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 [8] for Runge-Kutta methods and in [9] 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 an (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 [8] and for LMMs in [9]) 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 containing also 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). Again, for the case of a linear constraint it can easily be verified that there exists an attractive invariant manifold for the discrete dynamical systems. Also in the nonlinear case, we prove the existence of such an invariant manifold and derive important additional properties for RKMs and 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. In the linear case, for index-2 DAEs of more general than Hessenberg form similar results as ours were obtained in [5] for the special schemes of BDF-methods and of stiffly accurate RKMs. The results and invariant manifold techniques given below 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 [8], [9]. There, RKMs and LMMs are applied to stiff systems of singular perturbation type of the form

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

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.

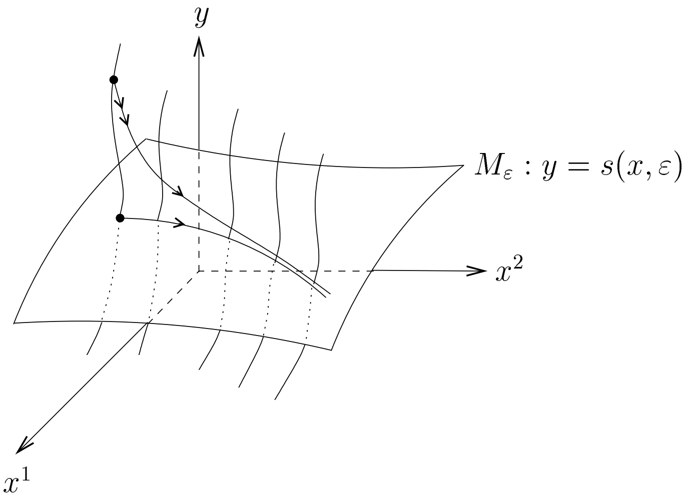

Fig. 1: The attractive invariant manifold M_ε of Eq. $(1)_\varepsilon$, stable foliation and 'asymptotic phase'

For RKMs applied to Eq. $(1)_\varepsilon$ it is assumed that the following assumptions hold.

Hypothesis $\mathrm{H_{RKM}}$

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 RKMs with $a_{si} = b_i, i = 1, \ldots, s$, this implies $R(\infty) = 0$. Under Hypothesis $\mathrm{H_{RKM}}$ 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 $(\mathrm{I})_{\mathrm{h},\varepsilon} :\ (\mathrm{x}, \mathrm{y}) \longmapsto (\bar{\mathrm{x}}, \bar{\mathrm{y}})$ from $\mathbb{R}^m \times \mathbb{R}^n$ into itself. (We have used the notation $X := (X_1, \ldots, X_s)^T \in \mathbb{R}^{sm}$, $f(X, Y) := (f(X_1, Y_1), \ldots, f(X_s, Y_s))^T \in \mathbb{R}^{sm}$, etc., $\otimes$ denotes the Kronecker product.) In coordinates measuring the difference to M_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)

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

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 $(\mathrm{I})_{\mathrm{h},\varepsilon}$ 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

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

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 $\widetilde{(\mathrm{I})}_{\mathrm{h},\varepsilon}$ 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 $jh \le Nh = T$ fixed

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

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

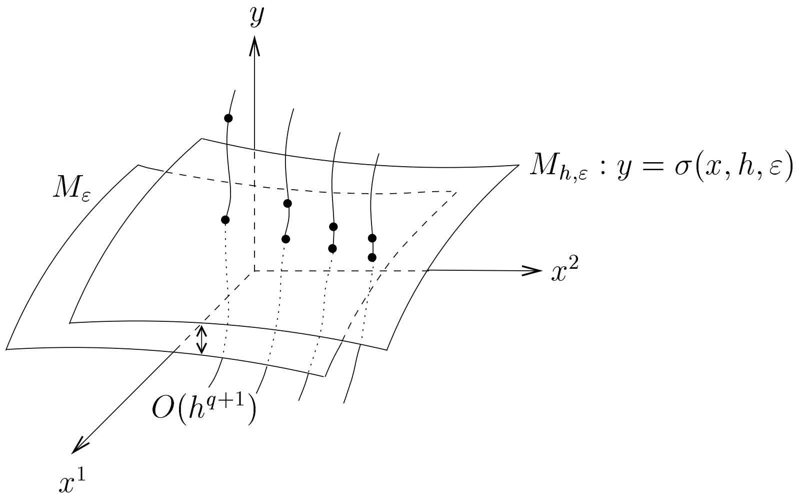

Fig. 2: The attractive invariant manifold $M_{h,\varepsilon}$ of the RKM-map $(\mathrm{I})_{\mathrm{h},\varepsilon}$, stable foliation and asymptotic phase and closeness to M_ε

