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Numerical integration of differential algebraic systems and invariant manifolds

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Abstract

The dynamics of a differential algebraic equation takes place on a lower dimensional manifold in phase space. Applying a numerical integration scheme, it is natural to ask if and how this geometric property is preserved by the discrete dynamical system. In the index-1 case answers to this question are obtained from the singularly perturbed case treated in [6] for Runge-Kutta methods and in [7] for linear multistep methods. As main result, it is shown that also for Runge-Kutta methods and linear multistep methods applied to an index-2 problem of Hessenberg form there is a (attractive) invariant manifold for the discrete dynamical system and this manifold is close to the manifold of the differential algebraic equation.
1 Introduction

The dynamics of a differential algebraic equation (DAE) is restricted to a manifold. When applying a numerical integration scheme to a DAE, does the discrete dynamical system preserve this geometric property of the continuous dynamical system? We investigate Runge-Kutta methods (RKMs) and linear multistep methods (LMMs) applied to DAEs of index 1 and index 2.

In Section 2 we show that the existence of invariant manifolds for RKMs and LMMs applied to DAEs of index 1 as well as convergence results and global error estimates are obtained from the singularly perturbed case (treated for RKMs in [6] and for LMMs in [7]) just by putting the singular perturbation parameter $\varepsilon = 0$. Indeed, we show that there is a commuting diagram for the two cases.

In Section 3 we consider index-2 problems of Hessenberg form. In Paragraph 3.1 we first deal with RKMs and LMMs applied to the index-1 formulation and show that at least for the case of a linear constraint the commuting diagram of Section 2 still exists also containing the additional ‘index-2 submanifolds’. In the nonlinear case we prove a linear (in $t$) drift off the index-2 submanifold of the DAE. In Paragraph 3.2 we consider RKMs and LMMs applied to the index-2 formulation of the DAE which is preferred in practice (no reduction to index 1). Here, the question of interest is the existence of an attractive invariant ‘index-1 manifold’. Again, for the case of a linear constraint it can easily be verified that there is such a manifold. In the nonlinear case, we prove the existence of such an invariant manifold and derive important additional properties for BDF-like RKMs and for LMMs.

For DAEs of index 2 we follow the lines of [2] and [4] where also a standard bibliography for DAEs may be found. It is to mention that in [1] invariant manifold techniques similar to ours have been applied to the index-1 formulation of index-2 DAEs in order to investigate stabilizations of the linear drift mentioned above. The results and invariant manifold techniques of this paper may also be applied to index-3 problems of Hessenberg form (cf. [2], [4]) which admit three types of manifolds that may or may not ‘persist’ under numerical approximation.

In this introductory section, in order to introduce the notation and to keep the paper mostly self-contained and legible, we first summarize the results for singularly perturbed ODEs and their approximations by RKMs and LMMs given in [6], [7]. There, RKMs and LMMs are applied to stiff systems of singular perturbation type of the form

$$(1)_\varepsilon \quad \begin{align*} \dot{x} &= f(x, y) \\ \varepsilon y &= g(x, y) \end{align*}$$

satisfying

**Hypothesis $H_\varepsilon$**

1) $f$ and $g$ are bounded and there is $r$ with $r \geq 2$ such that $f \in C_r^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $g \in C_r^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)$.

2) There is a function $s_0 \in C_r^r(\mathbb{R}^m, \mathbb{R}^n)$ such that $g(x, s_0(x)) = 0$ for $x \in \mathbb{R}^m$. 

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3) There is a positive constant \( b_0 \) such that all eigenvalues of the Jacobian \( g_y(x, s_0(x)) \) have real parts smaller than \(-b_0\) for all \( x \in \mathbb{R}^m\).

By \( C^r_b \) we denote spaces of functions of class \( C^r \) with bounded derivatives.

Under these assumptions Eq. (1)_\( \varepsilon \) admits, for all \( \varepsilon > 0 \) small enough, an attractive invariant manifold \( M_\varepsilon \) which is the graph over \( x \)-space of a smooth function \( s \)

\[
M_\varepsilon = \{(x, y) | x \in \mathbb{R}^m, \ y = s(x, \varepsilon)\}
\]

with \( s \) of class \( C^r_b \) with respect to \( x \) and \( \varepsilon \) (for \( \varepsilon \in (-\varepsilon_0, \varepsilon_0), \varepsilon_0 \) small) and \( s(x, 0) = s_0(x) \).

\( M_\varepsilon \) is highly attractive, i.e.,

\[
|y(t) - s(x(t), \varepsilon)| \leq K \chi^t_\varepsilon |y(0) - s(x(0), \varepsilon)|, \quad t \geq 0,
\]

where \( \chi^t_\varepsilon := e^{-\beta t/\varepsilon} \) with \( \beta \in (0, b_0) \).

\( M_\varepsilon \) possesses a stable foliation, i.e., there exists a positively invariant family of stable fibers which are smooth manifolds over \( y \)-space. The ‘steepness’ of the fibers is of the order of \( L^{12}_\varepsilon = \varepsilon Lip_y(f) \), i.e., if \( (x, y) \) and \( (\bar{x}, \bar{y}) \) are two points on a fiber then \( \bar{x} - x = O(\varepsilon) \). As a consequence, the property of ‘asymptotic phase’ holds: For every trajectory of Eq. (1)_\( \varepsilon \) there exists a unique trajectory on \( M_\varepsilon \) such that the two trajectories tend to each other exponentially with rate \( \chi^t_\varepsilon \). The whole situation is sketched in Fig. 1.

![Diagram](image-url)

**Fig. 1:** The attractive invariant manifold \( M_\varepsilon \) of Eq. (1)_\( \varepsilon \), stable foliation and ‘asymptotic phase’

For RKM’s applied to Eq. (1)_\( \varepsilon \) it is assumed that the following assumptions hold.

**Hypothesis H_{RKM}**

1) The RKM has order \( p \) and stage order \( 1 \leq q < p \).

2) The RKM-matrix \( A \) is invertible.
3) The stability function \( R(z) := 1 + zb^T(I_s - zA)^{-1}\mathbb{1}_s, \) \( z \in \mathbb{C}, \) where \( \mathbb{1}_s := (1, \ldots, 1)^T \in \mathbb{R}^s, \) satisfies \( |R(\infty)| < 1. \)

Here, \( s \) is the number of stages of the RKM. Since \( A \) is invertible, \( R(\infty) = 1 - b^T A^{-1} \mathbb{1}_s \) holds. For RKM with \( a_{is} = b_i, i = 1, \ldots, s, \) this implies \( R(\infty) = 0. \) Under Hypothesis \( H_{RKM} \) the RKM

\[
X = \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y)
\]
\[
Y = \mathbb{1}_s \otimes y + \frac{h}{\varepsilon} (A \otimes I_n) g(X, Y)
\]
\[
\bar{x} = x + h(b^T \otimes I_m) f(X, Y)
\]
\[
\bar{y} = y + \frac{h}{\varepsilon} (b^T \otimes I_n) g(X, Y)
\]

defines a smooth map \( (I)_{h,\varepsilon} : (x, y) \mapsto (\bar{x}, \bar{y}) \) from \( \mathbb{R}^m \times \mathbb{R}^n \) into itself. (We have used the notation \( X := (X_1, \ldots, X_s)^T \in \mathbb{R}^{sm}, \ f(Y) := (f(X_1, Y_1), \ldots, f(X_s, Y_s))^T \in \mathbb{R}^{sm}, \) etc., \( \otimes \) denotes the Kronecker product.) In coordinates measuring the difference to \( M_\varepsilon \)

\[
y = s(x, \varepsilon) + z, \quad Y = s(X, \varepsilon) + Z
\]
this map may be written as (we often suppress the dependence of \( s(x, \varepsilon) \) on \( \varepsilon \) for short)

\[
\bar{x} = x + h(b^T \otimes I_m) f(X, s(X) + Z)
\]
\[
\bar{y} = (R(\infty) I_n + O(\varepsilon/h))z + ((b^T A^{-1} \otimes I_n) + O(\varepsilon/h)) E - \varepsilon
\]

where the stages \( X, Z \) satisfy

\[
X = \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, s(X) + Z)
\]
\[
Z = O(\varepsilon/h).
\]

The functions \( E \) and \( \varepsilon \) are defined as

\[
E(x, X) := s(X) - \mathbb{1}_s \otimes s(x) - \frac{h}{\varepsilon} (A \otimes I_n) g(X, s(X))
\]
\[
\varepsilon(x, \bar{x}, X) := s(\bar{x}) - s(x) - \frac{h}{\varepsilon} (b^T \otimes I_n) g(X, s(X))
\]

Note that \( g(X, s(X)) = O(\varepsilon). \)

The RKM-map \( (I)_{h,\varepsilon} \) admits an attractive invariant manifold \( M_{h,\varepsilon} \) which is the graph of a smooth function \( \sigma(x, h, \varepsilon) : \)

\[
M_{h,\varepsilon} = \{(x, y) | x \in \mathbb{R}^m, \ y = \sigma(x, h, \varepsilon)\}
\]

with \( \sigma \) of class \( C^r_b \) with respect to \( x \) and \( \varepsilon \) (also for \( \varepsilon = 0 \)) and

\[
\sigma(x, h, \varepsilon) = s(x, \varepsilon) + \begin{cases} O(h^{q+1}) \quad \text{if } b_i = a_{is}, i = 1, \ldots, s \\ O(\varepsilon h^q) \end{cases}
\]
The attractivity rate is $\chi_{h,\varepsilon} = |R(\infty)| + c \varepsilon/h < 1$. $M_{h,\varepsilon}$ again has a stable foliation with fibers of 'steepness' $O(\varepsilon)$ (since the Lipschitz constant $L^{h,\varepsilon}_{12}$ of the right-hand side of the first equation of $(\mathcal{I})_{h,\varepsilon}$ is $O(\varepsilon)$) and every RKM-orbit has an accompanying 'asymptotic phase' orbit on $M_{h,\varepsilon}$. In Fig. 2 a sketch of these results is given. For the global error of the RKM applied to Eq. (1)$_{\varepsilon}$ we have for $h$ and $\varepsilon/h$ small enough and for $jh \leq Nh = T$ fixed

$$
(GE)_{h,\varepsilon}
$$

$$
x_j - x(jh) = O(h^p) + O(\varepsilon^{q/2} + O(\varepsilon|y_0 - s(x_0, \varepsilon)|))
$$

$$
y_j - y(jh) = O(h^{q+1}) + O((\varepsilon + \chi_{h,\varepsilon}^j)|y_0 - s(x_0, \varepsilon)|)
$$

where for $b_i = a_{s_i}$, $i = 1, \ldots, s$, the term $O(h^{q+1})$ in the $y$-equation is replaced by $O(h^p) + O(\varepsilon h^q)$.

Fig. 2: The attractive invariant manifold $M_{h,\varepsilon}$ of the RKM-map $(\mathcal{I})_{h,\varepsilon}$, stable foliation and asymptotic phase and closeness to $M_\varepsilon$

For LMMs we have the analogous results although the situation is somewhat more complicated. This is due to the fact that LMMs cannot be considered as a map from phase space into itself. They are best described by a map in a high-dimensional space.

A $k$-step method applied to Eq. (1)$_{\varepsilon}$ is defined by

$$
\sum_{i=0}^{k} \alpha_i x_i = h \sum_{i=0}^{k} \beta_i f(x_i, y_i), \quad \alpha_k = 1,
$$

$$
\sum_{i=0}^{k} \alpha_i y_i = \frac{h}{\varepsilon} \sum_{i=0}^{k} \beta_i g(x_i, y_i)
$$

where $(x_i, y_i)$, $i = 0, \ldots, k - 1$, are given starting values. We make the following assumption.
**Hypothesis $H_{\text{LMM}}$**

1) The LMM is an irreducible $k$-step method of order $p \geq 1$.

