

Numerical integration of differential algebraic systems and invariant manifolds

K. Nipp

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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

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

satisfying

Hypothesis H_ε

- 1) f and g are bounded and there is r with $r \geq 2$ such that $f \in C_b^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $g \in C_b^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)$.
- 2) There is a function $s_0 \in C_b^r(\mathbb{R}^m, \mathbb{R}^n)$ such that $g(x, s_0(x)) = 0$ for $x \in \mathbb{R}^m$.

- 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_b^r 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_ε 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_b^r with respect to x and ε (for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, ε_0 small) and $s(x, 0) = s_0(x)$. M_ε is highly attractive, i.e.,

$$|y(t) - s(x(t), \varepsilon)| \leq K \chi_\varepsilon^t |y(0) - s(x(0), \varepsilon)|, \quad t \geq 0,$$

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

M_ε 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_ε such that the two trajectories tend to each other exponentially with rate χ_ε^t . The whole situation is sketched in Fig. 1.

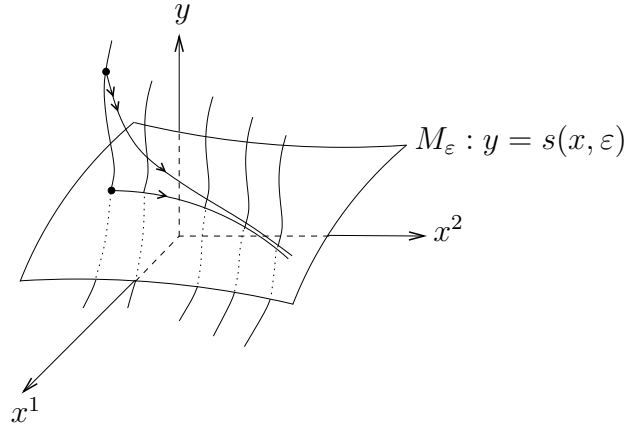


Fig. 1: The attractive invariant manifold M_ε of Eq. (1) $_\varepsilon$, stable foliation and 'asymptotic phase'

For RKMs 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 $\mathbb{1}_s := (1, \dots, 1)^T \in \mathbb{R}^s$, 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 RKMs with $a_{si} = b_i, i = 1, \dots, s$, this implies $R(\infty) = 0$. Under Hypothesis H_{RKM} the RKM

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

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 $X := (X_1, \dots, X_s)^T \in \mathbb{R}^{sm}$, $f(X, Y) := (f(X_1, Y_1), \dots, f(X_s, Y_s))^T \in \mathbb{R}^{sm}$, etc., \otimes denotes the Kronecker product.) In coordinates measuring the difference to M_ε

$$y = s(x, \varepsilon) + z, \quad Y = s(X, \varepsilon) + Z$$

this map may be written as (we often suppress the dependence of $s(x, \varepsilon)$ on ε for short)

$$(I)_{h,\varepsilon} \quad \begin{aligned} \bar{x} &= x + h(b^T \otimes I_m) f(X, s(X) + Z) \\ \bar{z} &= (R(\infty)I_n + O(\varepsilon/h))z + ((b^T A^{-1} \otimes I_n) + O(\varepsilon/h)) E - e \end{aligned}$$

where the stages X, Z satisfy

$$\begin{aligned} X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, s(X) + Z) \\ Z &= O(\varepsilon/h). \end{aligned}$$

The functions E and e are defined as

$$\begin{aligned} E(x, X) &:= s(X) - \mathbb{1}_s \otimes s(x) - \frac{h}{\varepsilon} (A \otimes I_n) g(X, s(X)) \\ e(x, \bar{x}, X) &:= s(\bar{x}) - s(x) - \frac{h}{\varepsilon} (b^T \otimes I_n) g(X, s(X)). \end{aligned}$$

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 σ of class C_b^r with respect to x and ε (also for $\varepsilon = 0$) and

$$\sigma(x, h, \varepsilon) = s(x, \varepsilon) + \begin{cases} O(h^{q+1}) \\ O(\varepsilon h^q), \text{ if } b_i = a_{si}, i = 1, \dots, s. \end{cases}$$

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 $L_{12}^{h,\varepsilon}$ of the right-hand side of the first equation of $(\tilde{I})_{h,\varepsilon}$ 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 ε/h small enough and for $jh \leq Nh = T$ fixed

$$(GE)_{h,\varepsilon} \quad \begin{aligned} x_j - x(jh) &= O(h^p) + O(\varepsilon h^{q+1}) + O(\varepsilon |y_0 - s(x_0, \varepsilon)|) \\ y_j - y(jh) &= O(h^{q+1}) + O((\varepsilon + \chi_{h,\varepsilon}^j) |y_0 - s(x_0, \varepsilon)|) \end{aligned}$$

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

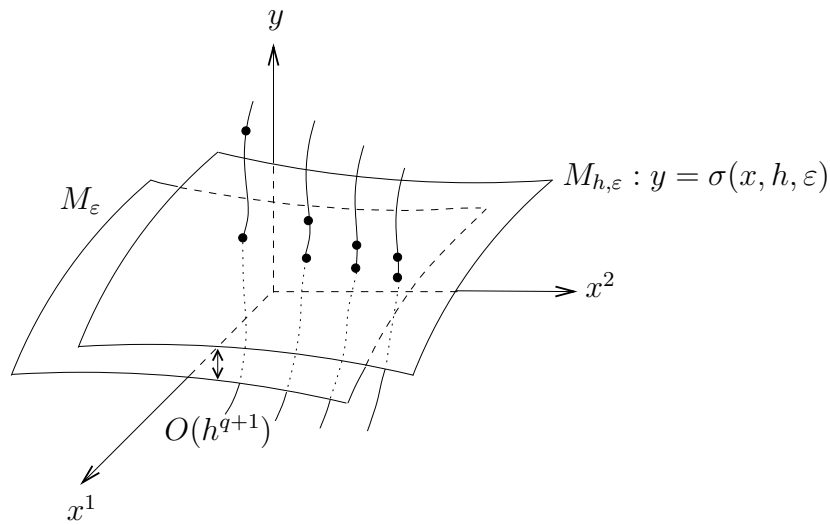


Fig. 2: The attractive invariant manifold $M_{h,\varepsilon}$ of the RKM-map $(I)_{h,\varepsilon}$, stable foliation and asymptotic phase and closeness to M_ε

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

$$\begin{aligned} \sum_{i=0}^k \alpha_i x_i &= h \sum_{i=0}^k \beta_i f(x_i, y_i) \\ \sum_{i=0}^k \alpha_i y_i &= \frac{h}{\varepsilon} \sum_{i=0}^k \beta_i g(x_i, y_i) \end{aligned} \quad , \quad \alpha_k = 1 ,$$

where (x_i, y_i) , $i = 0, \dots, k-1$, are given starting values. We make the following assumption.