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

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

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

Hypothesis $\mathrm{H_{LMM}}$

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 $(\mathrm{I})_{\mathrm{h},\varepsilon}$ 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

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

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

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

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

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

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

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

is invariant under the map $(\mathrm{I})_{\mathrm{h},\varepsilon}$ 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 $(\widetilde{\mathrm{I}})_{\mathrm{h},\varepsilon}$ giving the y-attractivity $const \cdot \varepsilon/h \cdot \chi^j_{h,\varepsilon}$, $j \geq k$. Again there exists a stable foliation ($L^{h,\varepsilon}_{12} = O(\varepsilon)$, 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:

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

For $\beta = 0$ the factor h in the x-equation is replaced by ε and the factor $(h + \chi^j_{h,\varepsilon})$ 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_ε), its invariant manifold by M_ε with attractivity χ^t_ε and 'steepness' of the stable fibers L^ε_{12}. Similarly, for *both* RKMs *and* LMMs applied to $(1)_\varepsilon$ we denote the discrete dynamical system by $(\mathrm{I})_{\mathrm{h},\varepsilon}$, its invariant manifold by $M_{h,\varepsilon}$ with attractivity $\chi_{h,\varepsilon}$ and 'steepness' of the stable fibers $L^{h,\varepsilon}_{12}$, and the global error estimate by $(\mathrm{GE})_{\mathrm{h},\varepsilon}$. If we consider the variable z (instead of y) measuring the distance to M_ε we put a $\tilde{}$ on $(\mathrm{I})_{\mathrm{h},\varepsilon}$, i.e., we write $(\widetilde{\mathrm{I}})_{\mathrm{h},\varepsilon}$.

In the DAE case, we replace the ε by 0 for index 1: $(1)_0$ (satisfying Hypothesis H_0), M_0, χ^t_0, L^0_{12}; $(\mathrm{I})_{\mathrm{h},0}$, $M_{h,0}$, $\chi_{h,0}$, $L^{h,0}_{12}$, $(\mathrm{GE})_{\mathrm{h},0}$ and $(\widetilde{\mathrm{I}})_{\mathrm{h},0}$. For index 2 we keep the notation but put a $\bar{}$ on top, i.e., $(\bar{1})_0$ (satisfying Hypothesis $\overline{\mathrm{H}}_0$), $\overline{M}_0$; $(\bar{\mathrm{I}})_{\mathrm{h},0}$, $\overline{M}_{h,0}$, etc. ⊣

2 Systems of index 1

Consider the DAE

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

satisfying

Hypothesis H_0

1) f and g are bounded and $f \in C^r_b(R^m \times \mathbb{R}^n, \mathbb{R}^m)$, $g \in C^r_b(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)$ 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 $(x,y)\in\Omega_d:=\{x\in\mathbb{R}^m,\ |y-s_0(x)|\le d\}$ 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 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_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. $(1)_\varepsilon$ 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 RKMs and LMMs applied to Eq. $(1)_\varepsilon$ one has to consider solutions of $(1)_\varepsilon$ on the stable manifold of M_ε, however. $\dashv$

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 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 $(\mathrm{I})_{\mathrm{h},\varepsilon}$ and putting $\varepsilon=0$. For the RKM assume Hypothesis $\mathrm{H}_{\mathrm{RKM}}$. If we put $\varepsilon=0$ in Hypothesis H_ε, in the differential equation $(1)_\varepsilon$ and in the map $(\widetilde{\mathrm{I}})_{\mathrm{h},\varepsilon}$, 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 H_0, Eq. $(1)_0$, the map

