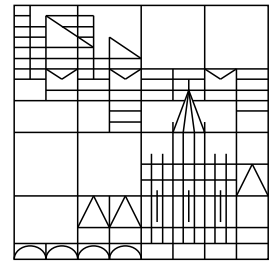


Universität Konstanz



Attracting sets in index 2 Differential Algebraic Equations and in their Runge-Kutta Discretizations

Johannes Schropp

Konstanzer Schriften in Mathematik und Informatik

Nr. 152, Juli 2001

ISSN 1430-3558

© Fachbereich Mathematik und Statistik
© Fachbereich Informatik und Informationswissenschaft
Universität Konstanz
Fach D 188, 78457 Konstanz, Germany
Email: preprints@informatik.uni-konstanz.de
WWW: <http://www.fmi.uni-konstanz.de/Schriften>

Attracting sets in index 2 Differential Algebraic Equations and in their Runge-Kutta Discretizations

Johannes Schropp

Dept. of Mathematics and Computer Science

University of Konstanz

P.O. Box 5560

D-78434 Konstanz

Abstract

We analyze Runge-Kutta discretizations applied to index 2 differential algebraic equations (DAE's) in the vicinity of attracting sets. We compare the geometric properties of the numerical and the exact solutions and show that projected and half-explicit Runge-Kutta methods reproduce the qualitative features of the continuous system correctly. The proof combines invariant manifold results of Schropp [13] and classical results for discretized ordinary differential equations of Kloeden, Lorenz [10].

1 Introduction

The treatment of index 2 differential algebraic problems gains more and more importance in numerical analysis. Classes of problems which serve as sources are, e.g, multibody systems with constraints on the velocity level or in the GGL-formulation (see, e.g., Gear [5] or Gear, Gupta, Leimkuhler [6]). Index 2 DAE's 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 [11]).

In the present paper we analyze the behaviour of projected and half-explicit Runge-Kutta discretizations applied to index 2 DAE's near stable attracting sets. It is well known that the dynamics of an index 2 problem in Hessenberg form takes place in a submanifold of the space times control space (see Hairer, Wanner [9], Ch. 7.1). Additionally, the phase space of the discrete dynamics for fixed step size is an open neighborhood of that submanifold. In Schropp [13] it is shown that discrete schemes satisfying the first order constraint admit a submanifold too which is attractive, invariant and close to the continuous one. Here, we compare the geometric properties of a Runge-Kutta method restricted to the discrete invariant manifold with the properties of the continuous solution flow on its phase space. To be more precise, we analyze the behaviour of the discrete and continuous dynamics near stable attracting sets, a

characterization in a neighborhood of hyperbolic equilibria can be found in Schropp [12] and the analysis for period orbits is presented in Schropp [13]. We show, that in the vicinity of an uniformly stable attracting set Γ_0 the discrete Runge-Kutta time h-map restricted to its invariant manifold admits a discrete attractor $\Gamma_{0,h}$ which converges in the Hausdorff metric towards its continuous counterpart Γ_0 as the step size h tends to zero. This generalizes the well known Kloeden, Lorenz result [10] for ordinary differential equations (ODEs) to index 2 DAEs.

Our main tools are embedding and invariant manifold techniques. We embed the original index 2 DAE into a DAE of the same index such that the corresponding index 0 ODE admits a representation as dynamical system on the euclidian space \mathbb{R}^N . Then, we mimic that approach for the projected and half-explicit Runge-Kutta dynamics. This will allow us to apply the results of Kloeden, Lorenz [10] for one-step methods in \mathbb{R}^N and using invariance results a drawback to DAEs is possible.

2 The main results

We consider the autonomous DAE

$$\begin{aligned} \dot{u} &= f(u, \lambda), \quad u(0) = u_0, \\ 0 &= g(u), \quad \lambda(0) = \lambda_0, \end{aligned} \tag{2.1}$$

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

(A1) $f \in C_b^\nu(\mathbb{R}^{N+l}, \mathbb{R}^N)$, $g \in C_b^{\nu+1}(\mathbb{R}^N, \mathbb{R}^l)$ for some sufficiently big ν .

(A2) There is a C_b^ν -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 and consistent initial values must satisfy $g(u_0) = 0$, $Dg(u_0)f(u_0, \lambda_0) = 0$. Additionally, $Dg(u)$ is of full rank for $u \in D_\tau$ so that the second equation of (2.1) defines the $(N - l)$ -dimensional submanifold $S := \{u \in \mathbb{R}^N \mid g(u) = 0\}$ of \mathbb{R}^N and the underlying index 0 ODE reads

$$\dot{u} = f(u, \psi_0(u)), \quad u(0) = u_0 \in S. \tag{2.2}$$

Note that by virtue of (A2) equation (2.2) describes a dynamical system on the manifold $g(u) = 0$. We denote the solution flow of (2.2) with $\bar{u}(t, u_0)$, $u_0 \in S$. Then, the solution flow of (2.1) has the form

$$\varphi(t, u_0, \lambda_0) = (\bar{u}(t, u_0), \psi_0(\bar{u}(t, u_0)))$$

for initial values $(u_0, \lambda_0) = (u_0, \psi_0(u_0))$ in the phase space

$$M_0 := \{(u, \lambda) \in \mathbb{R}^{N+l} \mid g(u) = 0, \lambda = \psi_0(u)\}. \quad (2.3)$$

In order to avoid inconvenient technicalities we assume $\varphi(t, u_0, \lambda_0)$ to exist for $t \geq 0$. This holds, e.g., if S is compact.