Hypothesis H_{LMM}

- 1) The LMM is an irreducible k -step method of order $p \geq 1$.
- 2) The LMM is ρ_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 σ_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 $(\mathbf{I})_{h,\varepsilon}$ from $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ into itself. Defining $\alpha := (\alpha_0, \dots, \alpha_{k-1})^T \in \mathbb{R}^k$, $\beta := (\beta_0, \dots, \beta_{k-1})^T \in \mathbb{R}^k$ and

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

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

$$\begin{aligned} X_1 &= ((R - L_\alpha) \otimes I_m) X_0 + h(L_\beta \otimes I_m) f(X_0, s(X_0) + Z_0) \\ &\quad + h\beta_k(e_k \otimes f(x_k, s(x_k) + z_k)) \\ (\tilde{\mathbf{I}})_{h,\varepsilon} \quad Z_1 &= \left[(R \otimes I_n) - \frac{1}{\beta_k} (L_\beta \otimes I_n) + |\beta| O(\max_{0 \leq i < k} |x_i - x_0|) \right. \\ &\quad \left. + h + d + \varepsilon/h + O(\varepsilon/h) \right] Z_0 + O(\varepsilon/h) \end{aligned}$$

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

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

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

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

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

$$M_{h,\varepsilon} = \{(x, y) \mid x \in \mathbb{R}^m, \quad y = \sigma(x, h, \varepsilon)\}$$

is invariant under the map $(I)_{h,\varepsilon}$ and is $O(\varepsilon h^p)$ -close to M_ε . 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 $\chi_{h,\varepsilon} = \rho_1 + O(h + \varepsilon/h) < 1$ and $y_j - \sigma(x_j, h, \varepsilon) = z_j + O(\varepsilon h^p) = O(\varepsilon/h)$ for $j \geq k$ as seen from $(\tilde{I})_{h,\varepsilon}$ giving the y -attractivity $\text{const} \cdot \varepsilon/h \cdot \chi_{h,\varepsilon}^j$, $j \geq k$. Again there exists a stable foliation ($L_{12}^{h,\varepsilon} = O(\varepsilon)$, i.e., '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 ε/h small enough and for $jh \leq T$ fixed:

$$\begin{aligned}
x_j - x(jh) &= O(h^p) + O(\max_{0 \leq i < k} \{|x_i - x(ih)|\}) \\
&+ O(h [\max_{0 \leq i < k} \{|y_i - y(ih)|\} + |y_0 - s(x_0, \varepsilon)|]) \\
(\text{GE})_{h,\varepsilon} \quad y_j - y(jh) &= O(h^p) + O(\max_{0 \leq i < k} \{|x_i - x(ih)|\}) \\
&+ O((h + \chi_{h,\varepsilon}^j) [\max_{0 \leq i < k} \{|y_i - y(ih)|\} + |y_0 - s(x_0, \varepsilon)|]) .
\end{aligned}$$

For $\beta = 0$ the factor h in the x -equation is replaced by ε and the factor $(h + \chi_{h,\varepsilon}^j)$ 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_ε), its invariant manifold by M_ε with attractivity χ_ε^t and 'steepness' of the stable fibers L_{12}^ε . 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 $(\text{GE})_{h,\varepsilon}$. If we consider the variable z (instead of y) measuring the distance to M_ε we put a \sim on $(I)_{h,\varepsilon}$, i.e., we write $(\tilde{I})_{h,\varepsilon}$.

In the DAE case, we replace the ε by 0 for index 1: $(1)_0$ (satisfying Hypothesis H_0), M_0 , χ_0^t , L_{12}^0 ; $(I)_{h,0}$, $M_{h,0}$, $\chi_{h,0}$, $L_{12}^{h,0}$, $(\text{GE})_{h,0}$ and $(\tilde{I})_{h,0}$. For index 2 we keep the notation but put a $\bar{}$ on top, i.e., $(\bar{1})_0$ (satisfying Hypothesis \bar{H}_0), \bar{M}_0 ; $(\bar{I})_{h,0}$, $\bar{M}_{h,0}$, etc. \dashv

2 Systems of index 1

Consider the DAE

$$\begin{aligned}
(1)_0 \quad \dot{x} &= f(x, y) \\
0 &= g(x, y)
\end{aligned}$$

satisfying

Hypothesis H_0

- 1) f and g are bounded and $f \in C_b^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $g \in C_b^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)$ for $r \geq 2$.
- 2) There is a function $s_0 \in C_b^r(\mathbb{R}^m, \mathbb{R}^n)$ 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 Ω_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 ($L_{12}^0 = 0$, 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 H₀ 3)).

ii) Note that in Hypothesis H₀ 3) we do not assume that $g_y(x, s_0(x))$ has eigenvalues with negative real part as we did in Hypothesis H_ε 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)_ε in the case of H₀ 3) which is hyperbolic, however, all assertions of Section 2 hold under Hypothesis H₀ 3). In this case, for the global error of RKMs and LMMs applied to Eq. (1)_ε one has to consider solutions of (1)_ε on M_{ε} , however. ⊥