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

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

$$M_{h,0} = \{(x,y) \,|\, x \in \mathbb{R}^m,\ y = \sigma_0(x,h) := \sigma(x,h,0)\}$$

with attractivity $\chi_{h,0} = |R(\infty)|$, and $L_{12}^{h,0} = 0$. From [8] 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

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

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

Hence, we have shown that the RKM-map $(\mathrm{I})_{\mathrm{h},0}$ 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* $\mathrm{H}_{\mathrm{RKM}}$ *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_b^r *with respect to* x*, such that for* $h \le h_0$ *and for* $(x,y) \in \Omega_d := \{(x,y) \,|\, x \in \mathbb{R}^m,$ $|y - s_0(x)| \le d\} \subset \mathbb{R}^m \times \mathbb{R}^n$ *the following assertions hold.*

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

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.,*

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

holds.

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

$$W^s(x,y) = \{(\xi,\eta) \,|\, \xi = x, \quad |\eta - s_0(\xi)| \le d\}\ ,$$

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*

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

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 $|Q| \le K$, 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

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

for $jh \le T$.

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

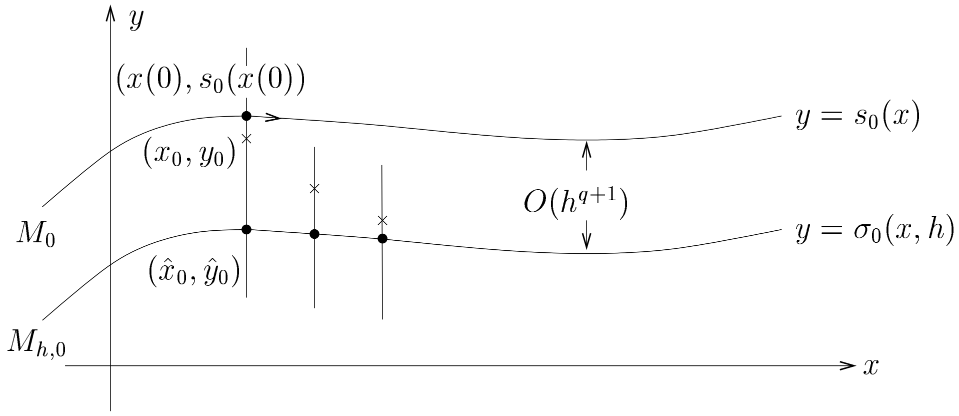

Fig. 3: The invariant manifolds for the DAE $(1)_0$ and the RKM-map $(\mathrm{I})_{\mathrm{h},0}$

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 $(\mathrm{I})_{\mathrm{h},0}$ 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

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

For $a_{s_i} = b_i$, $i = 1, \ldots, s$, 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. $(1)_\varepsilon$ just by putting $\varepsilon = 0$. Of course, the DAE-results could be derived by directly applying the invariant manifold theory for maps (cf. [7]) to the map $(\widetilde{\mathrm{I}})_{\mathrm{h},0}$. However, on the one hand, the results for the singularly perturbed case have been derived before (cf. [8]) and, on the other hand, the diagram of Fig. 4 gives additional insight.

$$
\begin{tikzcd}[column sep=huge]
\begin{array}{l} (1)_\varepsilon; \\ M_\varepsilon, \chi_\varepsilon^t, L_{12}^\varepsilon \end{array} \arrow[d, "\mathrm{RKM}"'] \arrow[r, dashed, shift right, "\varepsilon = 0"'] & \begin{array}{l} (1)_0\,; \\ M_0, \chi_0^t, L_{12}^0 \end{array} \arrow[l, shift right, "\varepsilon \dot{y}"'] \arrow[d, "\mathrm{RKM}"] \\
\begin{array}{l} (\mathrm{I})_{\mathrm{h},\varepsilon}; \\ M_{h,\varepsilon}, \chi_{h,\varepsilon}, L_{12}^{h,\varepsilon};\ (\mathrm{GE})_{\mathrm{h},\varepsilon} \end{array} \arrow[r, "\varepsilon = 0"] & \begin{array}{l} (\mathrm{I})_{\mathrm{h},0}; \\ M_{h,0}, \chi_{h,0}, L_{12}^{h,0};\ (\mathrm{GE})_{\mathrm{h},0} \end{array}
\end{tikzcd}
$$