2) The LMM is $\rho_1$-strictly stable, i.e., the polynomial $\rho(z) := \sum_{j=0}^{k} \alpha_j z^j$ has 1 as a simple zero and all other zeros have modulus smaller than $\rho_1 < 1$.

3) The LMM is $\sigma_1$-stiffly stable, i.e., $\beta_k \neq 0$ and all zeros of the polynomial $\sigma(z) := \sum_{j=0}^{k} \beta_j z^j$ have modulus smaller than $\sigma_1 < 1$.

Note that $\sum_{i=0}^{k} \alpha_i = 0$ and since $\alpha_k = 1$ this implies $\sum_{i=0}^{k-1} \alpha_i = -1$. Under the above assumptions, the LMM defines a smooth map $(I)_{h,\varepsilon}$ from $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ into itself. Defining $\alpha := (\alpha_0, \ldots, \alpha_{k-1})^T \in \mathbb{R}^k$, $\beta := (\beta_0, \ldots, \beta_{k-1})^T \in \mathbb{R}^k$ and

$$\begin{align*}
R := \begin{pmatrix}
0 & 1 & 0 \\
0 & \ddots & 1 \\
0 & & 1
\end{pmatrix}, &
X_i := \begin{pmatrix}
x_i \\
\vdots \\
x_{i+k-1}
\end{pmatrix}, &
L_\alpha := \alpha_k \alpha^T = \begin{pmatrix}
0 \\
\alpha_0 & \cdots & \alpha_{k-1}
\end{pmatrix},
\end{align*}$$

etc., and again measuring the difference to $M_\varepsilon$ by the change of coordinates $y = s(x, \varepsilon) + z$ this map has the form

$$X_1 = ((R - L_\alpha) \otimes I_m) X_0 + h(L_\beta \otimes I_m) f(X_0, s(X_0) + Z_0) + h\beta_k (\varepsilon_k \otimes f(x_k, s(x_k) + z_k))$$

$$\begin{align*}
(I)_{h,\varepsilon} Z_1 = & \left[ (R \otimes I_n) - \frac{1}{\beta_k} (L_\beta \otimes I_n) + |\beta| O \left( \max_{0 \leq i < k} |x_i - x_0| \
+ h + d + \varepsilon/h \right) + O(\varepsilon/h) \right] Z_0 + O(\varepsilon/h)
\end{align*}$$

mapping $(X_0, Z_0) \in \mathbb{R}^{km} \times \mathbb{R}^{kn} \cap \{ |Z_0|_\infty \leq d \}$ to $(X_1, Z_1) \in \mathbb{R}^{km} \times \mathbb{R}^{kn}$.

The LMM-map $(I)_{h,\varepsilon}$ admits an $m$-dimensional attractive invariant manifold $S_{h,\varepsilon}$ in $\mathbb{R}^{km} \times \mathbb{R}^{kn}$

$$S_{h,\varepsilon} = \{ x_0, \ldots, x_{k-1}, y_0, \ldots, y_{k-1} \mid x_0 \in \mathbb{R}^m, \ x_i = \Phi^i(x_0, h, \varepsilon), \ y_i = \sigma(x_i, h, \varepsilon), \ i = 0, \ldots, k-1 \}.$$

The function $\Phi$ is a one-step method of order $p$ for the differential equation $\dot{x} = f(x, s(x, \varepsilon))$ (by $\Phi^i$ we denote the $i$-th iterate) and

$$\sigma(x, h, \varepsilon) = s(x, \varepsilon) + O(\varepsilon h^p).$$

If started appropriately, i.e., $x_i = \Phi^i(x_0, h, \varepsilon), \ i = 0, \ldots, k-1$, the manifold

$$M_{h,\varepsilon} = \{ (x, y) \mid x \in \mathbb{R}^m, \ y = \sigma(x, h, \varepsilon) \}.$$
is invariant under the map \((I)_{h,\varepsilon}\) and is \(O(\varepsilon h^p)\)-close to \(M_\varepsilon\). The attractivity rate in \(y\)-direction is \(\chi_{h,\varepsilon} = \max\{\rho_1, \sigma_1\} + O(h + \varepsilon / h + d < 1\) and for \(\beta = 0\) one has \(\chi_{h,\varepsilon} = \rho_1 + O(h^\beta + \varepsilon / h) < 1\) and \(y_j - \sigma(x_j, h, \varepsilon) = y_j + O(\varepsilon h^p) = O(\varepsilon / h)\) for \(j \geq k\) as seen from \((\hat{I})_{h,\varepsilon}\) giving the \(y\)-attractivity const \cdot \varepsilon / h - \chi_{j,\varepsilon}, j \geq k\). Again there exists a stable foliation \((L_{12}^{h,\varepsilon} = O(\varepsilon), i.e., \text{‘steepness’ of the fibers } O(\varepsilon))\) implying the property of asymptotic phase. Hence, Fig. 2 again gives the right picture also for LMMs (after the \(k\)-th step). For the global error of the LMM applied to Eq. (1)\(_\varepsilon\) we have for \(h\) and \(\varepsilon / h\) small enough and for \(jh \leq T\) fixed:

\[
x_j - x(jh) = O(h^p) + O\left(\max_{0 \leq i < k} \{|x_i - x(ih)|\}\right)
+ O\left(h\left[\max_{0 \leq i < k} \{|y_i - y(ih)| + |y_0 - s(x_0, \varepsilon)|\}\right]\right)
\]

\[
(GE)_{h,\varepsilon}
\]

\[
y_j - y(jh) = O(h^p) + O\left(\max_{0 \leq i < k} \{|x_i - x(ih)|\}\right)
+ O\left((h + \chi_{j,\varepsilon})\left[\max_{0 \leq i < k} \{|y_i - y(ih)| + |y_0 - s(x_0, \varepsilon)|\}\right]\right).
\]

For \(\beta = 0\) the factor \(h\) in the \(x\)-equation is replaced by \(\varepsilon\) and the factor \((h + \chi_{j,\varepsilon})\) in the \(y\)-equation is replaced by the factor \((\varepsilon + O(\varepsilon / h)[j/k])\).

**Notation:** Throughout this paper, we denote the continuous dynamical system of singular perturbation type by \((1)\_\varepsilon\) (satisfying Hypothesis \(H_\varepsilon\)), its invariant manifold by \(M_\varepsilon\) with attractivity \(\chi_{\varepsilon}^t\) and ‘steepness’ of the stable fibers \(L_{12}^t\). Similarly, for both RKMs and LMMs applied to \((1)\_\varepsilon\) we denote the discrete dynamical system by \((I)_{h,\varepsilon}\), its invariant manifold by \(M_{h,\varepsilon}\) with attractivity \(\chi_{h,\varepsilon}\) and ‘steepness’ of the stable fibers \(L_{12}^{h,\varepsilon}\), and the global error estimate by \((GE)_{h,\varepsilon}\). If we consider the variable \(z\) (instead of \(y\)) measuring the distance to \(M_\varepsilon\) we put a \(\sim\) on \((I)_{h,\varepsilon}\), i.e., we write \((\hat{I})_{h,\varepsilon}\).

In the DAE case, we replace the \(\varepsilon\) by 0 for index 1: \((1)\_0\) (satisfying Hypothesis \(H_0\)), \(M_0, \chi_0, L_{12}^0; (I)_{h,0}, M_{h,0}, \chi_{h,0}, L_{12}^{h,0}, (GE)_{h,0}\) and \((\hat{I})_{h,0}\). For index 2 we keep the notation but put a \(\sim\) on top, i.e., \((\hat{I})_0\) (satisfying Hypothesis \(\bar{H}_0\)), \(\bar{M}_0; (\hat{I})_{h,0}, \bar{M}_{h,0}, \text{etc.}\). 

## 2 Systems of index 1

Consider the DAE

\[
(1)\_0 \quad \begin{align*}
\dot{x} &= f(x, y) \\
0 &= g(x, y)
\end{align*}
\]

satisfying

**Hypothesis \(H_0\)**

1) \(f\) and \(g\) are bounded and \(f \in C^r_b(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m), g \in C^r_b(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)\) for \(r \geq 2\).

2) There is a function \(s_0 \in C^r_b(\mathbb{R}^m, \mathbb{R}^n)\) such that \(g(x, s_0(x)) = 0\) for \(x \in \mathbb{R}^m\).

3) The matrix \(g_y(x, s_0(x))\) is invertible and \(g_y(x, s_0(x))^{-1}\) is bounded for \(x \in \mathbb{R}^m\).
Under these assumptions, Eq. (1)_0 is of index 1 since \( g(x, y) = 0 \) has a unique solution \( y = s_0(x) \) for \( (x, y) \in \Omega_d := \{ x \in \mathbb{R}^m, |y - s_0(x)| \leq d \} \) if \( d \) is small enough. All solutions of the DAE (1)_0 in \( \Omega_d \) lie on the \( m \)-dimensional surface

\[
M_0 = \{(x, y)| x \in \mathbb{R}^m, y = s_0(x)\} \subset \mathbb{R}^m \times \mathbb{R}^n.
\]

Remark 1: i) If, for \((x_0, y_0) \in \Omega_d\), we define the ‘impulse solution’ \((x(t), y(t))\) with \(x(0) = x_0\), \(y(0) = s_0(x_0)\) the set \(M_0\) may be viewed as ‘infinitely attractive invariant manifold’ of (1)_0 (there is no dynamics off \(M_0\)) with a vertical stable foliation \((L^0_{\bar{I}_2} = 0\), i.e., all points on a fiber have the same \(x\)-coordinate). Note that the index-1 case is just the limit case \((\varepsilon = 0)\) of the singularly perturbed case (except for Hypothesis H_0 3)).

ii) Note that in Hypothesis H_0 3) we do not assume that \(g_y(x, s_0(x))\) has eigenvalues with negative real part as we did in Hypothesis H_2 3). \(M_0\) is ‘infinitely attractive’ independently of the sign of the real part of the eigenvalues as is the invariant manifold \(M_{h,\varepsilon}\) (and \(M_{h,0}\) below) of the discrete dynamical system (since \(|R(\infty)| < 1\)). Hence, since there is also an invariant manifold of Eq. (1)_\varepsilon in the case of H_0 3) which is hyperbolic, however, all assertions of Section 2 hold under Hypothesis H_0 3). In this case, for the global error of RKM’s and LMMs applied to Eq. (1)_\varepsilon one has to consider solutions of (1)_\varepsilon on \(M_\varepsilon\), however.