2.1 RKMs

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

a) *The indirect approach.* The RKM

$$\begin{aligned} X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\ 0 &= g(X, Y) \\ \bar{x} &= x + h(b^T \otimes I_m) f(X, Y) \\ 0 &= g(\bar{x}, \bar{y}) \end{aligned}$$

is, due to Hypothesis H₀, 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)_ε and (I)_{h,ε} and putting $\varepsilon = 0$. For the RKM assume Hypothesis H_{RKM}. If we put $\varepsilon = 0$ in Hypothesis H_ε, in the differential equation (1)_ε and in the map $(\tilde{I})_{h,\varepsilon}$, in the invariant manifolds M_{ε} and $M_{h,\varepsilon}$, in the attractivity constants χ_{ε}^t and $\chi_{h,\varepsilon}$, and in the Lipschitz constants L_{12}^{ε} and $L_{12}^{h,\varepsilon}$ we obtain Hypothesis H₀, Eq. (1)₀, the map

$$\begin{aligned} X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, s_0(X) + Z) \\ 0 &= Z \\ (\tilde{I})_{h,0} \quad \bar{x} &= x + h(b^T \otimes I_m) f(X, s_0(X) + Z) \\ \bar{z} &= (1 - b^T A^{-1} \mathbb{1}_s) z + (b^T A^{-1} \otimes I_n) E_0 - e_0 \end{aligned}$$

where $E_0 := s_0(X) - \mathbb{1}_s \otimes s_0(x)$, $e_0 := s_0(\bar{x}) - s_0(x)$, and the invariant manifolds M_0 with attractivity $\chi_0^t = 0$ 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 Ω_d) the RKM-map has the form

$$(I)_{h,0} \quad \begin{aligned} X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\ O &= g(X, Y) \\ \bar{x} &= x + h(b^T \otimes I_m) f(X, Y) \\ \bar{y} &= (1 - b^T A^{-1} \mathbb{1}_s) y + (b^T A^{-1} \otimes I_n) Y \end{aligned}$$

considered in [2] and [4]. The global error $(GE)_{h,0}$ of $(I)_{h,0}$ is also obtained from $(GE)_{h,\varepsilon}$ 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)₀ satisfy Hypothesis H_0 , apply a RKM satisfying Hypothesis H_{RKM} and assume $r < p$.*

Then there exist positive constants d, h_0, K and a function $\sigma_0 : \mathbb{R}^m \times (0, h_0] \rightarrow \mathbb{R}^n$, of class C_b^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 Ω_d the invariant manifold $M_{h,0}$ is attractive with attractivity constant $\chi_{h,0} = |R(\infty)|$, i.e.,*

$$|\bar{y} - \sigma_0(\bar{x}, h)| \leq \chi_{h,0} |y - \sigma_0(x, h)|$$

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

$$\begin{aligned} \hat{x}_j &= x_j \\ |\hat{y}_j - y_j| &\leq K \chi_{h,0}^j |y_0 - \sigma_0(x_0, h)| \end{aligned}$$

for $j \in \mathbb{N}_0$.

iv)

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

with σ_0 of class C_b^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

$$(GE)_{h,0} \quad \begin{aligned} |x_j - x(jh)| &\leq K h^p \\ |y_j - y(jh)| &\leq K(h^{q+1} + \chi_{h,0}^j |y_0 - s_0(x_0)|) \end{aligned}$$

for $jh \leq T$.

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

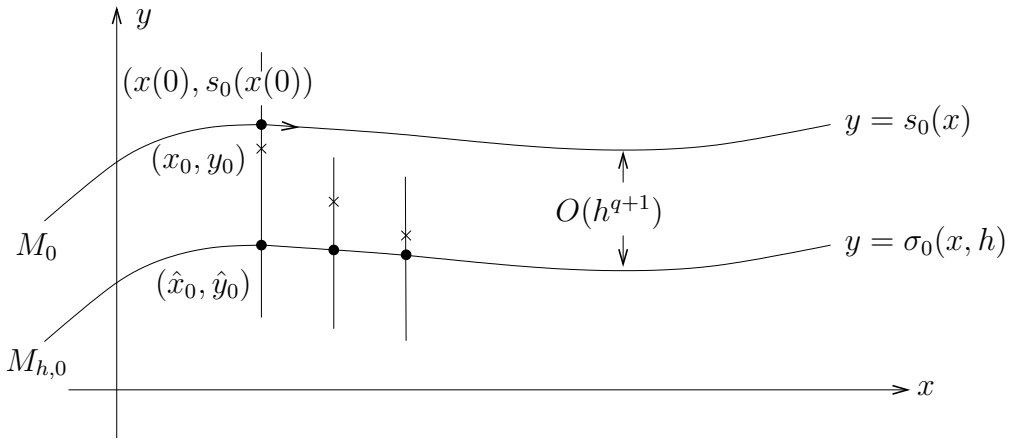


Fig. 3: The invariant manifolds for the DAE (1)₀ and the RKM-map (I)_{h,0}

Remark 2): In the case where the RKM satisfies $a_{s_i} = b_i$, $i = 1, \dots, s$ (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

$$(GE)_{h,0} \quad \begin{aligned} |x_j - x(jh)| &\leq K h^p \\ |y_j - y(jh)| &\leq K h^p \end{aligned} , \quad jh \leq T .$$

For $a_{s_i} = b_i$, $i = 1, \dots, s$, the direct and the indirect approach are identical. \dashv

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) _{ε} 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 $(\tilde{I})_{h,0}$. 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.

$$\begin{array}{ccc}
(1)_\varepsilon; & \varepsilon \dot{y} & (1)_0; \\
M_\varepsilon, \chi_\varepsilon^t, L_{12}^\varepsilon & \varepsilon = 0 \dashrightarrow & M_0, \chi_0^t, L_{12}^0 \\
\text{RKM} \downarrow & & \downarrow \text{RKM} \\
(I)_{h,\varepsilon}; & \varepsilon = 0 & (I)_{h,0}; \\
M_{h,\varepsilon}, \chi_{h,\varepsilon}, L_{12}^{h,\varepsilon}; (\text{GE})_{h,\varepsilon} & & M_{h,0}, \chi_{h,0}, L_{12}^{h,0}; (\text{GE})_{h,0}
\end{array}$$

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 RKMs 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)

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

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 $j \leq N$:

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

Remark 3): For $\beta = 0$ (BDF-like methods, corresponding to $a_{s_i} = b_i$, $i = 1, \dots, s$, 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, \dots, y_{k-1} (this is easily seen from $(\tilde{\mathbf{I}})_{h,0}$ with $\beta = 0$).
- Global error for $j \leq N$:

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

–

3 Systems of index 2

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

$$\begin{aligned}
 (\bar{\mathbf{I}})_0 \quad \dot{x} &= f(x, y) \\
 0 &= G(x)
 \end{aligned}$$

satisfying

Hypothesis $\bar{\mathbf{H}}_0$

- 1) f is bounded and $f \in C_b^{r+1}(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $G \in C_b^{r+1}(\mathbb{R}^m, \mathbb{R}^n)$, $r \geq 2$.
- 2) There is a function $s_0 \in C_b^r(\mathbb{R}^m, \mathbb{R}^n)$ 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. $(\bar{\mathbf{I}})_0$ 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 $\bar{\mathbf{H}}_0$. 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 Ω_d of the index-1 DAE (the so-called index-1 formulation of the index-2 problem $(\bar{\mathbf{I}})_0$)