One of the most interesting topics related to a DAE is to analyze the longtime behaviour of its evolutions. This behaviour is governed in a decisive way by its stable attracting subsets. For a nonempty, compact subset Γ_0 of \mathbb{R}^N and a point $u \in \mathbb{R}^N$

$$\text{dist}(u, \Gamma_0) := \inf\{\|u - \tilde{u}\| \mid \tilde{u} \in \Gamma_0\}$$

describes the distance of u to Γ_0 . Now, let Γ_0 be a compact, invariant subset of S for the index 0 equation (2.2) and let $B_\alpha(\Gamma_0) := \{u \in \mathbb{R}^N \mid \text{dist}(u, \Gamma_0) < \alpha\}$. Following Kloeden, Lorenz [10] we call Γ_0 uniformly stable, if for each $\epsilon > 0$ there is $\delta = \delta(\epsilon) > 0$ such that

$$\text{dist}(\bar{u}(t, u), \Gamma_0) \leq \epsilon \text{ for } t \geq 0 \text{ and } u \in B_\delta(\Gamma_0) \cap S.$$

The set Γ_0 is uniformly attractive if there is a $\delta_0 > 0$ and for each ϵ a time $T = T(\epsilon) > 0$ satisfying

$$\text{dist}(\bar{u}(t, u), \Gamma_0) < \epsilon \text{ for all } t \geq T(\epsilon).$$

An uniformly stable, attractive set Γ_0 is called uniformly asymptotically stable for the ODE (2.2). Alternatively, we say $(\Gamma_0, \psi_0(\Gamma_0))$ is uniformly asymptotically stable for the DAE (2.1).

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

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}, \quad A = (a_{ij})_{1 \leq i, j \leq s} \in \mathbb{R}^{s,s}, \quad b, c \in \mathbb{R}^s \quad (2.4)$$

and constant step size h when applied to the DAE (2.1) in the vicinity of an asymptotically stable set $(\Gamma_0, \psi_0(\Gamma_0))$. Our goal here to show is that appropriate Runge-Kutta schemes reproduce the phase portrait of a DAE correctly. To avoid drift phenomena in the longtime behaviour of the numerical methods we restrict ourselves to discrete schemes which retain the constraint $g(u) = 0$. This leads us to the widely spread projected Runge-Kutta methods due to Ascher, Petzold [1] and the half-explicit methods introduced by Hairer, Lubich, Roche [8]. The Runge-Kutta method (2.4) possesses stage order q , if

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

For the Butcher tableau (2.4) of the Runge-Kutta method we impose the following conditions:

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

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

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

If we denote the Runge-Kutta approximation of (2.1) at the time $t_n = nh$ with (u_n, λ_n) the projected Runge-Kutta method has the form

$$\begin{aligned}\tilde{u}_{n+1} &= u_n + h(b^T \otimes I) \bar{f}(U^n, \Lambda^n), \\ \lambda_{n+1} &= R(\infty) \lambda_n + (b^T A^{-1} \otimes I) \Lambda^n\end{aligned}\tag{2.5}$$

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

$$\begin{aligned}U - (\mathbb{I} \otimes u_n) &= h(A \otimes I) \bar{f}(U, \Lambda), \\ 0 &= \bar{g}(U).\end{aligned}\tag{2.6}$$

Here, \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

$$\begin{aligned}u_{n+1} &= \tilde{u}_{n+1} + \frac{\partial}{\partial \lambda} f(u_{n+1}, \lambda_{n+1}) \gamma \\ 0 &= g(u_{n+1})\end{aligned}\tag{2.7}$$

completes the numerical scheme. The extra variable γ is needed for the projection only. It measures the deviation of \tilde{u}_{n+1} from the manifold S .

An important subclass of the projected Runge-Kutta methods are the stiffly accurate ones which are defined by $a_{sj} = b_j$, $j = 1, \dots, s$. The iterates of these Runge-Kutta methods satisfy $g(u) = 0$ by construction and, hence, the projection step is superfluous.

For the half-explicit scheme, 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 .