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 $\mathrm{H}_{\mathrm{LMM}}$ 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 $(\widetilde{\mathrm{I}})_{\mathrm{h},\varepsilon}$ 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)

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

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

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

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

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

Remark 3): For $\beta = 0$ (BDF-like methods, corresponding to $a_{s_i} = b_i$, $i = 1, \ldots, s$, in the RKM case) we have:

- $\chi^k_{h,0} = 0$ (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 $(\widetilde{\mathrm{I}})_{\mathrm{h},0}$ with $\beta = 0$).
- Global error for $j \leq N$:

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

⊣

3 Systems of index 2

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

$$(\bar{1})_0 \qquad \begin{aligned} \dot{x} &= f(x, y) \\ 0 &= G(x) \end{aligned}$$

satisfying

Hypothesis $\overline{\mathrm{H}}_0$

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. $(\bar{1})_0$ 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 $\overline{\mathrm{H}}_0$. 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 $(\bar{1})_0$)

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

lie in the m-dimensional surface

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

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

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

is invariant under $(1)_0$. Hence, we have shown that under Hypothesis $\overline{\mathrm{H}}_0$ all solutions of Eq. $(\bar{1})_0$ (in Ω_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)).

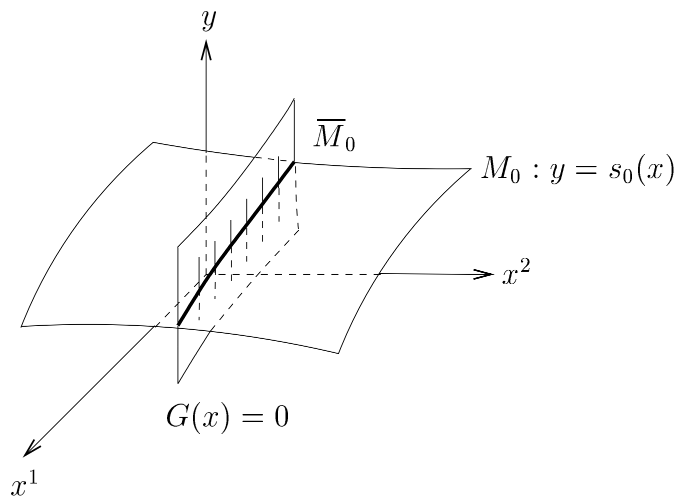

Fig. 5: The invariant manifold $\overline{M}_0$ of Eq. $(\bar{1})_0$

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

3.1 RKMs and LMMs applied to the index-1 formulation

Obviously, applying a RKM satisfying Hypothesis $\mathrm{H}_{\mathrm{RKM}}$ or a LMM satisfying Hypothesis $\mathrm{H}_{\mathrm{LMM}}$ 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 $(1)_\varepsilon$, $(\mathrm{I})_{\mathrm{h},\varepsilon}$ and $(\mathrm{I})_{\mathrm{h},0}$, respectively, also possess a 'first integral', i.e., a submanifold of M_ε, $M_{h,\varepsilon}$ 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

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

Of course, again any set

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

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

B.a) $(\mathrm{I})_{\mathrm{h},\varepsilon}$ *and* $(\mathrm{I})_{\mathrm{h},0}$ *for RKMs. 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 $g(x,y) = G_x(x) f(x,y) = B f(x,y)$. 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

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

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

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

for the RKM-map $(\mathrm{I})_{\mathrm{h},0}$. 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 $a_{s_i} = b_i$, $i = 1, \ldots, s$, 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.