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

lie in the m -dimensional surface

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

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

$$\int_0^t G_x(x(\tau)) f(x(\tau), s_0(x(\tau))) d\tau = 0$$

implying

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

This means that Eq. (1)₀ has G as first integral. The manifold

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

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

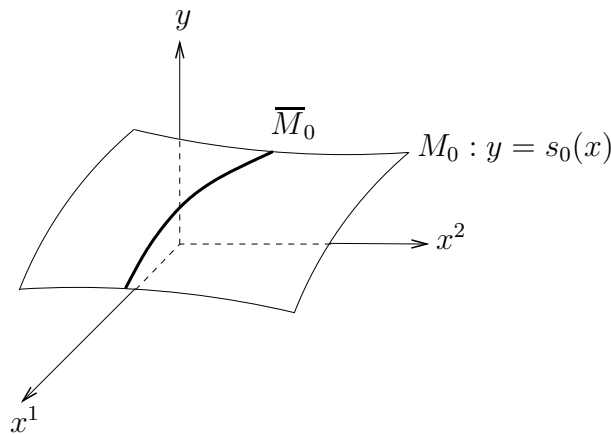


Fig. 5: The invariant manifold \bar{M}_0 of Eq. $(\bar{1})_0$

Remark 4): Note that every manifold $\bar{M}_0^{const} := \{(x, y) \mid G(x) = const, y = s_0(x)\}$ is invariant under Eq. (1)₀ and lies in M_0 , i.e., the m -dimensional surface M_0 consists of submanifolds \bar{M}_0^{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_{RKM} or a LMM satisfying Hypothesis H_{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)_ε, (I)_{h,ε} and (I)_{h,0}, respectively, also possess a ‘first integral’, i.e., a submanifold of $M_ε$, $M_{h,ε}$ and $M_{h,0}$, respectively.

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

$$\begin{aligned} \dot{x} &= f(x, s(x, \varepsilon)) \\ \varepsilon s_x(x, \varepsilon) f(x, s(x, \varepsilon)) &= g(x, s(x, \varepsilon)) . \end{aligned}$$

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

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

Of course, again any set

$$\bar{M}_\varepsilon^{const} = \{(x, y) \mid G(x) - \varepsilon s(x, \varepsilon) = const, y = s(x, \varepsilon)\} \subset M_\varepsilon$$

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

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

This implies the existence of the invariant manifold

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

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

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

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

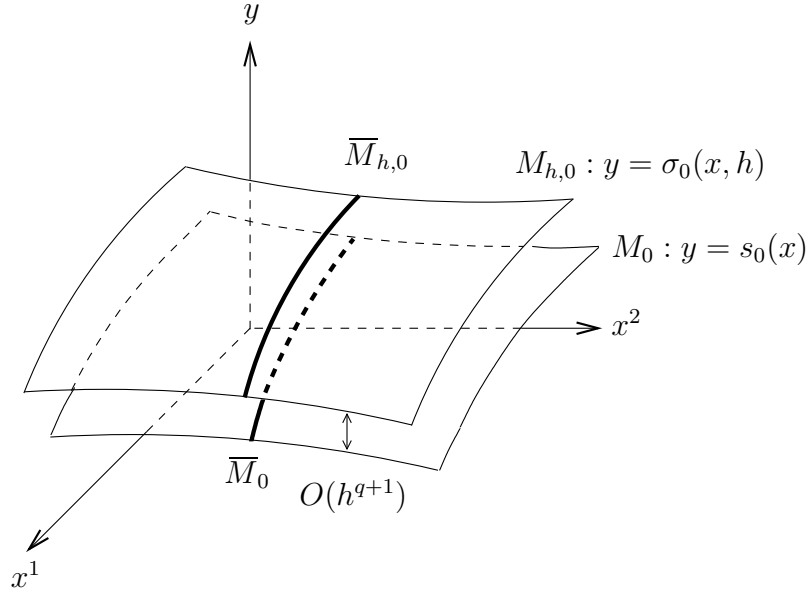


Fig. 6: The manifolds \bar{M}_0 and M_0 of Eq. (1)₀ and the invariant manifolds $\bar{M}_{h,0}$ and $M_{h,0}$ of the RKM-map (I)_{h,0} for $G(x) = Bx + c$

For RKMs 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 \bar{M}_0 , \bar{M}_ε , $\bar{M}_{h,\varepsilon}$ and $\bar{M}_{h,0}$, respectively, are added into the picture.

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

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

$$(2) \quad \begin{aligned} \bar{x} - x &= h \sum_{i=1}^s b_i f(X_i, Y_i) \\ \varepsilon [\sigma(\bar{x}) - \sigma(x)] &= h \sum_{i=1}^s b_i G_x(X_i) f(X_i, Y_i) \end{aligned}$$

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

$$(3) \quad Q(x; h, \varepsilon) := G(\bar{x}) - G(x) - h \sum_{i=1}^s b_i G_x(X_i) f(X_i, Y_i) .$$

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 $j \geq 1$

$$(4) \quad G(x_j) - \varepsilon \sigma(x_j, h, \varepsilon) = \sum_{\ell=0}^{j-1} Q(x_\ell; h, \varepsilon) + \Delta_0 .$$

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

$$(5) \quad G(x(h)) - G(x_\ell) = \int_0^h G_x(x(\tau)) f(x(\tau), y(\tau)) d\tau .$$

From the definition of Q we have

$$(6) \quad G(x_{\ell+1}) - G(x_\ell) = h \sum_{i=0}^s b_i G_x(X_i) f(X_i, Y_i) + Q(x_\ell; h, \varepsilon)$$

where X_i, Y_i are functions of x_ℓ, h and ε . From Eqs. (3) and (6) we obtain

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

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

$$\begin{aligned} x_{\ell+1} - x(h) &= O(h^{p+1}) + O(\varepsilon h^{q+1}) + O(\varepsilon |\sigma(x_\ell) - s(x_\ell)|) \\ &= O(h^{p+1}) + O(\varepsilon h^{q+1}) . \end{aligned}$$

