac{\partial f}{\partial \lambda}(\Gamma(0, u_0))S(u_0)^{-1}$ be the fundamental matrix of

$$\dot{w} = -B(\bar{u}(t, u_0))w.$$

Now we are in the situation to handle the special case of $\bar{u}(t, u_0)$ to be a T -periodic orbit. We split the whole space according to $\mathbb{R}^N = N(Dg(u_0)) \oplus R(\frac{\partial f}{\partial \lambda}(u_0, \psi_0(u_0))) =: R(V) \oplus R(W)$ and make the ansatz

$$Y(t)W = V\Lambda_{21}(t) + W\Lambda_{22}(t).$$

Using $Dg(u_0)V \equiv 0$ and $\bar{u}(T, u_0) = u_0$ for $t = T$ we end up with

$$Y(T)(V, W) = (V, W) \cdot \begin{pmatrix} X(T) & 0 \\ * & S(u_0)^{-1}Z(T)S(u_0) \end{pmatrix}. \quad (5.7)$$

Finally, from the solution representation

$$\|w(t)\|_2 = \|Z(t)w(0)\|_2 \leq \exp(-\eta t) \|w(0)\|_2$$

we can conclude $\|Z(t)\|_2 \leq \exp(-\eta t)$, that is, $\rho(S(u_0)^{-1}Z(T)S(u_0)) = \rho(Z(T)) \leq \exp(-\eta T)$. Together with formula (5.7) this finishes the proof.

Lemma 5.1 and Theorem 2.1 in Beyn [2] ensure the existence of an invariant curve $\bar{u}^h(\mathbb{R})$, $\bar{u}^h(t) = \bar{u}^h(t + T)$ for the one-step method (compare (4.5))

$$\begin{aligned} u_{n+1} &= u_n + h(b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n)) + h^{q+1}\hat{f}(h, u_n, \psi_h(u_n, g(u_n))) \\ &=: G_h(u_n) \end{aligned} \quad (5.8)$$

with the properties

$$\begin{aligned} \bar{u}^h(t + h + O(h^{q+1})) &= G_h(\bar{u}^h(t)), \\ \max\{\|\bar{u}(t, u_0) - \bar{u}^h(t)\| \mid t \in \mathbb{R}\} &\leq Ch^q. \end{aligned}$$

Obviously, we have $g(\bar{u}^h(\mathbb{R})) = 0$. This is a consequence of the fact that $\bar{u}^h(\mathbb{R})$ is an invariant set and every invariant set is located in the maximal invariant set $g^{-1}(0)$.

On the phase space $g^{-1}(0)$ the iteration scheme (5.8) coincides with the u -component of the projected Runge-Kutta method applied to $\dot{u} = f(u, \lambda)$, $g(u) = 0$. Thus, the discrete iteration scheme possesses an invariant curve which is $O(h^q)$ close to the periodic orbit.

An analogous argumentation also works for half-explicit Runge-Kutta methods and ensures the existence of an $O(h^r)$ close invariant curve to the periodic orbit.

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