2.1 RKM’s

We follow the lines of [2] and [4].

a) The indirect approach. The RKM

\[
X = \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\
0 = g(X, Y) \\
\bar{x} = x + h(b^T \otimes I_m) f(X, Y) \\
0 = g(\bar{x}, \bar{y})
\]

is, due to Hypothesis H_0, equivalent to applying a RKM to the \(m\)-dimensional system \(\dot{x} = f(x, s_0(x))\) and defining \(y_k = s_0(x_k)\). If the method is of order \(p\) the global error is \(O(h^p)\) (for a nonstiff vector field \(f\)).

b) The direct approach. Here, the RKM is derived via (1)_\varepsilon and (1)_h,\varepsilon and putting \(\varepsilon = 0\). For the RKM assume Hypothesis H_RKM. If we put \(\varepsilon = 0\) in Hypothesis H_\varepsilon, in the differential equation (1)_\varepsilon and in the map \((\bar{I})_{h,\varepsilon}\), in the invariant manifolds \(M_\varepsilon\) and \(M_{h,\varepsilon}\), in the attractivity constants \(\chi^\varepsilon\) and \(\chi_{h,\varepsilon}\), and in the Lipschitz constants \(L^\varepsilon_{12}\) and \(L^\varepsilon_{12}\) we obtain Hypothesis H_0, Eq. (1)_0, the map

\[
\tilde{I}_{h,0}
\]

\[
X = \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, s_0(X) + Z) \\
0 = Z \\
\bar{x} = x + h(b^T \otimes I_m) f(X, s_0(X) + Z) \\
\bar{z} = (1 - b^T A^{-1} \mathbb{1}_s) z + (b^T A^{-1} \otimes I_n) E_0 - e_0
\]

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where \( E_0 := s_0(X) - \Pi_s \otimes s_0(x), \) \( e_0 := s_0(\hat{x}) - s_0(x), \) and the invariant manifolds \( M_0 \) with attractivity \( \chi_0 = 0 \) and

\[
M_{h,0} = \{(x, y) \mid x \in \mathbb{R}^m, \; y = \sigma_0(x, h) := \sigma(x, h, 0)\}
\]

with attractivity \( \chi_{h,0} = |R(\infty)|, \) and \( L_{12}^{h,0} = 0. \) From [6] we know that \( (b^T A^{-1} \otimes I_n) E - e = O(h^{q+1}) + O(\varepsilon) \) and \( \sigma(x, h, \varepsilon) - s(x, \varepsilon) = O(h^{q+1}) \) implying \( (b^T A^{-1} \otimes I_n) E_0 - e_0 = O(h^{q+1}) \) and \( \sigma_0(x, h) - s_0(x) = O(h^{q+1}) \). Note that in the \( x, y \)-variables (in \( \Omega_d \)) the RKM-map has the form

\[
\begin{align*}
X &= \Pi_s \otimes x + h(A \otimes I_m) f(X, Y) \\
O &= g(X, Y) \\
\hat{x} &= x + h(b^T \otimes I_m) f(X, Y) \\
\hat{y} &= (1 - b^T A^{-1} \Pi_s) y + (b^T A^{-1} \otimes I_n) Y
\end{align*}
\]

considered in [2] and [4]. The global error \( \text{(GE)}_{h,0} \) of \( (I)_{h,0} \) is also obtained from \( (\text{GE})_{h,\varepsilon} \) by putting \( \varepsilon = 0. \)

Hence, we have shown that the RKM-map \( (I)_{h,0} \) admits an \( m \)-dimensional attractive invariant manifold \( M_{h,0} \) which is \( O(h^{q+1}) \)-close to \( M_0. \) The precise results are given in

**Theorem 1** Let Eq. (1) satisfy Hypothesis \( H_0 \), apply a RKM satisfying Hypothesis \( H_{\text{RKM}} \) and assume \( r < p. \)

Then there exist positive constants \( d, h_0, K \) and a function \( \sigma_0 : \mathbb{R}^m \times (0, h_0] \to \mathbb{R}^n, \) of class \( C^r \) with respect to \( x, \) such that for \( h \leq h_0 \) and for \( (x, y) \in \Omega_d := \{ (x, y) \mid x \in \mathbb{R}^m, \; |y - s_0(x)| \leq d \} \subset \mathbb{R}^m \times \mathbb{R}^n \) the following assertions hold.

i) The set \( M_{h,0} = \{(x, y) \mid x \in \mathbb{R}^m, \; y = \sigma_0(x, h)\} \) is invariant under the RKM-map \( (I)_{h,0}. \)

ii) For \( (x, y) \in \Omega_d \) the invariant manifold \( M_{h,0} \) is attractive with attractivity constant \( \chi_{h,0} = |R(\infty)|, \) i.e.,

\[
|\hat{y} - \sigma_0(\hat{x}, h)| \leq \chi_{h,0} |y - \sigma_0(x, h)|
\]

holds.

iii) \( M_{h,0} \) has a stable (vertical) foliation of the form

\[
W^s(x, y) = \{ (\xi, \eta) \mid \xi = x, \; |\eta - s_0(\xi)| \leq d \},
\]

implying the property of asymptotic phase, i.e., for \( (x_0, y_0) \in \Omega_d \) there is \( (\hat{x}, \hat{y}) \in M_{h,0} \) such that the RKM-orbits \( (x_j, y_j) \) and \( (\hat{x}_j, \hat{y}_j) \) satisfy

\[
\begin{align*}
\hat{x}_j &= x_j \\
|\hat{y}_j - y_j| &\leq K \chi_{h,0} |y_0 - \sigma_0(x_0, h)|
\end{align*}
\]

for \( j \in \mathbb{N}_0. \)
\( iv \)

\[ \sigma_0(x, h) = s_0(x) + h^{q+1} Q(x, h) , \]

with \( \sigma_0 \) of class \( C^r \) with respect to \( x \) and \( |Q| \leq K \), for all \( x \in \mathbb{R}^m \).

\( v \) Let \( (x(t), y(t)) \) be a solution of Eq. \((1)_0\) with \( x(0) = x_0 \) and let \( (x_0, y_0) \in \Omega_d \). Then for every \( T > 0 \) fixed, there is \( K > 0 \) such that the global error satisfies

\[ \begin{align*}
|x_j - x(jh)| & \leq K h^p \\
y_j - y(jh)| & \leq K(h^{q+1} + \chi_{h,0}^j |y_0 - s_0(x_0)|)
\end{align*} \]

for \( jh \leq T \).

The assertions of Theorem 1 are illustrated in Fig. 3.

Fig. 3: The invariant manifolds for the DAE \((1)_0\) and the RKM-map \((I)_{h,0}\)

**Remark 2:** In the case where the RKM satisfies \( a_{s_i} = b_i \), \( i = 1, \ldots, s \) (implying \( R(\infty) = 0 \), since \( A \) is invertible), we have \( \bar{y} = s_0(\bar{x}) \) in \((I)_{h,0}\) and therefore \( \sigma_0(x, h) = s_0(x) \) and \( M_{h,0} = M_0, \chi_{h,0} = 0 \) (infinite attractivity). The global error satisfies

\[ \begin{align*}
|x_j - x(jh)| & \leq K h^p \\
y_j - y(jh)| & \leq K h^p , \quad jh \leq T .
\end{align*} \]

For \( a_{s_i} = b_i \), \( i = 1, \ldots, s \), the direct and the indirect approach are identical.

Summarizing, we have shown for the direct approach that the diagram of Fig. 4 commutes, i.e., the results for the RKM applied to Eq. \((1)_0\) are obtained from the results of the RKM applied to Eq. \((1)_\varepsilon\) just by putting \( \varepsilon = 0 \). Of course, the DAE-results could be derived by directly applying the invariant manifold theory for maps (cf. [5]) to the map \((\bar{I})_{h,0}\). However, on the one hand, the results for the singularly perturbed case have been derived before (cf. [6]) and, on the other hand, the diagram of Fig. 4 gives additional insight.
\[ (1) \varepsilon; \quad \frac{\varepsilon \dot{y}}{1} \quad (1) 0; \]
\[ M_\varepsilon, \chi_\varepsilon^t, L_{12}^\varepsilon \quad \varepsilon \rightarrow 0 \quad M_0, \chi_0^t, L_{12}^0 \]
\[ \text{RKM} \quad \text{RKM} \]
\[ (I)_{h,\varepsilon}; \quad \varepsilon = 0 \quad (I)_{h,0}; \]
\[ M_{h,\varepsilon}, \chi_{h,\varepsilon}, L_{12}^{h,\varepsilon}; (GE)_{h,\varepsilon} \quad M_{h,0}, \chi_{h,0}, L_{12}^{h,0}; (GE)_{h,0} \]

Fig. 4: The correspondence between the DAE and the singularly perturbed differential equation and their RKM-maps

2.2 LMMs

For a LMM satisfying Hypothesis $H_{LMM}$ applied to Eq. $(1)_0$ we obtain analogous results as for the RKM of Paragraph 2.1, in particular, there is again a commuting diagram. There is one major difference, however, the ‘discrete’ manifold $M_{h,0}$ is always equal to the ‘continuous’ manifold $M_0$. More precisely, by putting $\varepsilon = 0$ in $(\tilde{I})_{h,\varepsilon}$ we obtain the LMM-map in $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ ($Y = s_0(X) + Z$, $|Z|_\infty \leq d$, $d$ small enough)

\[ X_1 = \left( (R - L_\alpha) \otimes I_m \right) X_0 + h(L_\beta \otimes I_m) f(X_0, s_0(X_0) + Z_0) \]
\[ \quad + h(\beta_k \otimes f(x_k, s_0(x_k) + z_k)) \]
\[ (\tilde{I})_{h,0} \]
\[ Z_1 = \{(R \otimes I_n) \left( (L_\beta \otimes C(x_k, z_k)^{-1}) \right) \text{diag}[B_0(X_0) + \hat{B}(X_0, Z_0)] \}\]

where $C(x_k, z_k) := -\beta_k (B_0(x_k) + \hat{B}(x_k, z_k))$, $B_0(x) := g_y(x, s_0(x))$, $\hat{B}(x, 0) = 0$. (Note that it can be seen directly that $Z = 0$ is an invariant manifold of $(\tilde{I})_{h,0}$).

Again, all results are inherited from the singularly perturbed case by putting $\varepsilon = 0$:

- Invariant manifold of $(I)_{h,0}$ : $M_{h,0} = M_0$.
- Attractivity in $y$-direction: $\chi_{h,0} = \max\{\rho_1, \sigma_1\} + O(h + |\beta|d)$.
- Stable (vertical) foliation and asymptotic phase.
- Global error for $j \leq N$:

\[ |x_j - x(jh)| \leq K_N \left[ \max_{0 \leq \ell < k} \{|x_\ell - x(\ell h)|\} + h \max_{0 \leq \ell < k} \{|y_\ell - y(\ell h)|\} \right. \]
\[ + \left. |y_0 - s_0(x_0)| + h^p \right] \]
\[ (GE)_{h,0} \]
\[ |y_j - y(jh)| \leq K_N \left[ \max_{0 \leq \ell < k} \{|x_\ell - x(\ell h)|\} + (h + \chi_{h,0}^j) \max_{0 \leq \ell < k} \{|y_\ell - y(\ell h)|\} \right. \]
\[ + \left. |y_0 - s_0(x_0)| + h^p \right] . \]
Remark 3): For $\beta = 0$ (BDF-like methods, corresponding to $a_{s_i} = b_i$, $i = 1, \ldots, s$, in the RKM case) we have:

- $\chi_{h,0}^k = 0$ (infinite attractivity in $y$-direction), i.e., $y_j = s_0(x_j)$ for $j \geq k$ independently of the starting values $y_0, \ldots, y_{k-1}$ (this is easily seen from $(\tilde{I})_{h,0}$ with $\beta = 0$).

- Global error for $j \leq N$:

$$
|x_j - x(jh)| \leq K_N \max_{0 \leq \ell < k} \{ |x_\ell - x(\ell h)| \} + h^p \\
(\text{GE})_{h,0} \quad |y_j - y(jh)| \leq K_N \max_{0 \leq \ell < k} \{ |x_\ell - x(\ell h)| \} + h^p \\
+ x_{h,0}^{[j/k]} \max_{0 \leq \ell < k} \{ |y_\ell - y(\ell h)| \} + |y_0 - s_0(x_0)| .
$$

\[\]

3 Systems of index 2

We consider the semi-explicit problem of so-called Hessenberg form

$$(\tilde{I})_0
\begin{align*}
\dot{x} &= f(x,y) \\
0 &= G(x)
\end{align*}
$$

satisfying

Hypothesis $\Pi_0$

1) $f$ is bounded and $f \in C^{r+1}_b(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $G \in C^{r+1}_b(\mathbb{R}^m, \mathbb{R}^n)$, $r \geq 2$.