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

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

$$(7) \quad \begin{aligned} u(c_i h) - u_0 &= h \sum_{j=1}^s a_{ij} f(u(c_j h), s(u(c_j h))) + O(h^{q+1}), \quad i = 1, \dots, s, \\ u(h) - u_0 &= h \sum_{i=1}^s b_i f(u(c_i h), s(u(c_i h))) + O(h^{p+1}) \end{aligned}$$

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.,

$$(8) \quad \begin{aligned} &\int_0^h G_x(u(\tau)) f(u(\tau), s(u(\tau))) d\tau = \\ &= h \sum_{i=1}^s b_i G_x(u(c_i h)) f(u(c_i h), s(u(c_i h))) + O(h^{p+1}) . \end{aligned}$$

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

$$P_1 - P_2 = P_1 - \bar{P}_1 + \bar{P}_1 - \bar{P}_2 + \bar{P}_2 - P_2$$

where

$$\begin{aligned} \bar{P}_1 &:= h \sum_{i=1}^s b_i G_x(U_i) f(U_i, s(U_i)) \\ \bar{P}_2 &:= h \sum_{i=1}^s b_i G_x(u(c_i h)) f(u(c_i h), s(u(c_i h))) . \end{aligned}$$

We have

$$\begin{aligned} P_1 - \bar{P}_1 &:= h O\left(\max_{1 \leq i \leq s} |X_i - U_i| + \max_{1 \leq i \leq s} |Z_i|\right), \\ \bar{P}_1 - \bar{P}_2 &:= h O\left(\max_{1 \leq i \leq s} |U_i - u(c_i h)|\right) \end{aligned}$$

and with (8)

$$\bar{P}_2 - P_2 = O(h^{p+1}) + h O\left(\max_{0 \leq t \leq h} |x(t) - u(t)| + \max_{0 \leq t \leq h} |z(t)|\right).$$

From [6] we know that

$$Z_i = O(\varepsilon h^q), \quad X_i - U_i = O(\varepsilon h^{q+1}), \quad i = 1, \dots, s.$$

The first relation of (7) implies

$$U_i - u(c_i h) = O(h^{q+1}), \quad i = 1, \dots, s,$$

and a simple Gronwall type argument yields

$$\max_{0 \leq t \leq h} |x(t) - u(t)| = h O\left(\max_{0 \leq t \leq h} |z(t)|\right).$$

For $z(t)$ we apply Theorems 1 and 3 of [6]:

$$\begin{aligned} z(t) &= x(t) - s(x(t)) = O(e^{-\text{const} \cdot t/\varepsilon} |y(0) - s(x(0))|) \\ &= O(|\sigma(x_\ell) - s(x_\ell)|) = O(h^{q+1}). \end{aligned}$$

Adding up, we finally have

$$Q(x_\ell; h, \varepsilon) = O(h^{q+2}).$$

(We have used the fact that the $\varepsilon \ll h$ and $q < p$ which cancels out the $O(h^{p+1})$ - and $O(\varepsilon h^{q+1})$ -terms). Hence, Eq. (4) implies for all $j \in \mathbb{N}$

$$(9) \quad G(x_j) - \varepsilon \sigma(x_j; h, \varepsilon) = \Delta_0 + jh \cdot O(h^{q+1})$$

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 $\bar{M}_{h,\varepsilon}$ has at worst a linear (in $t = jh$) 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 (GE) _{h,ε} 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. $(\bar{1})_0$ satisfy Hypothesis \bar{H}_0 , apply a RKM satisfying Hypothesis H_{RKM} to its ‘index-1 formulation’ $(1)_0$ and assume $r < p$. Consider for $\Delta_0 \in \mathbb{R}^n$ the set

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

with σ_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

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

for some constant K independent of j .

ii) If G is linear, $G(x) = Bx + c$, the set $\bar{M}_{h,0}^{\Delta_0}$ is an invariant manifold of the RKM-map $(I)_{h,0}$.

Remark 7): i) Note, that for $a_{s_i} = b_i$, $i = 1, \dots, s$, $\sigma_0(x, h) = s_0(x)$ and hence $\bar{M}_{h,0}^{\Delta_0} = \bar{M}_0^{\Delta_0} = \{(x, y) \mid G(x) = \Delta_0, y = s_0(x)\} \subset M_0$.

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 $\bar{M}_{h,0}^{\Delta_0}$ in y -direction (cf. Theorem 1). \dashv

iii) The global error is $(GE)_{h,0}$ 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

$$(10) \quad \begin{aligned} \sum_{i=0}^k \alpha_i x_i &= h \sum_{i=0}^k \beta_i f(x_i, \sigma(x_i)) \\ \varepsilon \sum_{i=0}^k \alpha_i \sigma(x_i) &= h \sum_{i=0}^k \beta_i G_x(x_i) f(x_i, \sigma(x_i)) \end{aligned}$$

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

$$(11) \quad Q(x_0; h, \varepsilon) := \sum_{i=0}^k \alpha_i G(x_i) - h \sum_{i=0}^k \beta_i G_x(x_i) f(x_i, \sigma(x_i)).$$

We will also need the fact that Φ 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 $j = 0, 1, 2, \dots$

$$\Delta_j := G(x_j) - \varepsilon\sigma(x_j)$$

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 $\delta^0 := (\Delta_0, \dots, \Delta_{k-1})^T \in \mathbb{R}^{kn}$, $\delta^1 := (\Delta_1, \dots, \Delta_k)^T$, $r^0 := (0, \dots, 0, Q_0)^T \in \mathbb{R}^{kn}$, $r^1 := (0, \dots, 0, Q_1)^T$, 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

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

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 $K_1 = \overline{K}_1 h^{p+1}$ and $\Delta_i = \Delta_0 + O(h^{p+1})$, $i = 1, \dots, k-1$. The role of Eq. (7) is taken by the relation

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

(cf. [3]).

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

$$|G(x_j) - \varepsilon\sigma(x_j, h, \varepsilon)| \leq jh \cdot Kh^p + K_0 \max_{0 \leq i < k} |\Delta_i|$$

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

$$(12) \quad |G(x_j) - \Delta_0| \leq jh \cdot Kh^p, \quad y_j = s_0(x_j)$$

for some constant K independent of j .