The application of a half-explicit Runge-Kutta method to (2.1) reads as follows. We solve (2.6) 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

$$\begin{aligned}u_{n+1} &= u_n + h(b^T \otimes I) \bar{f}(U^n, \Lambda^n), \\ 0 &= g(u_{n+1}).\end{aligned}\tag{2.8}$$

Introducing the matrix

$$\tilde{A} = \begin{pmatrix} a_{21} & & & & & \\ a_{31} & a_{32} & & & & \\ \vdots & & \ddots & & & \\ a_{s1} & \dots & \dots & a_{ss-1} & & \\ b_1 & \dots & \dots & b_{s-1} & b_s & \end{pmatrix} \in \mathbb{R}^{s,s}\tag{2.9}$$

and the vector $\tilde{U}^n := (U_2^n, \dots, U_s^n, u_{n+1})$ the half-explicit Runge-Kutta scheme can be written in the compact form

$$\begin{aligned}\tilde{U}^n - \mathbb{I} \otimes u_n &= h(\tilde{A} \otimes I) \bar{f}((u_n, \tilde{U}_1^n, \dots, \tilde{U}_{s-1}^n), \Lambda^n), \\ 0 &= \bar{g}(\tilde{U}^n)\end{aligned}\tag{2.10}$$

(see, e.g. formula (4.59) in Hairer, Lubich, Roche [8]).

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 $\lambda_n = \psi_{loc}(u_n)$. Here we follow the more efficient approach of Hairer, Lubich, Roche [8]. They propose to require $c_s = 1$ and take

$$\lambda_{n+1} = \Lambda_s^n.\tag{2.11}$$

In this case, we assume

(B3') $\Lambda_s^n - \bar{\lambda}(h, u_n) = O(h^r)$, $r \leq p$ (see, e.g., Hairer, Brasey [7] for sufficient conditions on A, b, c).

Sometimes when the dependence on the initial value (u_0, λ_0) and the step size h is important, we denote the numerical solution (u_n, λ_n) more precisely by

$$\Phi^h(nh, u_0, \lambda_0) = (u^h(nh, (u_0, \lambda_0)), \lambda^h(nh, (u_0, \lambda_0))).$$

The following Lemma (see Schropp [13]) characterizes the link between the discrete state and control flow u^h and λ^h .

Lemma 2.1 *Consider the DAE (2.1) and assume (A1)-(A3). Let (u_n, λ_n) denote the iterates 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^ν -function $\psi_{0,h} : S \rightarrow \mathbb{R}^l$, $S = \{u \in \mathbb{R}^N \mid g(u) = 0\}$ such that the following assertions hold.

i) The set $M_{0,h} = \{(u, \lambda) \in \mathbb{R}^{N+l} \mid g(u) = 0, \lambda = \psi_{0,h}(u)\}$ is invariant for the projected [half-explicit] Runge-Kutta map (2.5)-(2.6) [(2.8)-(2.11)].

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

$$\begin{aligned}\|u_i - \tilde{u}_i\| &\leq c\chi_h^i \|\lambda_0 - \psi_0(u_0)\|, \quad i \in \mathbb{N}, \\ \|\lambda_i - \tilde{\lambda}_i\| &\leq \hat{c}\chi_h^i \|\lambda_0 - \psi_0(u_0)\|, \quad i \in \mathbb{N}.\end{aligned}$$

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

Lemma 2.1 shows that the invariant manifold $M_{0,h}$ is the discrete analogue of the continuous phase space $M_0 = \{(u, \lambda) \in \mathbb{R}^{N+l} \mid g(u) = 0, \lambda = \psi_0(u)\}$. Our aim in the present paper is to compare the discrete flow $\Phi^h(nh, u_0, \lambda_0)$ on $M_{0,h}$ with its continuous counterpart $\varphi(t, u_0, \lambda_0)$ on M_0 in the neighborhood of an uniformly asymptotically stable set Γ_0 .

In order to measure the distance of two nonempty and compact subsets A and B of \mathbb{R}^N we define the Hausdorff separation

$$H^*(A, B) := \max\{\text{dist}(a, B) \mid a \in A\}$$

and the Hausdorff distance

$$H(A, B) := \max(H^*(A, B), H^*(B, A)).$$

Theorem 2.2 *Consider equation (2.1) under the assumptions (A1)-(A3) and let $(\Gamma_0, \psi_0(\Gamma_0))$ be a compact, uniformly asymptotically stable subset of the phase space. Let $\Phi^h(nh, u_0, \lambda_0) = (u^h(nh, (u_0, \lambda_0)), \lambda^h(nh, (u_0, \lambda_0)))$ denote the sequences generated by a projected [half-explicit] Runge-Kutta method satisfying (B1)-(B3) [(B1')-(B3')], when applied to (2.1) with initial values $(u_0, \lambda_0) = (u_0, \psi_{0,h}(u_0))$ on $M_{0,h}$ and let $\varphi(t, u_0, \lambda_0) = (\bar{u}(t, u_0), \psi_0(\bar{u}(t, u_0)))$ stand for the solution flow of (2.1).*

Then for $0 < h < h_0$, $h_0 > 0$ sufficiently small the discrete projected [half-explicit] Runge-Kutta dynamics possesses a compact, uniformly asymptotically stable set $(\Gamma_{0,h}, \psi_{0,h}(\Gamma_{0,h}))$, $\Gamma_{0,h} \subset S$ which contains Γ_0 and this set converges to $(\Gamma_0, \psi_0(\Gamma_0))$ in the Hausdorff metric as $h \rightarrow 0$.