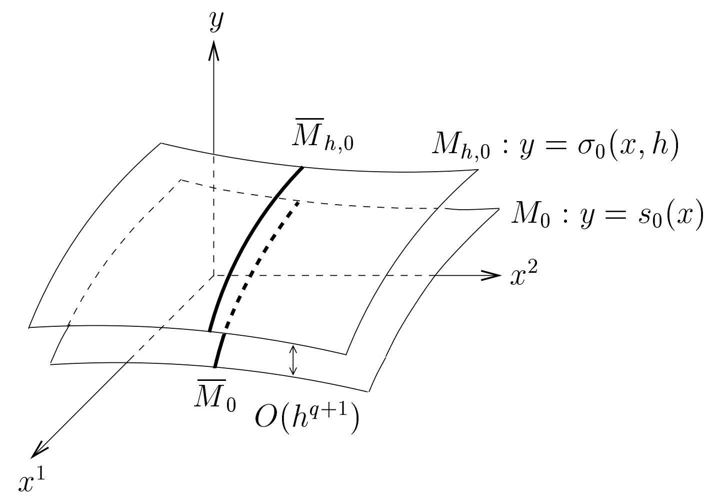

Fig. 6: The manifolds $\overline{M}_0$ and M_0 of Eq. $(1)_0$ and the invariant manifolds $\overline{M}_{h,0}$ and $M_{h,0}$ of the RKM-map $(\mathrm{I})_{\mathrm{h},0}$ for $G(x) = Bx + c$

For RKMs applied to the index-1 formulation of Eq. $(\bar{1})_0$ 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_ε, $M_{h,\varepsilon}$ and $M_{h,0}$, respectively, in y-direction. Moreover, every 'shifted manifold' $\overline{M}_0^{const} := \{(x,y) \,|\, G(x) = \text{const},\ y = s_0(x)\}$, $\overline{M}_\varepsilon^{const}$, $\overline{M}_{h,\varepsilon}^{const}$ and $\overline{M}_{h,0}^{const}$ (defined analogously) is also invariant. $\dashv$

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

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

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

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

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 $j \geq 1$

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

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

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

From the definition of Q we have

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

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 [8], 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

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

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

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

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

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

We have

$$\begin{aligned}P_1-\overline{P}_1 &:= h\,O\Big(\max_{1\le i\le s}\;|X_i-U_i|+\max_{1\le i\le s}\;|Z_i|\Big)\,,\\ \overline{P}_1-\overline{P}_2 &:= h\,O\Big(\max_{1\le i\le s}\;|U_i-u(c_ih)|\Big)\end{aligned}$$

and with (8)

$$\overline{P}_2-P_2=O(h^{p+1})+h\,O\Big(\max_{0\le t\le h}\;|x(t)-u(t)|+\max_{0\le t\le h}\;|z(t)|\Big)\;.$$

From [8] 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

$$U_i-u(c_ih)=O(h^{q+1})\,,\;\; i=1,\ldots,s\;,$$

and a simple Gronwall type argument yields

$$\max_{0\le t\le h}\;|x(t)-u(t)|=h\,O(\max_{0\le t\le h}\;|z(t)|)\;.$$

For $z(t)$ we apply Theorems 1 and 3 of [8]:

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

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 $j\in\mathbb{N}$

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

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 $t=jh$) 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 $(\mathrm{GE})_{\mathrm{h},\varepsilon}$ 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 Konst $\cdot\, e^{\mathrm{const}\cdot jh}$ 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.* $(\overline{1})_0$ *satisfy Hypothesis* $\overline{\mathrm{H}}_0$*, apply a* RKM *satisfying Hypothesis* $\mathrm{H}_{\mathrm{RKM}}$ *to its 'index-1 formulation'* $(1)_0$ *and assume* $r < p$*. Consider for* $\Delta_0 \in \mathbb{R}^n$ *the set*

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

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* $\overline{M}_{h,0}^{\Delta_0}$ *is an invariant manifold of the* RKM-*map* $(\mathrm{I})_{\mathrm{h},0}$.