- If G is linear, $G(x) = Bx + c$, and if in addition $Bx_i + c = \Delta_0$, $i = 1, \dots, k-1$, then the set $\overline{M}_0^{\Delta_0} = \{(x, y) \mid G(x) = \Delta_0, y = s_0(x)\} \in M_0$ is an invariant manifold of the LMM-map $(\mathbf{I})_{h,0}$.

If we take starting values off M_0 satisfying $x_i - x(ih) = O(h^{p+1})$, $i = 1, \dots, k-1$, where $x(t)$ is the solution of Eq. (1)₀ with $x(0) = x_0$, $G(x_0) = \Delta_0$ and/or $|y_i - s_0(x_i)| \leq d$, $i = 0, \dots, k-1$, d small enough, then the x -estimate (12) still holds and in y -direction one has exponential attractivity 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_{RKM} to the DAE of index 2

$$(\bar{\mathbf{I}})_0 \quad \begin{aligned} \dot{x} &= f(x, y) \\ 0 &= G(x) \end{aligned}$$

satisfying Hypothesis \overline{H}_0 . Following [2] and [4] we have

$$(13) \quad \begin{aligned} X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\ 0 &= G(X) \end{aligned}$$

for the stages and

$$(\bar{\mathbf{I}})_{h,0} \quad \begin{aligned} \bar{x} &= x + h(b^T \otimes I_m) f(X, Y) \\ \bar{y} &= (1 - b^T A^{-1} \mathbb{1}_s) y + (b^T A^{-1} \otimes I_n) Y \end{aligned}$$

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

$$(\tilde{\mathbf{I}})_{h,0} \quad \begin{aligned} \bar{x} &= x + h(b^T \otimes I_m) f(X, Y) \\ \bar{z} &= R(\infty) z + (b^T A^{-1} \otimes I_n)(Y - \mathbb{1}_s \otimes s_0(x)) + s_0(x) - s_0(\bar{x}). \end{aligned}$$

Of course, we have to show that $(\bar{\mathbb{I}})_{h,0}$ and $(\tilde{\mathbb{I}})_{h,0}$, 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 $\Delta : \mathbb{R}^m \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$ be a bounded function of class C_b^r .*

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

$$(14) \quad \begin{aligned} X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\ G(X) &= \mathbb{1}_s \otimes (G(x) - h^2 \Delta(x, h)) \end{aligned}$$

has a unique solution $(X, Y)(x, h)$, C_b^r with respect to x , satisfying

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

Proof: If we introduce $Z \in \mathbb{R}^{sn}$ 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 ($i = 1, \dots, s$) takes the following form

$$(15) \quad \begin{aligned} X_i &= x + h \sum_{j=1}^s a_{ij} f(X_j, s_0(X_j) + Z_j) \\ h \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j) &= G(x) - G(X_i) - h^2 \Delta(x, h) \\ &\quad + h \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j) . \end{aligned}$$

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

$$\begin{aligned} G(X_i) - G(x) &= \int_0^1 G_x(x + \tau(X_i - x)) d\tau \cdot (X_i - x) \\ &= h \sum_{j=1}^s a_{ij} \int_0^1 G_x(x + \tau(X_i - x)) d\tau \cdot f(X_j, s_0(X_j) + Z_j) . \end{aligned}$$

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

$$\begin{aligned} \frac{1}{h} \sum_{j=1}^s a_{ij} G_x(X_j) f(X_j, s_0(X_j) + Z_j) &= \frac{1}{h} \sum_{j=1}^s a_{ij} \int_0^1 [G_x(X_j) - G_x(x + \tau(X_i - x))] d\tau \cdot \\ &\quad \cdot f(X_j, s_0(X_j) + Z_j) - \Delta(x, h) \\ &=: Q_i(x, X, Z; h) . \end{aligned}$$

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 Δ is bounded by assumption, the functions Q_i , $i = 1, \dots, s$, 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

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

with Q bounded and of class C_b^r 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 $|X - \mathbb{1}_s \otimes x| \leq \text{const} \cdot h$, $|Z| \leq \text{const} \cdot h$. The smoothness follows from the implicit function theorem. \perp

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 $G_x(x) f(x, y) = O(h)$. \dashv

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 $(\mathbb{1}_s \otimes x, \mathbb{1}_s \otimes s_0(x))$. 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 $(\bar{I})_{h,0}$ (i.e., the RKM applied to the index-1 formulation of Eq. $(\bar{I})_0$) and $(\bar{I})_{h,0}$ create the same (\bar{x}, \bar{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 $(\bar{I})_{h,0}$

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

which is attractive in y -direction and satisfies $\sigma_0(x, h) = s_0(x) + O(h^{q+1})$. (Again, $\bar{M}_{h,0} = \bar{M}_0$ ($y = s_0(x)$) if $a_{s_i} = b_i$, $i = 1, \dots, s$.) 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 $(\bar{I})_0$ or its index-1 formulation $(1)_0$.

ii) The general case: For RKMs applied to Eq. $(\bar{I})_0$ which satisfy Hypothesis H_{RKM} and $a_{s_i} = b_i$, $i = 1, \dots, s$, 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.

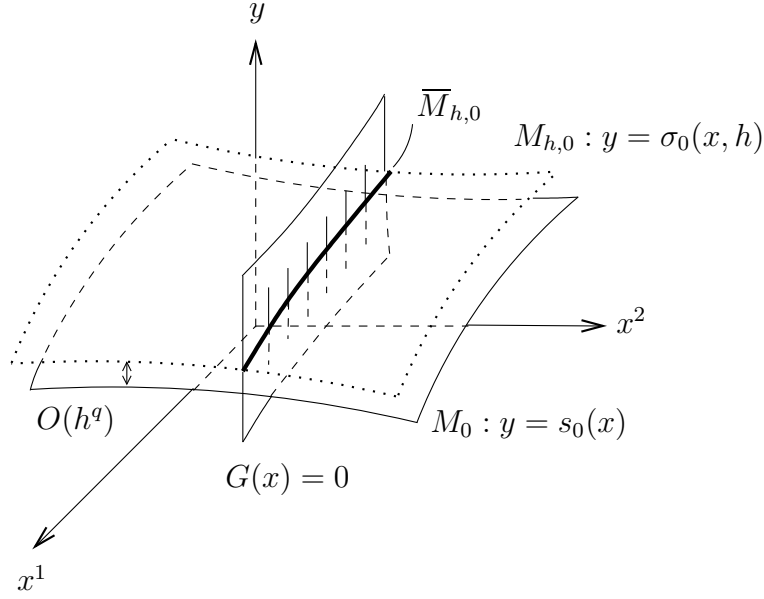


Fig. 7: The invariant manifolds of Eq. $(\bar{1})_0$ and of the RKM-map $(\bar{1})_{h,0}$ with $a_{s_i} = b_i$, $i = 1, \dots, s$

Theorem 4 Let Eq. $(\bar{1})_0$ satisfy Hypothesis \bar{H}_0 , apply a RKM satisfying Hypothesis H_{RKM} and $a_{s_i} = b_i$, $i = 1, \dots, s$, and assume $r < p$.