Theorem 2.2 confirms that the qualitative geometric properties of (2.1) are preserved under the discretization with projected and half-explicit Runge-Kutta methods in the vicinity of an asymptotically stable set. Hence stable phenomena of a DAE are reproduced correctly by its corresponding Runge-Kutta dynamics.

But we have said nothing about the dynamics on the invariant set $(\Gamma_0, \psi_0(\Gamma_0))$. Thus we cannot say anything about the discrete dynamics on its counterpart $(\Gamma_{0,h}, \psi_{0,h}(\Gamma_{0,h}))$. With additional assumptions about the dynamics within the attracting set $(\Gamma_0, \psi_0(\Gamma_0))$ in special cases one is able to characterize the discrete dynamics. This is done for the set Γ_0 to be a hyperbolic equilibrium in Schropp [12] or a hyperbolic periodic orbit (see Schropp [13]).

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 is useful to embed (2.1) into another DAE of the same index such that their corresponding index 0 ODE provides an embedding of (2.2) in an open neighborhood of S in \mathbb{R}^N . Assuming (A1)-(A3), an embedding of (2.2) into D_{τ_0} , $\tau_0 \in]0, \tau]$ sufficiently small can be established as follows.

Consider the DAE

$$\begin{aligned} \dot{u} &= f(u, \lambda), \quad u(0) = u_0, \\ \dot{v} &= -B(u)v, \quad \mu_2(-B(u)) \leq -\eta, \quad \eta > 0 \text{ for } u \in D_\tau, \quad v(0) = v_0, \\ 0 &= g(u) - v, \quad \lambda(0) = \lambda_0 \end{aligned} \tag{3.1}$$

with a C_b^ν -function $B(\cdot)$ on \mathbb{R}^N (e.g. choose $B \equiv I$). Here $\mu_2(C)$ stands for the logarithmic norm of a matrix $C \in \mathbb{R}^{l,l}$ (see, e.g., Dekker, Verwer [3], p. 27 for definition). In Schropp [13] it is shown that (A1)-(A3) imply the following assertions for the DAE (3.1).

(A1') $f \in C_b^\nu(\mathbb{R}^{N+l}, \mathbb{R}^N)$, $g \in C_b^{\nu+1}(\mathbb{R}^N, \mathbb{R}^l)$ and $B \in C_b^\nu(\mathbb{R}^N, \mathbb{R}^{l,l})$.

(A2') There is $\tau_0 \in]0, \tau]$ and a C_b^ν -function ψ satisfying $Dg(u)f(u, \psi(u, v)) + B(u)v = 0$ for $u \in D_{\tau_0}$ and $\|v\|_2 < \tau_0$.

(A3') $Dg(u)\frac{\partial f}{\partial \lambda}(u, \psi(u, v))$ is invertible for $u \in D_{\tau_0}$, $\|v\|_2 < \tau_0$ and the inverse has bounded norm.

(A1')-(A3') imply that equation (3.1) is of index 2. Consistent initial values must satisfy $g(u_0) - v_0 = 0$ and $Dg(u_0)f(u_0, \lambda_0) + B(u_0)v_0 = 0$. The solution flow of (3.1) has the form $(\tilde{u}(t, u_0), \tilde{v}(t, u_0), \tilde{\lambda}(t, u_0))$, $u_0 \in D_{\tau_0}$ with $\tilde{v}(t, u_0) = g(\tilde{u}(t, u_0))$ and $\tilde{\lambda}(t, u_0) = \psi(\tilde{u}(t, u_0), \tilde{v}(t, u_0))$. Moreover,

$$M_e := \{(u, v, \lambda) \in D_{\tau_0} \times \mathbb{R}^{2l} \mid g(u) - v = 0, \lambda = \psi(u, v)\}$$

is the phase space of equation (3.1). In particular, with $v(0) = v_0 = 0$ problem (3.1) reduces to (2.1). After eliminating the v -variables by $g(u) = v$ the u -component of the underlying index 0 ODE of (3.1) reads

$$\dot{u} = f(u, \psi(u, g(u))), \quad u(0) = u_0 \in D_{\tau_0} \subset \mathbb{R}^N \text{ open.} \tag{3.2}$$

In Schropp [13], Lemma 3.2 the qualitative properties of the solutions of (3.1) are summarized.

Lemma 3.1 *Consider equation (3.1) on the phase space M_e , and let (A1)-(A3) hold.*

Then every solution of (3.1) with initial value $u_0 \in D_{\tau_0}$, $v_0 = g(u_0)$ and $\lambda_0 = \psi(u_0, v_0)$ exists for all $t \geq 0$. Moreover, $M_{0,e} = \{(u, v, \lambda) \in D_{\tau_0} \times \mathbb{R}^{2l} \mid g(u) = v = 0, \lambda = \psi(u, 0)\}$ is an invariant and globally attractive subset of the phase space M_e .