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

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

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

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

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

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

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

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. [9], 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 $\delta^0 := (\Delta_0, \ldots, \Delta_{k-1})^T \in \mathbb{R}^{kn}$, $\delta^1 := (\Delta_1, \ldots, \Delta_k)^T$, $r^0 := (0, \ldots, 0, Q_0)^T \in \mathbb{R}^{kn}$, $r^1 := (0, \ldots, 0, Q_1)^T$, 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 $\mathrm{H}_{\mathrm{LMM}}$ 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 [9], one finds $K_1 = \overline{K}_1 \, h^{p+1}$ and $\Delta_i = \Delta_0 + O(h^{p+1})\,, \ i = 1, \ldots, k-1$. 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 $M_{h,0} = M_0 = \{(x,y) \,|\, x \in \mathbb{R}^m,\, y = s_0(x)\}$ satisfies

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

  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 $\overline{M}_0^{\Delta_0} = \{(x,y) \,|\, G(x) = \Delta_0,\, y = s_0(x)\} \in M_0$ is an invariant manifold of the LMM-map $(\mathrm{I})_{\mathrm{h},0}$.

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. $(1)_0$ with $x(0) = x_0$, $G(x_0) = \Delta_0$ and/or $|y_i - s_0(x_i)| \le d$, $i = 0, \ldots, k-1$, 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 $j \ge k$ (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 main point of interest is the existence of a y-attractive 'index-1 surface' which then implies the existence of an attractive invariant manifold for the discrete dynamical system.

a) RKMs. We apply a RKM satisfying Hypothesis $\mathrm{H}_{\mathrm{RKM}}$ to the DAE of index 2

$$(\bar{1})_0 \qquad \begin{aligned} \dot{x} &= f(x,y) \\ 0 &= G(x) \end{aligned}$$

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

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

for the stages and

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

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

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

Of course, we have to show that $(\bar{\mathrm{I}})_{\mathrm{h},0}$ and $(\tilde{\tilde{\mathrm{I}}})_{\mathrm{h},0}$, 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 a unique solution not only for x-starting values satisfying $G(x) = 0$ but also for perturbed values in an h-dependent 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_b^r.*

There are positive constants h_1, δ_1, K such that if $|\Delta| \le \delta_1$ then for $h \le h_1$ and $x \in \mathbb{R}^m$ the nonlinear system

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

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

$$|X(x,h) - \mathbb{1}_s \otimes x| \le Kh\,, \qquad |Y(x,h) - \mathbb{1}_s \otimes s_0(x)| \le K(h + |\Delta|)\ .$$

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 ($i = 1,\ldots,s$) takes the following form

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

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

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

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 f is bounded by assumption, the functions Q_i, $i = 1, \ldots, s$, are of the form $Q_i = -\Delta + O(h)$. Hence, back to the 'big space' and since the Runge-Kutta matrix A is invertible by Hypothesis $\mathrm{H_{RKM}}$, Eq. (15) has the form

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

with Q being $O(h + |\Delta|)$ and of class C_b^r with respect to x, X, Z. By Hypothesis $\overline{\mathrm{H}}_0$ we know that $\operatorname{diag}[G_x(X)]\, f(X, s_0(X)) = 0$ and that $\operatorname{diag}[G_x(X)]\, f_y(X, s_0(X))$ is invertible with bounded inverse. Hence, for $|Z| \leq d$, d small enough, the second equation can be written as

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

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

Remark 8): For an x-starting value such that $G(x) = O(h^2)$, i.e., $\Delta = O(h)$, Lemma 3 corresponds to Theorem 4.1 of [2] (cf. also [4], Theorem 7.1). We have given a different proof only needing $G(x) = O(\gamma h)$, γ small enough, instead of their assumption $G(x) = O(h^2)$ and $G_x(x)\, f(x, y) = O(h)$. $\dashv$

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 $g(X, Y) := \operatorname{diag}[G_x(X)]\, f(X, Y) = 0$ and vice versa. Hence, for $G(x) = 0$ and $|y - s_0(x)|$ small enough the maps $(\mathrm{I})_{\mathrm{h},0}$ (i.e., the RKM applied to the index-1 formulation of Eq. $(\bar{1})_0$) and $(\bar{\mathrm{I}})_{\mathrm{h},0}$ 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 $(\bar{\mathrm{I}})_{\mathrm{h},0}$

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

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 $(\bar{1})_0$ or its index-1 formulation $(1)_0$.

ii) The general case: For RKMs applied to Eq. $(\bar{1})_0$ which satisfy Hypothesis $\mathrm{H_{RKM}}$ and $a_{s_i} = b_i$, $i = 1, \ldots, s$, the existence of a y-attractive 'index-1 surface' can be proved by extending the RKM-map to all $\mathbb{R}^m$ and applying the invariant manifold theorems of [7] to this altered map. The restriction to the subspace $G(x) = 0$ then yields an invariant manifold for the RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$. The result is given in Theorem 4 below and is sketched in Fig. 7. If the RKM is not stiffly accurate the analogous approach may be applied as was pointed out by Ander Murua [6] implying a result analogous to the one for the case $a_{s_i} = b_i$, $i = 1, \ldots, s$.