2) There is a function $s_0 \in C^r_b(\mathbb{R}^m, \mathbb{R}^n)$ such that $G_x(x) f(x, s_0(x)) = 0$ for $x \in \mathbb{R}^m$.

3) The matrix $G_x(x) f_y(x, s_0(x))$ is invertible and the inverse is bounded for $x \in \mathbb{R}^m$.

Under these assumptions, Eq. $(\tilde{I})_0$ is of index 2 since differentiating $0 = G(x)$ with respect to $t$ yields $0 = G_x(x) f(x,y)$ which together with $\dot{x} = f(x,y)$ is an index-1 problem by Hypothesis $\Pi_0$. The algebraic system $0 = G_x(x) f(x,y)$ has a unique solution $y = s_0(x)$ for $(x,y) \in \Omega_d := \{ x \in \mathbb{R}^m, |y - s_0(x)| \leq d \}$, $d$ small enough. All solutions $(x(t), y(t))$ in $\Omega_d$ of the index-1 DAE (the so-called index-1 formulation of the index-2 problem $(\tilde{I})_0$)

$$(1)_0
\begin{align*}
\dot{x} &= f(x,y) \\
0 &= g(x,y) := G_x(x) f(x,y)
\end{align*}
$$

lie in the $m$-dimensional surface

$$
M_0 = \{(x,y) \mid x \in \mathbb{R}^m, y = s_0(x) \} \in \mathbb{R}^m \times \mathbb{R}^n .
$$

11
In addition, they satisfy for all $t \in \mathbb{R}$

$$\int_{0}^{t} G(x(\tau)) f(x(\tau), s_0(x(\tau)) \, d\tau = 0$$

implying

$$G(x(t)) - G(x(0)) = 0.$$ 

This means that Eq. (1)$_0$ has $G$ as first integral. The manifold

$$\overline{M}_0 = \{ (x, y) \mid G(x) = 0, \ y = s_0(x) \} \subset M_0 \subset \mathbb{R}^m \times \mathbb{R}^n.$$ 

is invariant under (1)$_0$. Hence, we have shown that under Hypothesis H$_0$ all solutions of Eq. (1)$_0$ (in $\Omega_d$) lie in the submanifold $\overline{M}_0$ of $M_0$ (cf. Fig. 5). Again the set $\overline{M}_0$ may be viewed as 'invariant manifold being infinitely attractive in $y$-direction with a vertical stable foliation' (cf. Remark 1)).

Fig. 5: The invariant manifold $\overline{M}_0$ of Eq. (1)$_0$

**Remark 4**: Note that every manifold $\overline{M}_0^{\text{const}} := \{ (x, y) \mid G(x) = \text{const}, \ y = s_0(x) \}$ is invariant under Eq. (1)$_0$ and lies in $M_0$, i.e., the $m$-dimensional surface $M_0$ consists of submanifolds $\overline{M}_0^{\text{const}}$. And, of course, all solutions of (1)$_0$ satisfy $\dot{x} = f(x, y), \ G(x) = G(x(0))$.

### 3.1 RKMs and LMMs applied to the index-1 formulation

Obviously, applying a RKM satisfying Hypothesis H$_{\text{RKM}}$ or a LMM satisfying Hypothesis H$_{\text{LMM}}$ to the index-1 formulation (1)$_0$ yields the results of Paragraphs 2.1 and 2.2, respectively, with the commuting diagram Fig. 4. However, the question of interest is if
the dynamical systems \((1)\varepsilon\), \((1)_{h,\varepsilon}\) and \((1)_{h,0}\), respectively, also possess a ‘first integral’, i.e., a submanifold of \(M_\varepsilon, M_{h,\varepsilon}\) and \(M_{h,0}\), respectively.

\(A\) \((1)\varepsilon\): The invariant manifold \(M_\varepsilon\) is the graph of the function \(s(x, \varepsilon)\) which satisfies the invariance equation

\[
\dot{x} = f(x, s(x, \varepsilon)) \quad \varepsilon \frac{s_x(x, \varepsilon) f(x, s(x, \varepsilon))}{f(x, s(x, \varepsilon))} = g(x, s(x, \varepsilon)).
\]

The second equation is equivalent to \(\varepsilon \dot{s} = G_x(x) \dot{x}\) implying

\[
\varepsilon [s(x(t), \varepsilon) - s(x(0), \varepsilon)] = G(x(t)) - G(x(0)).
\]

Hence, Eq. \((1)\varepsilon\) with \(g(x, y) = G_x(x)f(x, y)\) admits the invariant manifold

\[
\overline{M}_\varepsilon = \{(x, y) \mid G(x) - \varepsilon s(x, \varepsilon) = 0, \ y = s(x, \varepsilon)\} \subset M_\varepsilon.
\]

Of course, again any set

\[
\overline{M}_\varepsilon^{\text{const}} = \{(x, y) \mid G(x) - \varepsilon s(x, \varepsilon) = \text{const}, \ y = s(x, \varepsilon)\} \subset M_\varepsilon
\]

is an invariant manifold of Eq. \((1)\varepsilon\). Putting \(\varepsilon = 0\) one obtains \(\overline{M}_0 \subset M_0\) or \(\overline{M}_0^{\text{const}} \subset M_0\), respectively.

\(B\) \(a\) \((I)_{h,\varepsilon}\) and \((I)_{h,0}\) for RKM. \(i\) The linear case: We assume

\[
G(x) = Bx + c
\]

where \(B\) is a \(n \times m\)-matrix and \(c\) is a \(n\)-vector both independent of \(x\). This implies \(g(x, y) = G_x(x)f(x, y) = Bf(x, y)\). In the RKM case the discrete invariant manifold \(M_{h,\varepsilon}\) is the graph of the function \(\sigma(x, h, \varepsilon)\) satisfying the invariance equation

\[
\bar{x} - x = h \sum_{i=1}^{s} b_i f(X_i, Y_i)
\]

\[
\varepsilon [\sigma(\bar{x}, h, \varepsilon) - \sigma(x, h, \varepsilon)] = h \sum_{i=1}^{s} b_i g(X_i, Y_i) = B(\bar{x} - x).
\]

This implies the existence of the invariant manifold

\[
\overline{M}_{h,\varepsilon} = \{(x, y) \mid G(x) - \varepsilon \sigma(x, h, \varepsilon) = 0, \ y = \sigma(x, h, \varepsilon)\} \subset M_{h,\varepsilon}
\]

for the RKM-map \((I)_{h,\varepsilon}\). Putting \(\varepsilon = 0\) we obtain the invariant manifold

\[
\overline{M}_{h,0} = \{(x, y) \mid G(x) = 0, \ y = \sigma_0(x, h)\} \subset M_{h,0}
\]

for the RKM-map \((I)_{h,0}\). We know that \(\sigma_0(x, h) = s_0(x) + O(h^{a+1})\). The situation for the DAE in the linear case is sketched in Fig. 6. Note that if \(a_{s_i} = b_i, i = 1, \ldots, s\), we have \(M_{h,0} = M_0\) and \(\overline{M}_{h,0} = \overline{M}_0\), i.e., the continuous and the discrete manifolds are the same.
Fig. 6: The manifolds $\overline{M}_0$ and $M_0$ of Eq. (1)$_0$ and the invariant manifolds $\overline{M}_{h,0}$ and $M_{h,0}$ of the RKM-map $(\mathcal{I})_{h,0}$ for $G(x) = Bx + c$

For RKM applied to the index-1 formulation of Eq. (1)$_0$ we have shown that in the linear case the commuting diagram of Fig. 4 also holds if the submanifolds $\overline{M}_0$, $\overline{M}_\varepsilon$, $\overline{M}_{h,\varepsilon}$ and $\overline{M}_{h,0}$, respectively, are added into the picture.

Remark 5): The invariant manifolds $\overline{M}_0$, $\overline{M}_\varepsilon$, $\overline{M}_{h,\varepsilon}$ and $\overline{M}_{h,0}$, respectively, inherit the attractivity of the invariant manifolds $M_0$, $M_\varepsilon$, $M_{h,\varepsilon}$ and $M_{h,0}$, respectively, in $y$-direction. Moreover, every ‘shifted manifold’ $\overline{M}_0^{\text{const}} := \{ (x, y) \mid G(x) = \text{const}, y = s_0(x) \}$, $\overline{M}_\varepsilon^{\text{const}}$, $\overline{M}_{h,\varepsilon}^{\text{const}}$ and $\overline{M}_{h,0}^{\text{const}}$ (defined analogously) is also invariant.

ii) The nonlinear case: For RKM applied to Eq. (1)$_\varepsilon$ we have the following invariance equation for $M_{h,\varepsilon}$

$$\bar{x} - x = h \sum_{i=1}^{s} b_i f(X_i, Y_i)$$

$$\varepsilon [\sigma(\bar{x}) - \sigma(x)] = h \sum_{i=1}^{s} b_i G_x(X_i) f(X_i, Y_i)$$

where we have suppressed the dependence of $\sigma$ on $h, \varepsilon$. The stages $X_i, Y_i$, $i = 1, \ldots, s$, are functions of $x, h$ and $\varepsilon$ (smooth with respect to $x, \varepsilon$). We define the function $Q(x; h, \varepsilon)$ by

$$Q(x; h, \varepsilon) := G(\bar{x}) - G(x) - h \sum_{i=1}^{s} b_i G_x(X_i) f(X_i, Y_i) .$$

Starting the RKM with $G(x_0) - \varepsilon \sigma(x_0) = \Delta_0$ we obtain using the definition of $Q$ and Eq. (2) that for $j \geq 1$

$$G(x_j) - \varepsilon \sigma(x_j, h, \varepsilon) = \sum_{\ell=0}^{j-1} Q(x_\ell; h, \varepsilon) + \Delta_0 .$$
We want to estimate the function $Q(x_t; h, \varepsilon)$. Let $(x(t), y(t))$ be a solution of Eq. (1) with initial values $x(0) = x_t, y(0) = y_t = \sigma(x_t)$. Integrating $\frac{d}{dt} G(x(t)) = G_x(x(t)) f(x(t), y(t))$ between 0 and $h$ we get

\begin{equation}
G(x(h)) - G(x_t) = \int_0^h G_x(x(\tau)) f(x(\tau), y(\tau)) \, d\tau.
\end{equation}

From the definition of $Q$ we have

\begin{equation}
G(x_{t+1}) - G(x_t) = h \sum_{i=0}^s b_i G_x(X_i) f(X_i, Y_i) + Q(x_t; h, \varepsilon)
\end{equation}

where $X_i, Y_i$ are functions of $x_t$, $h$ and $\varepsilon$. From Eqs. (3) and (6) we obtain

\[ Q(x_t; h, \varepsilon) = G(x_{t+1}) - G(x(h)) - [P_1 - P_2] \]

with $P_1 := h \sum_{i=0}^s b_i G_x(X_i) f(X_i, Y_i)$ and $P_2 := \int_0^h G_x(x(\tau)) f(x(\tau), y(\tau)) \, d\tau$. From [6], Theorem 2 and Theorem 3 (with proof) we know that

\[ x_{t+1} - x(h) = O(h^{p+1}) + O(\varepsilon h^{q+1}) + O(\varepsilon |\sigma(x_t) - s(x_t)|) \]

\[ = O(h^{p+1}) + O(\varepsilon h^{q+1}). \]

Since $G$ is of class $C^1_b$ this implies $G(x_{t+1}) - G(x(h)) = O(h^{p+1}) + O(\varepsilon h^{q+1})$.