We are interested in the behaviour of s -stage projected and half-explicit Runge-Kutta type methods of order p with Butcher tableau (2.4) and constant step size h when applied to (3.1). The projected Runge-Kutta method has the form

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + h(b^T \otimes I)\bar{f}(U^n, \Lambda^n), \\ v_{n+1} &= v_n - h(b^T \otimes I)\bar{B}(U^n)V^n, \\ \lambda_{n+1} &= (1 - b^T A^{-1}\mathbb{I})\lambda_n + (b^T A^{-1} \otimes I)\Lambda^n \end{aligned} \tag{3.3}$$

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

$$\begin{aligned} U - (\mathbb{I} \otimes u_n) &= h(A \otimes I)\bar{f}(U, \Lambda), \\ V - (\mathbb{I} \otimes v_n) &= -h(A \otimes I)\bar{B}(U)V, \\ 0 &= \bar{g}(U) - V \end{aligned} \quad (3.4)$$

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

$$\begin{aligned} u_{n+1} &= \tilde{u}_{n+1} + \frac{\partial}{\partial \lambda} f(u_{n+1}, \lambda_{n+1})\gamma, \\ 0 &= g(u_{n+1}) - v_{n+1} \end{aligned} \quad (3.5)$$

is used to compute u_{n+1} .

With \tilde{A} from (2.9), $\tilde{U}^n := (U_2^n, \dots, U_s^n, u_{n+1})$ and $\tilde{V}^n = (V_2^n, \dots, V_s^n, v_{n+1})$ the application of half-explicit Runge-Kutta methods to (3.1) reads as follows.

$$\begin{aligned} \tilde{U}^n - \mathbb{I} \otimes u_n &= h(\tilde{A} \otimes I)\bar{f}((u_n, \tilde{U}_1^n, \dots, \tilde{U}_{s-1}^n), \Lambda^n), \\ \tilde{V}^n - \mathbb{I} \otimes g(u_n) &= -h(\tilde{A} \otimes I)\bar{B}((u_n, \tilde{U}_1^n, \dots, \tilde{U}_{s-1}^n))(g(u_n), \tilde{V}_1^n, \dots, \tilde{V}_{s-1}^n), \\ 0 &= \bar{g}(\tilde{U}^n) - \tilde{V}^n. \end{aligned} \quad (3.6)$$

This has to be completed by $\lambda_{n+1} = \psi(u_{n+1}, v_{n+1})$ or more efficiently by $\lambda_{n+1} = \Lambda_s^n$ provided $c_s = 1$ holds. Finally, the reader may notice that (3.3)-(3.5) and (3.6) reduce to (2.5)-(2.7) and (2.10), respectively, when initialized with $g(u_0) = v_0 = 0$.

Lemma 3.2 *Let the assumptions of Theorem 2.1 hold and let $u_0 \in D_{\tau_0}$, $v_0 = g(u_0)$, $\lambda_0 = \psi(u_0, v_0)$ be a consistent initial value for the DAE (3.1).*

Then for $0 < h \leq h_0$, $h_0 > 0$ sufficiently small the projected and half-explicit Runge-Kutta iterates (u_n, v_n, λ_n) exist for $n \in \mathbb{N}$. Moreover, the projected or half-explicit Runge-Kutta scheme reproduces the phase portrait of (3.1) in the state variables (u, v) correctly, that is, $M_{0,\epsilon,\epsilon} := \{(u, v, \lambda) \in D_{\tau_0} \times \mathbb{R}^{2l} \mid g(u) = v = 0, \|\lambda - \psi(u, v)\| < \epsilon\}$ is a positive invariant and globally attractive subset for the discrete dynamics.

For a proof of Lemma 3.2 see Schropp [13], section 3.

It is shown in Schropp [13], section 4 that the projected Runge-Kutta iteration with eliminated v -variables has the form

$$\begin{aligned} u_{n+1} &= u_n + h[(b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n)) + h^q \hat{f}(h, u_n, \lambda_n)], \\ \lambda_{n+1} &= R(\infty)\lambda_n + (b^T A^{-1} \otimes I)\Lambda(h, u_n) \end{aligned} \quad (3.7)$$

with a smooth and bounded function \hat{f} . Moreover, for $0 < h \leq h_0$, $h_0 > 0$ sufficiently small there is a C_b^r -function $\psi_h : D_{\tau_0} \rightarrow \mathbb{R}^l$ with the following properties:

- i) The set $M_h = \{(u, \lambda) \in D_{\tau_0} \times \mathbb{R}^l \mid \lambda = \psi_h(u)\}$ is invariant for the projected Runge-Kutta map (3.7).
- ii) The manifold M_h is uniformly attractive with attractivity constant $\chi_h = |R(\infty)| + O(h^{q+1})$.
- iii) For every initial value (u_0, λ_0) with $\|\lambda_0 - \psi(u_0, g(u_0))\|$ sufficiently small there is $(\tilde{u}_0, \tilde{\lambda}_0) \in M_h$ and $c, \hat{c} > 0$ such that the corresponding evolutions (u_n, λ_n) and $(\tilde{u}_n, \tilde{\lambda}_n)$ satisfy

$$\begin{aligned} \|u_i - \tilde{u}_i\| &\leq c\chi_h^i \|\lambda_0 - \psi(u_0, g(u_0))\|, \quad i \in \mathbb{N}, \\ \|\lambda_i - \tilde{\lambda}_i\| &\leq \hat{c}\chi_h^i \|\lambda_0 - \psi(u_0, g(u_0))\| \quad i \in \mathbb{N}. \end{aligned}$$

- iv) $\|\psi(u, g(u)) - \psi_h(u)\| \leq Ch^q$.

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

$$u_{n+1} = u_n + h[(b^T \otimes I)\bar{f}(U(h, u_n), \Lambda(h, u_n)) + h^q \hat{f}(h, u_n, \psi_h(u_n))]. \quad (3.8)$$

Obviously, the iteration scheme (3.8) can be regarded as a q th order one-step method applied to the initial value problem (3.2).

An analogous result holds for the half-explicit Runge-Kutta schemes with $O(h^r)$ instead of $O(h^q)$.

4 Discretization near stable attracting sets

In this section we give a proof of Theorem 2.2. We make essential use of the embedding techniques and their results displayed in section 3.

Let $\varphi(t, u_0, \lambda_0) = (\bar{u}(t, u_0), \psi_0(\bar{u}(t, u_0)))$ denote the solution flow of the DAE (2.1), and let $(\Gamma_0, \psi_0(\Gamma_0))$ be uniformly asymptotically stable for that DAE. Thus, Γ_0 is uniformly asymptotically stable for the corresponding index 0 equation (2.2). By definition this means that for every $\epsilon > 0$ there is a $\delta > 0$ such that

$$\text{dist}(\bar{u}(t, u), \Gamma_0) \leq \epsilon$$

for $t \geq 0$ and $u \in B_\delta(\Gamma_0) \cap S$. Additionally, there is a $\delta_0 > 0$ such that for each ϵ

$$\text{dist}(\bar{u}(t, u), \Gamma_0) \leq \epsilon$$

holds for all $t \geq T(\epsilon)$ and $u \in B_\delta(\Gamma_0) \cap S$.

We want to apply the Kloeden, Lorenz results [10] for one-step discretizations of dynamical systems on \mathbb{R}^N in the vicinity of uniformly asymptotically stable sets. To this purpose, our first goal in this section is to show that Γ_0 is a uniformly asymptotically stable set for the dynamics of equation (3.2) on D_{τ_0} too. This is the content of

Lemma 4.1 *Let (A1)-(A3) hold and let Γ_0 be uniformly asymptotically stable for equation (2.2). Then Γ_0 is uniformly asymptotically stable for the ODE (3.2).*

Proof: We prove Lemma 4.1 indirect and in two parts.

Assumption 1: Γ_0 is not uniformly stable for the dynamics of (3.2).

Then there is $\epsilon_0 > 0$, a sequence $(\delta_n)_{n \in \mathbb{N}}$, $\delta_n \rightarrow 0$ as $n \rightarrow \infty$, sequences $(t_n)_{n \in \mathbb{N}}$, $t_n > 0$, $(u_n)_{n \in \mathbb{N}}$, $u_n \in B_{\delta_n}(\Gamma_0)$ such that

$$\bar{u}(t_n, u_n) \notin B_{\epsilon_0}(\Gamma_0), \quad n \in \mathbb{N}$$

holds. Moreover, $(t_n)_{n \in \mathbb{N}}$ cannot be bounded, because otherwise for a convergent subsequence $(t_n)_{n \in \mathbb{N}_1}$, $\mathbb{N}_1 \subset \mathbb{N}$, $t_n \rightarrow \tilde{t}$, $u_n \rightarrow \tilde{u} \in \Gamma_0$ the relation

$$\bar{u}(t_n, u_n) \rightarrow \bar{u}(\tilde{t}, \tilde{u}) \notin B_{\epsilon_0}(\Gamma_0), \quad n \rightarrow \infty, \quad n \in \mathbb{N}_1$$

holds in contradiction to $\bar{u}(\tilde{t}, \tilde{u}) \in \Gamma_0$ due to the invariance of Γ_0 . Thus, we can assume without loss of generality $\lim_{n \rightarrow \infty} t_n = \infty$.

Since Γ_0 is uniformly asymptotically stable for (2.2) on S for $\epsilon_0/2$ there is $\tilde{\delta} := \delta(\epsilon_0/2)$ such that the flow with initial values in $B_{\tilde{\delta}}(\Gamma_0) \cap S$ remains in $B_{\epsilon_0/2}(\Gamma_0) \cap S$ for $t \geq 0$. Due to $u_n \in B_{\delta_n}(\Gamma_0)$ and $\delta_n \rightarrow 0$ as $n \rightarrow \infty$ we may assume $u_n \in B_{\tilde{\delta}}(\Gamma_0)$ for $n \in \mathbb{N}$ without loss of generality.