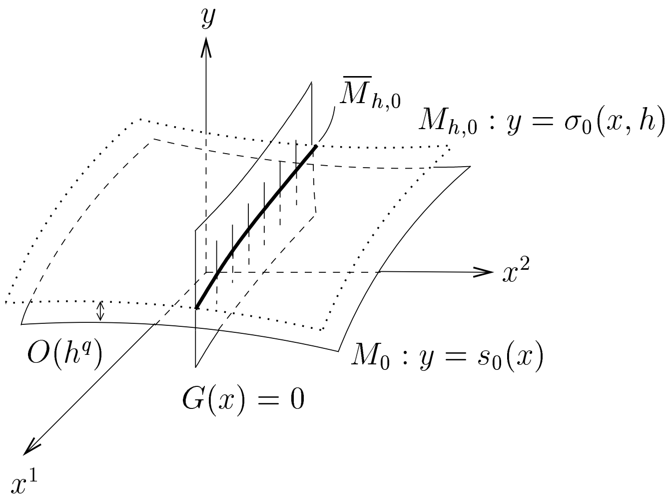

Fig. 7: The invariant manifold $\overline{M}_{h,0}$ of the RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$ with $a_{s_i} = b_i,\ i = 1, \ldots, s$

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

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

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

ii) $\overline{M}_{h,0}$ *is 'infinitely attractive', i.e.,* $(x,y) \in \{\, |G(x)| \le \gamma h\} \times \mathbb{R}^n$ *implies for the image* $(\bar{x}, \bar{y})$ *under* $(\bar{\mathrm{I}})_{\mathrm{h},0}$

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

iii) $\overline{M}_{h,0}$ *has a vertical stable foliation implying the existence of an 'asymptotic phase' orbit* $(\hat{x}_j, \hat{y}_j)$ *with* $\hat{x}_j = x_j$*,* $j \ge 0$*, and* $\hat{y}_j = y_j = \sigma_0(x_j, h)$*,* $j \ge 1$*.*

iv) Closeness to $\overline{M}_0$ *:*

$$|\sigma_0(x,h) - s_0(x)| \le K h^q\ .$$

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

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

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

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

By means of Lemma 3 and since $R(\infty) = 0$ by Hypothesis $\mathrm{H}_{\mathrm{RKM}}$ and $a_{s_i} = b_i$, $i = 1, \cdots, s$, we have for every $d > 0$ that for h small enough Eq. (17) defines a smooth map from $\mathbb{R}^m \times \mathbb{R}^n \cap \{|z| \le d\}$ into itself. We apply the invariant manifold theorems of [7] 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 [7] are satisfied and we obtain the existence of an m-dimensional invariant manifold $M_{h,0} = \{(x,y) \,|\, x \in \mathbb{R}^m,\ y = \sigma_0(x,h)\}$ 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) $G(X) = \mathbb{1}_s \otimes G(x)$ there is for every $\bar{x}$ with $G(\bar{x}) = 0$ a pre-image x with $G(x) = 0$ obtained by iteration of $x^{\ell+1} = \bar{x} - h(b^T \otimes I_m)\, f(X(x^\ell,h),\ Y(x^\ell,h))$, $\ell \ge 0$, $x^0 = \bar{x}$. Hence, we have shown the existence of the invariant manifold

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

From Lemma 3 we know that for a starting value (x_0, y_0) with $G(x_0) = h\,\Delta^*$, $|\Delta^*|$ sufficiently small, 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 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