It remains to estimate $P_1 - P_2$. From nonstiff RKM-theory (cf. [3]) we know that for a RKM applied to $\dot{u} = f(u, s(u))$, $u(0) = u_0 := x_t$ the relations

\begin{equation}
\begin{aligned}
u(c_i h) - u_0 &= h \sum_{j=1}^s a_{ij} f(u(c_j h), s(u(c_j h))) + O(h^{q+1}), \quad i = 1, \ldots s, \\
u(h) - u_0 &= h \sum_{i=1}^s b_i f(u(c_i h), s(u(c_i h))) + O(h^{p+1})
\end{aligned}
\end{equation}

hold. Moreover, for the function $G_x(u(t)) f(u(t), s(u(t)))$ the RKM is a quadrature formula of order $p$, i.e.,

\begin{equation}
\begin{aligned}
\int_0^h G_x(u(\tau)) f(u(\tau), s(u(\tau))) \, d\tau &= h \sum_{i=1}^s b_i G_x(u(c_i h)) f(u(c_i h), s(u(c_i h))) + O(h^{p+1}).
\end{aligned}
\end{equation}

We introduce $Z_i, i = 1, \ldots, s$, and $z(t)$ by $Y_i = s(X_i) + Z_i$ and $y(t) = s(x(t)) + z(t)$ and we estimate

\[ P_1 - P_2 = P_1 - \overline{P}_1 + \overline{P}_1 - \overline{P}_2 + \overline{P}_2 - P_2 \]
where
\[ \mathcal{P}_1 := h \sum_{i=1}^{s} b_i G_x(U_i) f(U_i, s(U_i)) \]
\[ \mathcal{P}_2 := h \sum_{i=1}^{s} b_i G_x(u(c_i h)) f(u(c_i h), s(u(c_i h))) . \]

We have
\[ P_1 - \mathcal{P}_1 := h O \left( \max_{1 \leq i \leq s} |X_i - U_i| + \max_{1 \leq i \leq s} |Z_i| \right) , \]
\[ \mathcal{P}_1 - \mathcal{P}_2 := h O \left( \max_{1 \leq i \leq s} |U_i - u(c_i h)| \right) \]
and with (8)
\[ \mathcal{P}_2 - P_2 = O(h^{p+1}) + h O \left( \max_{0 \leq t \leq h} |x(t) - u(t)| + \max_{0 \leq t \leq h} |z(t)| \right) . \]

From [6] we know that
\[ Z_i = O(\varepsilon h^q), \quad X_i - U_i = O(\varepsilon h^{q+1}), \quad i = 1, \ldots, s . \]

The first relation of (7) implies
\[ U_i - u(c_i h) = O(h^{q+1}), \quad i = 1, \ldots, s , \]
and a simple Gronwall type argument yields
\[ \max_{0 \leq t \leq h} |x(t) - u(t)| = h O(\max_{0 \leq t \leq h} |z(t)|) . \]

For \( z(t) \) we apply Theorems 1 and 3 of [6]:
\[ z(t) = x(t) - s(x(t)) = O \left( e^{-\text{const} \cdot t/\varepsilon} |y(0) - s(x(0))| \right) \]
\[ = O(|\sigma(x_t) - s(x_t)|) = O(h^{q+1}) . \]

Adding up, we finally have
\[ Q(x_t; h, \varepsilon) = O(h^{q+2}) . \]

(We have used the fact that \( \varepsilon \ll h \) and \( q < p \) which cancels out the \( O(h^{p+1}) \)- and \( O(\varepsilon h^{q+1}) \)-terms). Hence, Eq. (4) implies for all \( j \in \mathbb{N} \)
\[ (9) \quad G(x_j) - \varepsilon \sigma(x_j; h, \varepsilon) = \Delta_0 + j h \cdot O(h^{q+1}) \]

where the constant in \( O(h^{q+1}) \) is independent of \( j \). This means a RKM-orbit starting on \( M_{h, \varepsilon} \) and \( O(h^{q+1}) \)-close to \( \overline{M}_{h, \varepsilon} \) has at worst a linear (in \( t = j h \)) drift off in the \( x \)-component. (Of course, starting off \( M_{h, \varepsilon} \) there is the attractivity in the \( y \)-component with \( \chi_{h, \varepsilon} \).)
Remark 6): Using the global error estimate \((\text{GE})_{h,\varepsilon}\) it is simple to get the estimate

\[ G(x_j) - \varepsilon \sigma(x_j, h, \varepsilon) = \Delta_0 + O(h^p) + O(\varepsilon h^{q+1}) . \]

However, here the constants in the \(O\)-terms are of the form \(\text{Konst} \cdot e^{\text{const} \cdot jh}\) which is a much weaker result than the one of Eq. (9).

The above results also hold for \(\varepsilon = 0\). We state the DAE case in

**Theorem 2** Let Eq. \((1)_{0}\) satisfy Hypothesis \(\overline{H}_0\), apply a RKM satisfying Hypothesis \(H_{\text{RKM}}\) to its \('\text{index-1 formulation}'\) \((1)_{0}\) and assume \(r < p\). Consider for \(\Delta_0 \in \mathbb{R}^n\) the set

\[ \mathcal{M}^0_{h,0} = \{(x, y) \mid G(x) = \Delta_0, y = \sigma_0(x, h)\} \subset M_{h,0} \]

with \(\sigma_0\) and \(M_{h,0}\) from Theorem 1. Then the following assertions hold.

i) A RKM-orbit \((x_j, y_j), j \in \mathbb{N}, \) with \(G(x_0) = \Delta_0, y_0 = \sigma(x_0, h)\) satisfies

\[ |G(x_j) - \Delta_0| \leq jh \cdot K h^{q+1}, \quad y_j = \sigma_0(x_j, h) \]

for some constant \(K\) independent of \(j\).

ii) If \(G\) is linear, \(G(x) = Bx + c\), the set \(\mathcal{M}^0_{h,0}\) is an invariant manifold of the RKM-map \((I)_{h,0}\).

Remark 7): i) Note, that for \(a_{x_i} = b_i, i = 1, \ldots, s, \sigma_0(x, h) = s_0(x)\) and hence \(\mathcal{M}^0_{h,0} = \mathcal{M}^0_{0} = \{(x, y) \mid G(x) = \Delta_0, y = s_0(x)\} \subset M_0\).

ii) If the RKM-orbit is started such that \(|y_0 - s_0(x_0)| \leq d\) small enough, one obtains due to the vertical stable foliation of \(M_{h,0}\) the same \(x\)-estimates as in Theorem 2 and exponential attractivity to \(\mathcal{M}^0_{h,0}\) in \(y\)-direction (cf. Theorem 1).

iii) The global error is \((\text{GE})_{h,0}\) of the index-1 problem as given in Theorem 1 v) and in Remark 2).

**B.b)** \((I)_{h,\varepsilon}\) and \((I)_{h,0}\) for LMMs. The invariance equation for \(M_{h,\varepsilon}\) is

\[
\sum_{i=0}^{k} \alpha_i x_i = h \sum_{i=0}^{k} \beta_i f(x_i, \sigma(x_i))
\]

\[
\varepsilon \sum_{i=0}^{k} \alpha_i \sigma(x_i) = h \sum_{i=0}^{k} \beta_i G_x(x_i) f(x_i, \sigma(x_i))
\]

(10)

together with \(x_i = \Phi^i(x_0, h, \varepsilon), i = 1, 2, \ldots\). Here, we again have suppressed the dependence of \(\sigma\) on \(h\) and \(\varepsilon\). We define the function

\[
Q(x_0; h, \varepsilon) := \sum_{i=0}^{k} \alpha_i G(x_i) - h \sum_{i=0}^{k} \beta_i G_x(x_i) f(x_i, \sigma(x_i)) .
\]

(11)
We will also need the fact that \( \Phi \) is a one-step method of order \( p \) for \( \dot{u} = f(u, s(u, \varepsilon)) \) (cf. [7], Theorem 2). For \( \Delta_0 \in \mathbb{R}^n \) we take \( x_0 \) such that \( G(x_0) - \varepsilon \sigma(x_0) = \Delta_0 \) and we define for \( j = 0, 1, 2, \ldots \)

\[
\Delta_j := G(x_j) - \varepsilon \sigma(x_j)
\]

and

\[
Q_j := Q(x_j; h, \varepsilon)
\]

where \( Q(x_j; h, \varepsilon) \) is defined as in (11) with \( x_i \) replaced by \( x_{j+i} \). From Eqs. (10) and (11) we have for \( j \geq 0 \)

\[
\sum_{i=0}^{k} \alpha_i \Delta_{j+i} = Q_j
\]

or with \( \delta^0 := (\Delta_0, \ldots, \Delta_{k-1})^T \in \mathbb{R}^n \), \( \delta^1 := (\Delta_1, \ldots, \Delta_k)^T \), \( r^0 := (0, \ldots, 0, Q_0)^T \in \mathbb{R}^n \), \( r^1 := (0, \ldots, 0, Q_1)^T \), etc.,

\[
\delta^j = ((R - L_\alpha) \otimes I_n) \delta^{j-1} + r^{j-1}, \quad j \geq 1,
\]

and, therefore,

\[
\delta^j = ((R - L_\alpha) \otimes I_n)^j \delta^0 + \sum_{\ell=0}^{j-1} ((R - L_\alpha) \otimes I_n)^\ell r^{j-\ell-1}, \quad j \geq 1.
\]

By Hypothesis H_{LMM} the \( k \times k \)-matrix \( R - L_\alpha \) has one eigenvalue 1 and all others have modulus smaller than \( \rho_1 < 1 \). Hence, we have

\[
|\Delta_{j+k-1}| \leq |\delta^j|_\infty \leq K_0 |\delta^0|_\infty + j \cdot K_0 K_1, \quad j = 1, 2, \ldots,
\]

if \( K_0 > 0 \) is such that \( |((R - L_\alpha) \otimes I_n)^j| \leq K_0 \) for \( j > 0 \) and if we assume that \( |Q_j| \leq K_1 \) for all \( j \). This second assumption has to be verified. In fact, with similar techniques as for RKMs using the results in [7], one finds \( K_1 = K_1 h^{p+1} \) and \( \Delta_i = \Delta_0 + O(h^{p+1}), \quad i = 1, \ldots, k - 1 \). The role of Eq. (7) is taken by the relation

\[
L(G(u), t; h) = \sum_{i=0}^{k} [\alpha_i G(u(ih)) - \beta_i G_x(u(ih)) f(u(ih), s(u(ih)))] = O(h^{p+1})
\]

(cf. [3]).

Summarizing, we have for \( j \in \mathbb{N} \)

\[
|G(x_j) - \varepsilon \sigma(x_j, h, \varepsilon)| \leq j h \cdot K h^p + K_0 \max_{0 \leq i < k} |\Delta_i|
\]

with constants \( K, K_0 \) independent of \( j \). This, of course, again means at worst a linear drift (in \( t = jh \)) off \( G(x) - \varepsilon \sigma(x, h, \varepsilon) = \Delta_0 \). For \( G \) linear, \( G(x) = Bx + c \), it is easy to see that the set \( G(x) - \varepsilon \sigma(x, h, \varepsilon) = \Delta_0 \) is an invariant set of the LMM-map.
In the DAE case ($\varepsilon = 0$), we thus have analogously to Theorem 2 in the RKM case:

- The LMM-orbit $(x_j, y_j)$, $j \in \mathbb{N}$, with $G(x_0) = \Delta_0$ and lying in $M_{h,0} = M_0 = \{(x, y) \mid x \in \mathbb{R}^m, y = s_0(x)\}$ satisfies

$$|G(x_j) - \Delta_0| \leq jh \cdot Kh^p, \quad y_j = s_0(x_j)$$

for some constant $K$ independent of $j$.