Then there exist positive constants h_0, γ, K and a function $\sigma_0 : \mathbb{R}^m \times (0, h_0] \rightarrow \mathbb{R}^n$, of class C_b^r with respect to x , such that for $h \leq h_0$ the following assertions hold.

i) The set $\bar{M}_{h,0} = \{(x, y) \mid G(x) = 0, y = \sigma_0(x, h)\}$ is an invariant manifold for the RKM-map $(\bar{1})_{h,0}$.

ii) $\bar{M}_{h,0}$ 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 $(\bar{1})_{h,0}$

$$G(\bar{x}) = 0, \quad \bar{y} = \sigma_0(\bar{x}, h).$$

iii) $\bar{M}_{h,0}$ 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 $\hat{y}_j = y_j = \sigma_0(x_j, h)$, $j \geq 1$.

iv) Closeness to \bar{M}_0 :

$$|\sigma_0(x, h) - s_0(x)| \leq Kh^q.$$

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

$$\begin{aligned}
X &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(X, Y) \\
G(X) &= \mathbb{1}_s \otimes G(x) \\
\bar{x} &= x + h(b^T \otimes I_m) f(X, Y) \\
\bar{y} &= (1 - b^T A^{-1} \mathbb{1}_s) y + (b^T A^{-1} \otimes I_n) Y.
\end{aligned}
\tag{16}$$

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

$$(17) \quad \begin{aligned} \bar{x} &= x + h(b^T \otimes I_m) f(X, s_0(X) + Z) \\ \bar{z} &= R(\infty) z + (b^T A^{-1} \otimes I_n) Z + (b^T A^{-1} \otimes I_n)(s_0(X) - \mathbb{1}_s \otimes s_0(x)) \\ &\quad + s_0(x) - s_0(\bar{x}) . \end{aligned}$$

By means of Lemma 3 and since $R(\infty) = 0$ by Hypothesis H_{RKM} and $a_{s_i} = b_i$, $i = 1, \dots, s$, 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

$$\begin{aligned} \bar{x} &= x + hF_1(x, h) \\ \bar{z} &= F_2(x, h) . \end{aligned}$$

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 $\Gamma_{11} = 1 + O(h)$. 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 $B1, B2, B3(r)$ 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 $a_{s_i} = b_i$, $i = 1, \dots, s$, that this subspace is positively invariant under (16). On the other hand, since in Eq. (16) $G(X) = \mathbb{1}_s \otimes G(x)$ 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 $a_{s_i} = b_i$, $i = 1, \dots, s$, 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 σ_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 $\hat{x}_j = x_j$, $j \geq 0$. Due to the infinite attractivity in y -direction we also have $\hat{y}_j = y_j = \sigma_0(x_j, h)$, $j \geq 1$. 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

$$\begin{aligned} U &= \mathbb{1}_s \otimes x + h(A \otimes I_m) f(U, s_0(U)) \\ \bar{u} &= x + h(b^T \otimes I_m) f(U, s_0(U)) . \end{aligned}$$

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

$$\begin{aligned} \bar{z} &= R(\infty)z + (b^T A^{-1} \otimes I_n)Z \\ &\quad + (b^T A^{-1} \otimes I_n)(s_0(X) - s_0(U)) + s_0(\bar{u}) - s_0(\bar{x}) \\ &\quad + (b^T A^{-1} \otimes I_n)(s_0(U) - \mathbb{1}_s \otimes s_0(x)) + s_0(x) - s_0(\bar{u}) . \end{aligned}$$

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

$$\bar{z} = R(\infty)z + O(1)Z + O(h^{q+1}) .$$

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. $(\bar{1}_0)$ at the t -values $c_i h$

$$Z_i = Y_i - s_0(X_i) = Y_i - s_0(x(c_i h)) + s_0(x(c_i h)) - s_0(X_i), \quad i = 1, \dots, s .$$

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

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

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

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 $j \geq 1$

$$\begin{aligned} |y_j - y(jh)| &\leq |y_j - \sigma_0(x_j, h)| + |\sigma_0(x_j, h) - s_0(x_j)| \\ &\quad + |s_0(x_j) - s_0(x(jh))| + |s_0(x(jh)) - y(jh)| \end{aligned}$$

where $(x(t), y(t))$ is a solution of $(\bar{1})_0$ 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. \dashv

In the case of general RKMs (i.e., $b_i \neq a_{si}$ for at least one $i \in \{1, \dots, s\}$ and Hypothesis $H_{\text{RK M}}$) 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. $(\bar{\Gamma})_0$ we have (cf. [4])

$$(19) \quad \begin{aligned} \sum_{i=0}^k \alpha_i x_i &= h \sum_{i=0}^k \beta_i f(x_i, y_i) \\ 0 &= G(x_k) \end{aligned}$$

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 $i, \ell = 0, \dots, k-1$, and let $\Delta : \mathbb{R}^{kn} \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$ be a bounded function of class C_b^r .*

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

$$(20) \quad \begin{aligned} \sum_{i=0}^k \alpha_i x_i &= h \sum_{i=0}^k \beta_i f(x_i, y_i) \\ G(x_k) &= - \sum_{i=0}^{k-1} G(x_i) - h^2 \Delta(x_0, \dots, x_{k-1}; h) \end{aligned}$$

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

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

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

$$(21) \quad 0 = \sum_{i=0}^{k-1} \alpha_i [G(x_k) - G(x_i)] - h^2 \Delta$$

where we have skipped the arguments of Δ for short. We may write

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

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

$$\begin{aligned} \frac{1}{h} \sum_{i=0}^k \beta_i G_x(x_k) f(x_i, y_i) &= \frac{1}{h^2} \sum_{i=0}^{k-1} \alpha_i \int_0^1 [G_x(x_i + \tau(x_k - x_i)) - G_x(x_k)] d\tau \cdot (x_k - x_i) - \Delta \\ &=: Q(x_0, \dots, x_k; h) . \end{aligned}$$