Next for a fixed $n \in \mathbb{N}$ we define the time points τ_n, σ_n and the space points v_n, w_n as follows.

$$\begin{aligned} \tau_n &:= \inf\{t > 0 \mid \bar{u}(t, u_n) \notin B_{\epsilon_0}(\Gamma_0)\}, \quad v_n := \bar{u}(\tau_n, u_n) \in \partial B_{\epsilon_0}(\Gamma_0), \\ \sigma_n &:= \inf\{\hat{t} \in [0, \tau_n] \mid \bar{u}(t, u_n) \notin B_{\tilde{\delta}}(\Gamma_0) \text{ for } t \in]\hat{t}, \tau_n]\}, \quad w_n := \bar{u}(\sigma_n, u_n) \in B_{\tilde{\delta}}(\Gamma_0). \end{aligned} \quad (4.1)$$

The compactness of $B_{\tilde{\delta}}(\Gamma_0)$ ensures $w_n \rightarrow \tilde{w} \in B_{\tilde{\delta}}(\Gamma_0)$ for $n \rightarrow \infty$ eventually after choosing a subsequence $\mathbb{N}_2 \subset \mathbb{N}_1$. The sequence $(\sigma_n)_{n \in \mathbb{N}}$ cannot be bounded, because this leads to a contradiction to the invariance of Γ_0 . Hence, $\lim_{n \rightarrow \infty} \sigma_n = \infty$ holds. This ensures

$$\|g(w_n)\|_2 = \|g(\bar{u}(\sigma_n, u_n))\|_2 \leq \exp(-\sigma_n \eta) \|g(u_n)\|_2 \rightarrow 0 \text{ as } n \rightarrow \infty,$$

that is, $\tilde{w} \in S \cap B_{\tilde{\delta}}(\Gamma_0)$. Then the uniform asymptotic stability of Γ_0 for the ODE (2.2) implies that $\bar{u}(t, \tilde{w})$ exists for $t \geq 0$ in $B_{\epsilon_0/2}(\Gamma_0)$ and $\text{dist}(\bar{u}(t, \tilde{w}), \Gamma_0) \leq \hat{\epsilon}$ holds for $t \geq T(\hat{\epsilon})$, $\hat{\epsilon} > 0$ arbitrary.

Now we consider the sequence $(s_n)_{n \in \mathbb{N}}$, $s_n := \tau_n - \sigma_n \geq 0$, $n \in \mathbb{N}$. Again $(s_n)_{n \in \mathbb{N}}$ cannot be bounded, because convergence towards a finite number \tilde{s} would lead to $\bar{u}(\tilde{s}, \tilde{w}) \in \partial B_{\epsilon_0}(\Gamma_0)$ which stands in contradiction to $\bar{u}(t, \tilde{w}) \in B_{\epsilon_0/2}(\Gamma_0)$. This implies

$$\lim_{n \rightarrow \infty} s_n = \infty. \quad (4.2)$$

Finally, let \hat{T} be defined via

$$\bar{u}(t, \tilde{w}) \in B_{\tilde{\delta}/2}(\Gamma_0) \text{ for } t \geq \hat{T} \quad (4.3)$$

and let $N_0 \in \mathbb{N}$ satisfy $s_n > \hat{T}$ for $n \geq N_0$. We obtain $\bar{u}(\hat{T}, w_n) \rightarrow \bar{u}(\hat{T}, \tilde{w}) \notin B_{\tilde{\delta}}(\Gamma_0)$ in contradiction to $\bar{u}(\hat{T}, \tilde{w}) \in B_{\tilde{\delta}/2}(\Gamma_0)$. Thus Assumption 1 cannot hold and we have shown that Γ_0 is uniformly stable for the dynamics of ODE (3.2).

Assumption 2: Γ_0 is not uniformly attractive for the dynamics of (3.2).

Assumption 2 implies that there is $\epsilon_0 > 0$ and sequences $(\delta_n)_{n \in \mathbb{N}}$, $\delta_n \rightarrow 0$ as $n \rightarrow \infty$, $(u_n)_{n \in \mathbb{N}}$, $u_n \in B_{\delta_n}(\Gamma_0)$, $(t_n)_{n \in \mathbb{N}}$, $t_n \geq n$ satisfying