- If $G$ is linear, $G(x) = Bx + c$, and if in addition $Bx_i + c = \Delta_0$, $i = 1, \ldots, k - 1$, then the set $\mathcal{M}_{\Delta_0} = \{(x, y) \mid G(x) = \Delta_0, y = s_0(x)\} \in M_0$ is an invariant manifold of the LMM-map $\mathcal{I}_{h,0}$.

If we take starting values off $M_0$ satisfying $x_i - x(ih) = O(h^{p+1})$, $i = 1, \ldots, k - 1$, where $x(t)$ is the solution of Eq. (1) with $x(0) = x_0$, $G(x_0) = \Delta_0$ and/or $|y_i - s_0(x_i)| \leq d$, $i = 0, \ldots, k - 1$, $d$ small enough, then the $x$-estimate (12) still holds and in $y$-direction one has exponential attractiveness to $M_0$. For $\beta = 0$, $M_0$ is ‘infinitely $y$-attractive’, i.e., $y_j = s_0(x_j)$ for $j \geq k$ (cf. Paragraph 2.2, Remark 3)).

### 3.2 RKMs and LMMs applied to the index-2 formulation

While appropriate numerical integration of the index-2 formulation preserves $G(x) = 0$, here, the point of interest is the existence of a $y$-attractive invariant index-1 manifold for the discrete dynamical system.

- **a) RKMs.** We apply a RKM satisfying Hypothesis $H_{\text{RKM}}$ to the DAE of index 2

\[
\begin{align*}
\dot{x} &= f(x,y) \\
0 &= G(x)
\end{align*}
\]

satisfying Hypothesis $H_0$. Following [2] and [4] we have

$$X = \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y)$$

$$0 = G(X)$$

for the stages and

$$\bar{x} = x + h(b^T \otimes I_m) f(X, Y)$$

$$\bar{y} = (1 - b^T A^{-1} \mathbb{1}_s) y + (b^T A^{-1} \otimes I_n) Y$$

for one step of the RKM. Introducing the variable $z$ by means of $y = s_0(x) + z$ and similarly for $\bar{z}$ this is equivalent to

$$\bar{x} = x + h(b^T \otimes I_m) f(X, Y)$$

$$\bar{z} = R(\infty) z + (b^T A^{-1} \otimes I_n) (Y - \mathbb{1}_s \otimes s_0(x)) + s_0(x) - s_0(\bar{x}).$$

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Of course, we have to show that \((\tilde{I})_{h,0}\) and \((\tilde{I})_{h,0}\), respectively, are well defined maps in phase space, i.e., we have to show that Eq. (13) has a unique solution \((X, Y)\) given \(x\) appropriately in \(\mathbb{R}^m\). This is done in Lemma 3 below. There, we consider an altered system (Eq. (14)) and show that for all \(x \in \mathbb{R}^m\) it has a unique solution near \((\mathbb{1}_s \otimes x, \mathbb{1}_s \otimes s_0(x))\). For our original system (13) this implies the existence of unique solution not only for \(x\)-starting values satisfying \(G(x) = 0\) but also for perturbed values in a \(O(h^2)\)-neighbourhood of \(G(x) = 0\). Note that the solution does not depend on the \(y\)-starting value.

**Lemma 3** Let \(\Delta : \mathbb{R}^m \times \mathbb{R}_+ \to \mathbb{R}^n\) be a bounded function of class \(C^r_0\). Then, there are positive constants \(h_1, K\) such that for \(h \leq h_1\) and \(x \in \mathbb{R}^m\) the non-linear system

\[
\begin{align*}
X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\
G(X) &= \mathbb{1}_s \otimes (G(x) - h^2 \Delta(x, h))
\end{align*}
\]

has a unique solution \((X, Y)(x, h), C^r_0\) with respect to \(x\), satisfying

\[
|X(x, h) - \mathbb{1}_s \otimes x| \leq K h, \quad |Y(x, h) - \mathbb{1}_s \otimes s_0(x)| \leq K h.
\]

**Proof:** If we introduce \(Z \in \mathbb{R}^m\) by \(Y = s_0(X) + Z\) and add the term \(h \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j)\) on both sides of the second equation, Eq. (14) in components \((i = 1, \ldots, s)\) takes the following form

\[
X_i = x + h \sum_{j=1}^s a_{ij} f(X_j, s_0(X_j) + Z_j)
\]

(15) \[ h \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j) = G(x) - G(X_i) - h^2 \Delta(x, h) + h \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j). \]

Using the first equation of Eq. (15) we find

\[
G(X_i) - G(x) = \int_0^1 G_x(x + \tau(X_i - x))d\tau \cdot (X_i - x)
\]

(16) \[
= h \sum_{j=1}^s a_{ij} \int_0^1 G_x(x + \tau(X_i - x))d\tau \cdot f(X_j, s_0(X_j) + Z_j).
\]

Hence, the second equation of Eq. (15) is of the form

\[
\frac{1}{h} \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j) = \frac{1}{h} \sum_{j=1}^s a_{ij} \int_0^1 [G_x(X_j) - G_x(x + \tau(X_i - x))]d\tau \cdot \\
\cdot f(X_j, s_0(X_j) + Z_j) - \Delta(x, h)
\]

\[
=: Q_i(x, X, Z; h).
\]
Since the norm of the integrand is bounded by $L_{G_x}(|X_j - x| + |X_i - x|) \leq \text{const} \cdot h$ due to the first equation of (15) and since $\Delta$ is bounded by assumption, the functions $Q_i$, $i = 1, \ldots, s$, are bounded for all $h$ small. Hence, back to the ‘big space’ and since the Runge-Kutta matrix $A$ is invertible by Hypothesis $H_{RKM}$, Eq. (15) has the form

$$X = 1_s \otimes x + h(A \otimes I_m) f(X, s_0(X) + Z)$$

$$\text{diag}[G_x(X)] f(X, s_0(X) + Z) = h(A^{-1} \otimes I_n) Q(x, X, Z; h)$$

with $Q$ bounded and of class $C^r_b$ with respect to $x, X, Z$. By Hypothesis $\bar{H}_0$ we know that $\text{diag}[G_x(X)] f(X, s_0(X)) = 0$ and that $\text{diag}[G_x(X)] f_y(X, s_0(X))$ is invertible with bounded inverse. Hence, for $|Z| \leq d, d$ small enough, the second equation can be written as

$$Z = h C(X, Z)^{-1}(A^{-1} \otimes I_n) Q(x, X, Z; h)$$

with $C(X, Z) = \text{diag}[G_x(X)] f_y(X, s_0(X)) + O(|Z|)$ and $C(X, Z)^{-1}$ bounded. Considering the two equations as a fixed point equation (for some map) the contraction principle implies the existence of a unique solution $(X, Z)(x, h)$ satisfying $|X - 1_s \otimes x| \leq \text{const} \cdot h$, $|Z| \leq \text{const} \cdot h$. The smoothness follows from the implicit function theorem. \hfill \qed

Remark 8): For an $x$-starting value such that $G(x) = h^2 \Delta(x, h)$, Lemma 3 corresponds to Theorem 4.1 of [2] (cf. also [4], Theorem 7.1). We have given a different proof and we do not need their assumption $G_x[f(x, y)] = O(h)$.

i) The linear case: We assume that $G(x) = Bx + c$ for the function $G$ and that the starting values $x$ and $y$ are such that $G(x) = 0$ and $|y - s_0(x)| \leq d, d$ small enough. From Lemma 3 with $\Delta \equiv 0$ it follows that Eq. (13) has a unique solution $(X, Y)(x, h)$ near $(1_s \otimes x, 1_s \otimes s_0(x))$. It is easy to see that by our assumptions $G(X) = 0$ implies $g(X, Y) := \text{diag}[G_x(X)] f(X, Y) = 0$ and vice versa. Hence, for $G(x) = 0$ and $|y - s_0(x)|$ small enough the maps $(\tilde{I})_{h,0}$ (i.e., the RKM applied to the index-1 formulation of Eq. (13)) and $(\tilde{I})_{h,0}$ create the same $(\tilde{x}, \tilde{y})$ and therefore the same orbit. Moreover, $G(x_j) = 0$ for all $j \geq 0$. Summarizing (cf. Theorem 1), we have the existence of an invariant manifold for the map $(\tilde{I})_{h,0}$

$$\overline{M}_{h,0} = \{(x, y) | G(x) = 0, y = \sigma_0(x, h)\}$$

which is attractive in $y$-direction and satisfies $\sigma_0(x, h) = s_0(x) + O(h^{q+1})$. (Again, $\overline{M}_{h,0} = \overline{M}_0 (y = s_0(x))$ if $a_{s_i} = b_i, i = 1, \ldots, s$.) Hence, for linear $G$ and $x$-starting value such that $G(x) = 0$ it does not matter if we approximate numerically by an appropriate RKM the index-2 problem $(\tilde{I})_{h,0}$ or its index-1 formulation (13).

ii) The general case: For RKMs applied to Eq. (13) which satisfy Hypothesis $H_{RKM}$ and $a_{s_i} = b_i, i = 1, \ldots, s$, we are also able to prove the existence of an attractive invariant (‘index-1’) manifold. This is done by first extending the RKM-map to all $\mathbb{R}^m$, applying the invariant manifold theorems of [5] to this altered map and then taking the restriction to the subspace $G(x) = 0$. The result is given in Theorem 4 below and is sketched in Fig. 7.
Fig. 7: The invariant manifolds of Eq. (I)₀ and of the RKM-map (I)ₜ₀ with \( a_{s_i} = b_i, \ i = 1, \ldots, s \)

**Theorem 4** Let Eq. (I)₀ satisfy Hypothesis \( \Pi₀ \), apply a RKM satisfying Hypothesis \( \Pi_{\text{RKM}} \) and \( a_{s_i} = b_i, \ i = 1, \ldots, s \), and assume \( r < p \).