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

$$\begin{aligned} (22) \quad x_k &= - \sum_{i=0}^{k-1} \alpha_i x_i + h \sum_{i=0}^k \beta_i f(x_i, y_i) \\ \beta_k G_x(x_k) f(x_k, y_k) &= - \sum_{i=0}^{k-1} \beta_i G_x(x_i) f(x_i, y_i) + hQ(x_0, \dots, x_k; h) \end{aligned}$$

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 $y_i = s_0(x_i) + z_i$, $i = 0, \dots, k$, with $|z_i| \leq d$, $i = 0, \dots, k-1$. Since, by Hypothesis \bar{H}_0 , $G_x(x)f(x, s_0(x)) = 0$ and $G_x(x)f_y(x, s_0(x))$ is invertible and its inverse is bounded for $x \in \mathbb{R}^m$ we can apply, for $|z_k| \leq d_k$ small enough, the Newton-Kantorovich theorem implying for h and $|\beta|d$ sufficiently small the existence of a unique solution $(x_k, y_k)(x_0, \dots, x_{k-1}; y_0, \dots, y_{k-1}; h)$ 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. ⊥

Remark 10): i) For x_i , $i = 0, \dots, k-1$, 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 $y_i - y(ih) = O(h)$, $i = 0, \dots, k-1$, 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 $y_i - s_0(x_i) = O(h)$, $i = 0, \dots, k-1$, we have

$$\left| x_k + \sum_{i=0}^{k-1} \alpha_i x_i \right| \leq Kh, \quad |y_k - s_0(x_k)| \leq Kh$$

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_i 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 $(\bar{I})_{h,0}$ create the same orbit if $G(x_i) = 0$, $i = 0, \dots, k-1$, implying the existence of the y -attractive

invariant manifold $\bar{M}_0 = \{(x, y) \mid G(x) = 0, y = s_0(x)\}$ (for $\beta = 0$ and $\beta \neq 0$) with the properties already derived in Paragraph 3.1 for $(\mathbf{I})_{h,0}$.

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

$$(23) \quad \begin{aligned} \sum_{i=0}^k \alpha_i x_i &= h\beta_k f(x_k, y_k) \\ G(x_k) &= -\sum_{i=0}^{k-1} \alpha_i G(x_i). \end{aligned}$$

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 $(x_k, z_k)(x_0, \dots, x_{k-1}; h)$ of Eq. (23) satisfies

$$(24) \quad \begin{aligned} x_k &= -\sum_{i=0}^{k-1} \alpha_i x_i + h\beta_k f(x_k, s_0(x_k) + z_k) \\ z_k &= h\bar{Q}(x_0, \dots, x_{k-1}; h) \end{aligned}$$

with $\bar{Q} = O(|Q|)$ (cf. Eq. (22) for $\beta = 0$). For every $x_0 \in \mathbb{R}^m$ and $\gamma > 0$ the function \bar{Q} is bounded and of class C_b^r with respect to x_0, \dots, x_{k-1} if $|x_i - x_0| \leq \gamma h, i = 1, \dots, k-1$. We extend \bar{Q} to all \mathbb{R}^{km} by modifying it in the following way: Inside the tube $\Omega_{\gamma/2} = \{X_0 \in \mathbb{R}^{km} \mid x_0 \in \mathbb{R}^m, |x_i - x_0| \leq \frac{\gamma}{2} h, i = 1, \dots, k-1\}$ we put $\hat{Q} := \bar{Q}$, outside the tube Ω_γ we put $\hat{Q} = 0$ and, in between, \hat{Q} is taken such that it is C_b^r . 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 $\mathbb{R}^{km} \times \{Z \in \mathbb{R}^{kn} \mid |Z|_\infty \leq d\}$ into itself of the form

$$(25) \quad \begin{aligned} X_1 &= ((R - L_\alpha) \otimes I_m) X_0 + h(e_k \otimes \hat{P}(X_0; h)) \\ Z_1 &= (R \otimes I_n) Z_0 + h(e_k \otimes \hat{Q}(X_0; h)). \end{aligned}$$

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., $x_i = \Phi^i(x_0, h), i = 0, \dots, k-1$. 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 $\chi_{h,0}^k = 0$ if $x_i = \Phi^i(x_0, h), i = 0, \dots, k-1$, 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 $x_i = \Phi^i(x_0, h), x_i - x_0 = O(h), i = 0, \dots, k-1$, it follows that for γ 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 RKMs. As seen in Paragraph 3.1 the solution $x(t)$ of Eq. $(\bar{\mathbf{I}})_0$ with $x(0) = x_0$ satisfies

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

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

$$h\beta_k G_x(x_k) f(x_k, s_0(x_k) + z_k) = h^2 Q(x_0, \dots, x_k; h)$$

that

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

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

$$\begin{aligned} z_k = y_k - s_0(x_k) &= y_k - s_0(x(kh)) + s_0(x(kh)) - s_0(x_k) \\ &= y_k - y(kh) + O(|x_k - x(kh)|). \end{aligned}$$

Since on $M_{h,0}$ we have $x_i = \Phi^i(x_0, h)$ with $x_i - x(ih) = O(h^{p+1})$, $i = 0, \dots, k-1$, 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 $G(x_i) = 0$, $i = 0, \dots, k-1$, 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 $(\bar{\Gamma})_{h,0}$:

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

- Closeness to M_0 :

$$\sigma_0(x, h) - s_0(x) = O(h^p).$$

- Infinite attractivity in x -direction:

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

- Attractivity in y -direction:

$$\text{infinite (i.e., } \chi_{h,0}^k = 0) \quad \text{if } x_i = \Phi^i(x_0, h) \quad \text{for } i = 0, \dots, k-1;$$

in any case,

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

- 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 $|y_j - \sigma(x_j, h)| \leq K \chi_{h,0}^j \max_{0 \leq i < k} \{|y_i - \sigma_0(x_i, h)|\}$ for $j \geq k$ with $\chi_{h,0} = \max\{\rho_1, \sigma_1\} + O(|\beta|h) + O(h) < 1$ if $x_i = \Phi^i(x_0, h)$, $i = 0, \dots, k-1$. The stable fibers are not vertical anymore.

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