$$\text{dist}(\bar{u}(t_n, u_n), \Gamma_0) \geq \epsilon_0.$$

Moreover, let $\tilde{\delta} > 0$ be defined via $\text{dist}(\bar{u}(t, u_0), \Gamma_0) \rightarrow 0$ as $t \rightarrow \infty$ for $u_0 \in B_{\tilde{\delta}}(\Gamma_0) \cap S$ due to the attractivity of Γ_0 for the dynamics of (2.2). With $\tilde{\delta}$, the time points τ_n, σ_n and the space points $v_n \in B_{\epsilon_0}(\Gamma_0)$, $w_n \in B_{\tilde{\delta}}(\Gamma_0)$ can be defined as in (4.1). Now we are in the situation to mimic the steps in the first part of our proof. Let $\tilde{w} = \lim_{n \rightarrow \infty} w_n \in \partial B_{\tilde{\delta}}(\Gamma_0)$ and let \hat{T} be defined as in (4.3). Again, we define $(s_n)_{n \in \mathbb{N}}$ by $s_n := \tau_n - \sigma_n$ and obtain (4.2). Finally, this leads us to $\bar{u}(\hat{T}, w_n) \rightarrow \bar{u}(\hat{T}, \tilde{w}) \notin B_{\tilde{\delta}}(\Gamma_0)$ as $n \rightarrow \infty$. This stands in contradiction to $\bar{u}(\hat{T}, \tilde{w}) \in B_{\tilde{\delta}/2}(\Gamma_0)$ and Lemma 4.1 is shown.

In the remainder of this section we give a proof of Theorem 2.2. By virtue of Lemma 4.1 the set Γ_0 is uniformly asymptotically stable for (3.2) and in section 3 we have seen that (3.8) is a smooth q -th order one-step method applied to (3.2). Thus, Theorem 1.1 in Kloeden, Lorenz [10] is applicable and ensures for sufficiently small step size h the existence of an uniformly asymptotically stable set Γ_h containing Γ_0 which converges towards Γ_0 in the Hausdorff metric as $h \rightarrow 0$.

The last step in our proof is to draw back the results from an open subset of \mathbb{R}^N to the manifold S . To that purpose we define $\Gamma_{0,h} := \Gamma_h \cap S$. Since S is invariant for the discrete dynamics and the dynamics coincides with the u -component of the projected Runge-Kutta method (2.5)-(2.7) applied to $\dot{u} = f(u, \lambda)$, $g(u) = 0$ the set $\Gamma_{0,h}$ is uniformly asymptotically stable for (2.5)-(2.7). Finally, with property iv) of Lemma 2.1 we obtain that $(\Gamma_{0,h}, \psi_{0,h}(\Gamma_{0,h}))$ possesses the desired properties for sufficiently small step size h .

An analogous argumentation works for the half-explicit Runge-Kutta methods too and finishes the proof of Theorem 2.2.

References

- [1] ASCHER, U., PETZOLD, L.R., *Projected Runge-Kutta methods for Differential-Algebraic Equations*, SIAM J. of Numer. Anal., **28** (1991), pp. 1097–1120.
- [2] BEYN, W.-J., *On the Numerical Approximation of Phase Portraits near Stationary Points*, SIAM J. Numer. Anal., **24** (1987), pp. 1095–1113.
- [3] DEKKER, K., VERWER, J.G., *Stability of Runge-Kutta methods for stiff nonlinear differential equations* (1984), CWI Monographs, North-Holland.

- [4] GARAY, B., *Discretization and some qualitative properties of ordinary differential equations about equilibria*, Acta Math. Com. Univ., **62** (1993), pp. 249–275.
- [5] GEAR, C.W., *Differential-Algebraic Systems under Index Transformations*, SIAM J. Sci. Statist. Comput. **9** (1988), pp. 39-47.
- [6] GEAR, C.W., GUPTA, G.K., LEIMKUHNER, B., *Automatic integration of Euler-Lagrange equations with constraints*, J. Comp. Math. **12 & 13** (1985), pp. 77-90.
- [7] HAIRER, E., BRASEY, V., *Half-explicit Runge-Kutta methods for Differential-Algebraic Systems of index 2*, SIAM J. of Numer. Anal., **30** (1993), pp. 538–552.
- [8] HAIRER, E., LUBICH, CH., ROCHE, M., *The Numerical Solution of Differential-Algebraic Systems by Runge-Kutta Methods*, Lecture Notes in Mathematics, 1409 (1989), Springer.
- [9] HAIRER, E., WANNER, G., *Solving Ordinary Differential Equations II*, second edition (1996), Springer.
- [10] KLOEDEN, P.E., LORENZ, J., *Stable attracting sets in dynamical systems and in their one-step discretizations*, SIAM J. of Numer. Anal., **23** (1986), pp. 986-995.
- [11] SCHROPP, J., *A dynamical systems approach to constrained minimization*, Numer. Funct. Anal. and Optimiz., **21** (2000), pp. 537–551.
- [12] SCHROPP, J., *Behavior of Runge-Kutta Discretizations near Equilibria of Index 2 Differential Algebraic Equations*, Appl. Numer. Math., to appear.
- [13] SCHROPP, J., *Geometric Properties of Runge-Kutta Discretizations for Index 2 Differential Algebraic Equations*, Konstanzer Schriften in Mathematik und Informatik **128**.