Then there exist positive constants \( h₀, \gamma, K \) and a function \( \sigma₀ : \mathbb{R}^m \times (0, h₀] \rightarrow \mathbb{R}^n \), of class \( C^r \) with respect to \( x \), such that for \( h \leq h₀ \) the following assertions hold.

i) The set \( \overline{M}_{h₀} = \{(x, y) \mid G(x) = 0, y = \sigma₀(x, h)\} \) is an invariant manifold for the RKM-map \((I)_{h₀}\).

ii) \( \overline{M}_{h₀} \) is ‘infinitely attractive’, i.e., \( (x, y) \in \{(G(x) \leq \gamma h^2 \times \mathbb{R}^n \) implies for the image \((\bar{x}, \bar{y})\) under \((I)_{h₀}\)

\[
G(\bar{x}) = 0, \quad \bar{y} = \sigma₀(\bar{x}, h) .
\]

iii) \( \overline{M}_{h₀} \) has a vertical stable foliation implying the existence of an ‘asymptotic phase’ orbit \((\hat{x}_j, \hat{y}_j)\) with \( \hat{x}_j = x_j, \ j \geq 0, \) and \( \hat{y}_j = y_j = \sigma₀(x_j, h), \ j \geq 1. \)

iv) Closeness to \( \overline{M}_0 \):

\[
|\sigma₀(x, h) - s₀(x)| \leq Kh^q .
\]

**Proof:** i), ii), iii) For \( x \in \mathbb{R}^m \) we consider

\[
X = \mathbf{1}_s \otimes x + h (A \otimes I_m) f(X, Y) \\
G(X) = \mathbf{1}_s \otimes G(x)
\]

(16)

\[
\bar{x} = x + h (b^T \otimes I_m) f(X, Y) \\
\bar{y} = (1 - b^T A^{-1} \mathbf{1}_s) y + (b^T A^{-1} \otimes I_n) Y .
\]
By means of Lemma 3 with $\Delta \equiv 0$ we know that Eq. (16) describes a well defined map from $\mathbb{R}^m \times \mathbb{R}^n$ into itself. Introducing $z$ by $y = s_0(x) + z$ and $Z$ by $Y = s_0(X) + Z$, this map has the form

$$\bar{x} = x + h(b^T \otimes I_m) f(X, s_0(X) + Z) \quad (17)$$

$$\bar{z} = R(\infty) z + (b^T A^{-1} \otimes I_n) Z + (b^T A^{-1} \otimes I_n)(s_0(X) - I_s \otimes s_0(x)) + s_0(x) - s_0(\bar{x}).$$

By means of Lemma 3 and since $R(\infty) = 0$ by Hypothesis H$_{\text{RKM}}$ and $a_{s_i} = b_i$, $i = 1, \ldots, s$, we have for every $d > 0$ that for $h$ small enough Eq. (17) defines a smooth map from $\mathbb{R}^m \times \mathbb{R}^n \cap \{ |z| \leq d \}$ into itself. We apply the invariant manifold theorems of [5] to this map of the form

$$\bar{x} = x + hF_1(x, h)$$

$$\bar{z} = F_2(x, h).$$

In the domain considered, $F_1$ is invertible with respect to $x$, i.e., for every $\bar{x}, z$ there is $x$ such that $\bar{x} = F_1(x, z, h)$. For the ‘lower’ Lipschitz constant of $F_1$ with respect to $x$ we find $G_{11} = 1 + O(h)$. For the Lipschitz constant of $F_1$ with respect to $z$ we have $L_{12} = 0$. For $F_2$ we have $L_{21} = O(h)$ and $L_{22} = |R(\infty)| = 0$. Hence, the conditions $B_1, B_2, B3(r)$ of [5] are satisfied and we obtain the existence of an $m$-dimensional invariant manifold $M_{h,0} = \{(x, y) \mid x \in \mathbb{R}^m, y = \sigma_0(x, h)\}$ for the map (16).

Now restricting the map (16) to the subspace $G(x) = 0$ it follows immediately since $a_{s_i} = b_i$, $i = 1, \ldots, s$, that this subspace is positively invariant under (16). On the other hand, since in Eq. (16) $G(X) = I_s \otimes G(x)$ there is for every $\bar{x}$ with $G(\bar{x}) = 0$ a pre-image $x$ with $G(x) = 0$ obtained by iteration of $x^{\ell+1} = \bar{x} - h(b^T \otimes I_m) f(X(x^\ell, h), Y(x^\ell, h))$, $\ell \geq 0$, $x^0 = \bar{x}$. Hence, we have shown the existence of the invariant manifold

$$\overline{M}_{h,0} = \{(x, y) \mid G(x) = 0, y = \sigma_0(x, h)\} \subset M_{h,0}.$$

From Lemma 3 we know that for a starting value $(x_0, y_0)$ with $G(x_0) = h^2 \Delta_0$ the RKM-image $(x_1, y_1)$ exists. Due to $a_{s_i} = b_i$, $i = 1, \ldots, s$, we have $G(x_1) = 0$. Due to $R(\infty) = 0$ and $L_{12} = 0$ we have $y_1 = \sigma_0(x_1, h)$. Together this gives an infinite attractivity to $\overline{M}_{h,0}$.

The smoothness of $\sigma_0$ as well as the foliation of $M_{h,0}$ follows from the invariant manifold results applied to Eq. (17). Due to $L_{12} = 0$ the foliation is vertical and the asymptotic phase orbit therefore satisfies $\dot{x}_j = x_j$, $j \geq 0$. Due to the infinite attractivity in $y$-direction we also have $\dot{y}_j = y_j = \sigma_0(x_j, h)$, $j \geq 1$. Hence, we have shown Assertions i), ii), iii) of the theorem.

iv) For the closeness of $M_{h,0}$ to $M_0$ we have to estimate the right-hand side of the $z$-equation of (17). We consider the nonstiff equation $\dot{u} = f(u, s_0(u))$ with initial condition $u(0) = x$. Applying the given RKM with $u_0 = u(0)$ we obtain

$$U = I_s \otimes x + h(A \otimes I_m) f(U, s_0(U))$$

$$\bar{u} = x + h(b^T \otimes I_m) f(U, s_0(U)).$$

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Taking into account the \(x\)-equation of (17) (with the corresponding \(X\)-equation) we therefore find

\[(18) \quad X - U = O(h)Z \quad \text{and} \quad \bar{x} - \bar{u} = O(h)Z.\]

Taking the \(z\)-equation of (17) and adding zero appropriately we have

\[
\tilde{z} = R(\infty)z + (b^T A^{-1} \otimes I_n)Z \\
+ (b^T A^{-1} \otimes I_n)(s_0(X) - s_0(U)) + s_0(\bar{u}) - s_0(\bar{x}) \\
+ (b^T A^{-1} \otimes I_n)(s_0(U) - \mathds{1} \otimes s_0(x)) + s_0(x) - s_0(\bar{u}).
\]

As seen in Paragraph 2.1 the last two terms together can be studied via the singularly perturbed case of \([6]\) and the limit \(\varepsilon \to 0\) yields the estimate \(O(h^{q+1})\). Thus, we have together with Eq. (18)

\[
\tilde{z} = R(\infty)z + O(1)Z + O(h^{q+1}).
\]

It remains to estimate \(|Z|\). Taking the components we have taking into account the solution \((x(t), y(t) = s_0(x(t)))\) of Eq. (11) at the \(t\)-values \(c_i h\)

\[
Z_i = Y_i - s_0(X_i) = Y_i - s_0(x(c_i h)) + s_0(x(c_i h)) - s_0(X_i), \quad i = 1, \ldots, s.
\]

From [2], Lemma 4.3 and proof (cf. also [4], Lemma 7.4) we have the ‘local error’ estimates

\[
X_i - x(c_i h) = O(h^{q+1}), \quad Y_i - y(c_i h) = O(h^q), \quad i = 1, \ldots, s,
\]

implying \(Z_i = O(h^q)\). Hence, we have \(\tilde{z} = R(\infty)z + O(h^q)\) and the invariant manifold results of [5] give the assertion claimed.

\(\square\)

**Remark 9:** Having an estimate for the global error of the \(x\)-component which is at least \(O(h^{q+1})\) for \(jh \leq \text{const}\) (see, e.g., the results in [2] or [4]) we may estimate for the \(y\)-component for \(j \geq 1\)

\[
|y_j - y(jh)| \leq |y_j - \sigma_0(x_j, h)| + |\sigma_0(x_j, h) - s_0(x_j)| \\
+ |s_0(x_j) - s_0(x(jh))| + |s_0(x(jh)) - y(jh)|
\]

where \((x(t), y(t))\) is a solution of (11) with \(|x_0 - x(0)| \leq \gamma h^2\). The first and the last term on the right-hand side are zero due to the infinite attractivity in \(y\)-direction of \(M_{h,0}\) and \(M_0\), respectively, the third term is of the order of \(|x_j - x(jh)|\). Hence, we have

\[
|y_j - y(jh)| \leq |\sigma_0(x_j, h) - s_0(x_j)| + K |x_j - x(jh)|
\]

and the \(x\)-estimate together with Assertion iv) of the theorem give an estimate \(O(h^q)\) for the \(y\)-component.

\(\square\)

In the case of general RKMs (i.e., \(b_i \neq a_{si}\) for at least one \(i \in \{1, \ldots, s\}\) and Hypothesis \(H_{RKM}\)) we are not able to prove the existence of an index-2 manifold. The \(y\)-attractive index-1 manifold \(M_{h,0}(y_0 = \sigma_0(x, h))\), however, exists in the following sense. If the
RKM orbit is started with $x$ such that $G(x) = O(h^2)$ then the orbit $(x_j, y_j)$ approaches exponentially the manifold $M_{h,0}$ which is $O(h^q)$-close to $M_0$. This holds for all $j > 0$ such that $|G(x_j)| \leq \gamma h^2$ for a given $\gamma > 0$.

b) LMMs. For LMMs applied to Eq. (11) we have (cf. [4])

$$
\sum_{i=0}^{k} \alpha_i x_i = h \sum_{i=0}^{k} \beta_i f(x_i, y_i) \\
0 = G(x_k)
$$

(19)

with $\sum_{i=0}^{k} \alpha_i = 0$, $\alpha_k = 1$, $\beta_k \neq 0$ by Hypothesis $H_{LMM}$. The existence of a unique solution $(x_k, y_k)$ for $h$ small enough follows from Lemma 5 below. As in the RKM case (cf. Lemma 3) we again consider an altered system (Eq. (20)) and thus obtain the existence of a solution of Eq. (19) for $x_i$-values in an $O(h^2)$-neighbourhood of $G(x) = 0$.

**Lemma 5** Let the $x$-starting values satisfy $|x_i - x_\ell| \leq \text{const} \cdot h$ for $i, \ell = 0, \ldots, k - 1$, and let $\Delta : \mathbb{R}^{kn} \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$ be a bounded function of class $C^r_0$.

Then, there are positive constants $h_1, d, K$ such that for $h \leq h_1$ and for $|y_k - s_0(x_i)| \leq d$, $i = 0, \ldots, k - 1$, the nonlinear system

$$
\sum_{i=0}^{k} \alpha_i x_i = h \sum_{i=0}^{k} \beta_i f(x_i, y_i) \\
G(x_k) = -\sum_{i=0}^{k-1} G(x_i) - h^2 \Delta(x_0, \ldots, x_{k-1}; h)
$$

(20)

has a unique solution $(x_k, y_k)(x_0, \ldots, x_{k-1}; y_0, \ldots, y_{k-1}; h), C^r_0$ with respect to the $x$- and $y$-arguments, satisfying

$$
|x_k + \sum_{i=0}^{k-1} \alpha_i x_i| \leq K(h + |\beta|d)
\quad \text{and} \quad
|y_k - s_0(-\sum_{i=0}^{k-1} \alpha_i x_i)| \leq K(h + |\beta|d)
$$

**Proof:** The second equation of (20) is equivalent to

$$
0 = \sum_{i=0}^{k-1} \alpha_i [G(x_k) - G(x_i)] - h^2 \Delta
$$

(21)

where we have skipped the arguments of $\Delta$ for short. We may write

$$
\sum_{i=0}^{k-1} \alpha_i [G(x_k) - G(x_i)] = \sum_{i=0}^{k-1} \alpha_i \int_0^1 G_x(x_i + \tau(x_k - x_i))d\tau \cdot (x_k - x_i)
$$

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Moreover, multiplying the first equation of (20) from the left by \( G_x(x_k) \) yields with \( \sum_{i=0}^{k-1} \alpha_i = -1 \)
\[
\sum_{i=0}^{k-1} \alpha_i G_x(x_k) x_i - \sum_{i=0}^{k-1} \alpha_i G_x(x_k) x_k = h \sum_{i=0}^{k} \beta_i G_x(x_k) f(x_i, y_i).
\]

Adding this equation to (21) and dividing by \( h^2 \) we thus obtain
\[
\frac{1}{h^2} \sum_{i=0}^{k} \beta_i G_x(x_k) f(x_i, y_i) = \frac{1}{h^2} \sum_{i=0}^{k-1} \alpha_i \int_0^{1} [G_x(x_i + \tau(x_k - x_i)) - G_x(x_k)] d\tau \cdot (x_k - x_i) - \Delta
\]
\[
=: Q(x_0, \ldots, x_k; h).
\]

We estimate
\[
x_k - x_i = x_k + \sum_{\ell=0}^{k-1} \alpha_{\ell} x_\ell + \sum_{\ell=0}^{k-1} \alpha_{\ell}[x_i - x_\ell] = O(h)
\]

by means of the first equation (20) and by our assumption on \( |x_i - x_\ell| \). We therefore conclude that the function \( Q \) is bounded. It remains to show that the nonlinear system
\[
x_k = -\sum_{i=0}^{k-1} \alpha_i x_i + h \sum_{i=0}^{k} \beta_i f(x_i, y_i)
\]
\[
(22) \quad \beta_k G_x(x_k) f(x_k, y_k) = -\sum_{i=0}^{k-1} \beta_i G_x(x_i) f(x_i, y_i) + hQ(x_0, \ldots, x_k; h)
\]

has a unique solution \((x_k, y_k)\) near \((-\sum_{i=0}^{k-1} \alpha_i x_i, s_0(-\sum_{i=0}^{k-1} \alpha_i x_i))\). We introduce the variables \( z_i \) by \( y_i = s_0(x_i) + z_i, \ i = 0, \ldots, k, \) with \( |z_i| \leq d_i \) small enough, the Newton-Kantorovich theorem implying for \( h \) and \( |\beta|d \) sufficiently small the existence of a unique solution \((x_k, y_k)(x_0, \ldots, x_{k-1}; y_0, \ldots, y_{k-1}; h)\) satisfying \( |x_k + \sum_{i=0}^{k-1} \alpha_i x_i| \leq \text{const} \cdot (h + |\beta|d), \ |z_k| \leq \text{const} \cdot (h + |\beta|d) \) (cf. [7]). The smoothness follows from the implicit function theorem.

\[ \square \]

Remark 10): i) For \( x_i, i = 0, \ldots, k - 1, \) such that \(-\sum_{i=0}^{k-1} \alpha_i G(x_i) = h^2 \Delta, \) Lemma 5 corresponds to Theorem 6.1 of [4]. With our type of proof we do not need their assumption \( y_i - y(ih) = O(h), i = 0, \ldots, k - 1, \) but only \( |y_i - s_0(x_i)| \leq d, d \) small enough (if \( \beta \neq 0 \)). If we choose the \( y_i \) such that \( y_i - s_0(x_i) = O(h), i = 0, \ldots, k - 1, \) we have
\[
|x_k + \sum_{i=0}^{k-1} \alpha_i x_i| \leq Kh, \quad |y_k - s_0(x_k)| \leq Kh
\]
as in [4]. For BDF-like methods, i.e., \( \beta = 0 \) in Eq. (19) this estimate holds independently of the \( y \)-starting values \( y_i \). In this case, there is no restriction on the \( y \) and the solution \((x_k, y_k)\) does not depend on the \( y \)-starting values \( y_i \) at all.
ii) In [4] also LMMs with 
\[ 0 = \sum_{i=0}^{k} \beta_i G(x_i) \] as second equation (in Eq. (19)) are considered. Lemma 5 yields a solution \((x_k, y_k)\) of such a method for \(x\)-starting values \(x_i\) such that 
\[ -\sum_{i=0}^{k-1} (\alpha_i - \frac{\beta_i}{\beta_k}) G(x_i) = h^2 \Delta. \]

In the linear case, it is again easy to verify that the maps \((I)_{h,0}\) and \((\overline{I})_{h,0}\) create the same orbit if \(G(x_i) = 0, i = 0, \ldots, k - 1\), implying the existence of the \(y\)-attractive invariant manifold \(M_0 = \{(x, y) \mid G(x) = 0, y = s_0(x)\}\) (for \(\beta = 0 \text{ and } \beta \neq 0\) with the properties already derived in Paragraph 3.1 for \((I)_{h,0}\).

In the nonlinear case we consider for \(\beta = 0\) (BDF-like methods)

\[ \sum_{i=0}^{k} \alpha_i x_i = h \beta_k f(x_k, y_k) \]

\[ G(x_k) = \sum_{i=0}^{k-1} \alpha_i G(x_i) \, . \]

For \(z_k\) defined by \(y_k = s_0(x_k) + z_k\) we know from the proof of Lemma 5 (with \(\Delta \equiv 0\)) that the solution \((x_k, z_k)(x_0, \ldots, x_{k-1}; h)\) of Eq. (23) satisfies

\[ x_k = -\sum_{i=0}^{k-1} \alpha_i x_i + h \beta_k f(x_k, s_0(x_k) + z_k) \]

\[ z_k = h \overline{Q}(x_0, \ldots, x_{k-1}; h) \]

with \(\overline{Q} = O(|Q|)\) (cf. Eq. (22) for \(\beta = 0\)). For every \(x_0 \in \mathbb{R}^m\) and \(\gamma > 0\) the function \(\overline{Q}\) is bounded and of class \(C^r_0\) with respect to \(x_0, \ldots, x_{k-1}\) if \(|x_i - x_0| \leq \gamma h, i = 1, \ldots, k - 1\). We extend \(\overline{Q}\) to all \(\mathbb{R}^{km}\) by modifying it in the following way: Inside the tube \(\Omega_{\gamma/2} = \{X_0 \in \mathbb{R}^{km} \mid x_0 \in \mathbb{R}^m, |x_i - x_0| \leq \frac{\gamma}{2} h, i = 1, \ldots, k - 1\}\) we put \(\hat{Q} := \overline{Q}\), outside the tube \(\Omega\) we put \(\hat{Q} = 0\) and, in between, \(\hat{Q}\) is taken such that it is \(C^r_0\). The first equation of (24) may be considered for all \(X_0 \in \mathbb{R}^{km}\). Hence, for \(d\) and \(h\) small enough we have a smooth map from \(\mathbb{R}^{km} \times \{Z \in \mathbb{R}^{km} \mid |Z|_\infty \leq d\}\) into itself of the form

\[ X_1 = ((R - L_0) \otimes I_m) X_0 + h (\epsilon_k \otimes \hat{P}(X_0; h)) \]

\[ Z_1 = (R \otimes I_n) Z_0 + h (\epsilon_k \otimes \hat{Q}(X_0; h)) \, . \]

As done in [7] we apply the invariant manifold theory of [5] and the analogous construction yields the existence of an \(m\)-dimensional attractive invariant manifold for the modified map (25) (in the \(x, y\)-variables)

\[ M_{h,0} = \{(x, y) \mid x \in \mathbb{R}^m, y = \sigma_0(x, h)\} \]

if started appropriately, i.e., \(x_i = \Phi^i(x_0, h), i = 0, \ldots, k - 1\). The closeness to \(M_0\) is \(\sigma_0(x, h) - s_0(x) = O(h |\hat{Q}|) = O(h |Q|)\), the attractivity in \(y\)-direction is \(y_j - \sigma_0(x_j, h) = z_j + \sigma_0(x_j, h) - s_0(x_j) = O(h |\hat{Q}|)\) for \(j \geq k\) and \(x_{h,0}^k = 0\) if \(x_i = \Phi^i(x_0, h), i = 0, \ldots, k - 1,\)

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and $M_{h,0}$ has a vertical stable foliation ($L_{12}^{h,0} = 0$, since the $O(h)$-terms in Eq. (25) do not depend on $Z_0$). Since on $M_{h,0}$ we have $x_i = \Phi^i(x_0, h)$, $x_i - x_0 = O(h)$, $i = 0, \ldots, k - 1$, it follows that for $\gamma$ large enough, $M_{h,0}$ is an invariant manifold for the original map (24).

For the closeness of $M_{h,0}$ to $M_0$ we have to get a better estimate for the function $Q$ established in the proof of Lemma 5. This is done using similar techniques as for RKM. As seen in Paragraph 3.1 the solution $x(t)$ of Eq. $(\tilde{\Gamma})_0$ with $x(0) = x_0$ satisfies

$$
\sum_{i=0}^{k} \alpha_i G(x(ih)) - h \beta_k G(x(kh)) f(x(kh), s_0(x(kh))) = O(h^{p+1}) .
$$

Since $G(x(t)) = 0$, $t \geq 0$, we thus have together with

$$
h \beta_k G(x(kh)) f(x_k, s_0(x_k) + z_k) = h^2 Q(x_0, \ldots, x_k; h)
$$

that

$$
hQ = \beta_k \left[ G(x(kh)) f(x_k, s_0(x_k) + z_k) - G(x(kh)) f(x(kh), s_0(x(kh))) \right] + O(h^p) .
$$

The term in brackets is of order $O(|z_k| + O(|x_k - x(kh)|))$. We estimate

$$
z_k = y_k - s_0(x_k) = y_k - s_0(x(kh)) + s_0(x(kh)) - s_0(x_k) = y_k - y(kh) + O(|x_k - x(kh)|) .
$$

Since on $M_{h,0}$ we have $x_i = \Phi^i(x_0, h)$ with $x_i - x(ih) = O(h^{p+1})$, $i = 0, \ldots, k - 1$, it follows from the results in [4] that

$$
x_k - x(kh) = O(h^p), \quad y_k - y(kh) = O(h^p) ,
$$

implying $hQ = O(h^p)$.

Taking the restriction to the subspace $G(x) = 0$, i.e., taking $G(x_i) = 0$, $i = 0, \ldots, k - 1$, it follows from Eq. (23) that $G(x_k) = 0$ and, hence, that this subspace is positively invariant under the LMM-map. It is easy to see that this subspace is indeed invariant. Summarizing we have:

- Invariant manifold of $(\tilde{\Gamma})_{h,0}$:
  $$
  \overline{M}_{h,0} = \{ (x, y) \mid G(x) = 0, \ y = \sigma_0(x, h) \} \subset M_{h,0} .
  $$

- Closeness to $M_0$:
  $$
  |\sigma_0(x, h) - s_0(x)| = O(h^p) .
  $$

- Infinite attractivity in $x$-direction:
  $$
  \left| - \sum_{i=0}^{k-1} \alpha_i G(x_i) \right| \leq const \cdot h^2 \ \text{implies} \ \ G(x_j) = 0 \ \text{for} \ j \geq k .
  $$

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• Attractivity in $y$-direction:

\[ x_i = \Phi^i(x_0, h) \quad \text{for} \quad i = 0, \ldots, k - 1; \]

in any case,

\[ |y_j - \sigma_0(x_j, h)| \leq K h^p \quad \text{for} \quad j \geq k. \]

• Stable (vertical) foliation and asymptotic phase.

Remark 11: i) We have shown that also for LMMs with $\beta = 0$ the situation of Fig. 7 holds (if started appropriately) but with closeness $O(h^p)$ instead of $O(h^q)$.

ii) As for RKMs the global error estimate for the $x$-component which is $O(h^p)$ (cf. [4]) immediately gives the estimate $O(h^p)$ for the $y$-component by means of

\[ |y_j - y(jh)| \leq |\sigma_0(x_j, h) - s_0(x_j)| + K |x_j - x(jh)|. \]

\[ - \]

In the case of general LMMs (i.e., $\beta \neq 0$ in Eq. (19) and Hypothesis H_{LMM}) the same invariant manifold result holds as in the BDF-like case (cf. also [7]). The attractivity in $y$-direction is $|y_j - \sigma(x_j, h)| \leq K \chi_{h,0} \max_{0 \leq i < k} \{|y_i - \sigma_0(x_i, h)|\}$ for $j \geq k$ with $\chi_{h,0} = \max\{\rho_1, \sigma_1\} + O(\|\beta\|h) + O(h) < 1$ if $x_i = \Phi^i(x_0, h), i = 0, \ldots k - 1$. The stable fibers are not vertical anymore.

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