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

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

$$X - U = O(h) Z \ \text{ and } \ \bar{x} - \bar{u} = O(h)\, Z \ . \tag{18}$$

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

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

As seen in Paragraph 2.1 the last two terms together can be studied via the singularly perturbed case of [8] and the limit $\varepsilon \to 0$ 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 $\big(x(t),\, y(t) = s_0(x(t))\big)$ of Eq. $(\overline{1}_0)$ at the t-values $c_i h$

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

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 $\bar{z} = R(\infty) z + O(h^q)$ and the invariant manifold results of [7] 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 $jh \leq$ const (see, e.g., the results in [2] or [4]) we may estimate for the y-component for $j \geq 1$

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

where $(x(t), y(t))$ is a solution of $(\bar{\mathrm{I}})_0$ with $|x_0 - x(0)| \le \gamma h$. 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

$$|y_j - y(jh)| \le |\sigma_0(x_j, h) - s_0(x_j)| + K\,|x_j - x(jh)|$$

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., $a_{si} \ne b_i$ for at least one $i \in \{1, \dots, s\}$ and Hypothesis $\mathrm{H_{RKM}}$) there also exists an attractive invariant manifold for the RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$. Since $G(x) = 0$ is not an invariant set in this case, $\Delta(x, h) \equiv 0$ in Lemma 3 is no longer appropriate. One has to show that there exists $\Delta(x, h)$ such that $G(x) = h\Delta(x, h)$ is an invariant set for the RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$. The idea of proof of A. Murua [6] was to consider the auxiliary map from $\mathbb{R}^m \times \mathbb{R}^n$ into itself

$$(17)^* \qquad \begin{aligned} \bar{x} \;&= x + h(b^T \otimes I_m)\, f(X, s_0(X) + Z) &&=:\; x \,+\, h\,\hat{F}(x, \Delta, h) \\ \bar{\Delta} \;&= \Delta + \frac{1}{h}\,[G(\bar{x}) - G(x)] &&=:\; H(x, \Delta, h) \end{aligned}$$

where $(X, Z)(x, \Delta, h)$ is the unique solution of Eq. (14) for h and $|\Delta|$ small enough. Note that the set $M_\Delta = \{(x, \Delta) \,|\, G(x) = h\Delta\}$ is an invariant set of the map $(17)^*$, and this particular case of the map $(17)^*$ corresponds to the x-part of the RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$ (cf. (13) and (14)). One easily finds that $H(x, \Delta, h) = R(\infty)\Delta + h\hat{H}(x, \Delta, h)$. Hence, the invariant manifold theory of [7] applies. One has $\Gamma_{11} = 1 + O(h)$, $L_{12} = O(h)$, $L_{21} = O(h)$ and $L_{22} = |R(\infty)| + O(h)$, giving the existence of an invariant manifold $\Delta = \Delta_0(x, h)$ for the map $(17)^*$ which is attractive with $\chi_h = |R(\infty)| + O(h) < 1$, i.e., $|\bar{\Delta} - \Delta_0(\bar{x}, h)| \le \chi_h\,|\Delta - \Delta_0(x, h)|$. For $(x, \Delta) \in M_\Delta$, i.e., for our RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$ (cf. (13), (14)) this implies

$$(19) \qquad |G(\bar{x}) - h\,\Delta_0(\bar{x}, h)| \;\le\; \chi_h\,|G(x) - h\,\Delta_0(x, h)|\,.$$

We now consider the map (17) with $(X, Z)(x, h)$ being the unique solution of Eq. (14) with $\Delta = \Delta_0(x, h)$. In exactly the same way as in the proof of Theorem 4 we get the existence of the invariant manifold $M_{h,0} = \{(x, y) \,|\, x \in \mathbb{R}^m,\ y = \sigma_0(x, h)\}$ with attractivity constant $|R(\infty)| < 1$, and the restriction to $G(x) = h\Delta_0(x, h)$ (which corresponds to our RKM-map $(\bar{\mathrm{I}})_{\mathrm{h},0}$) yields the invariant manifold

$$\overline{M}_{h,0} \;=\; \{(x, y) \,|\, G(x) = h\,\Delta_0(x, h),\ y = \sigma_0(x, h)\}\,.$$

The properties are as in Theorem 4 except for a 'finite' attractivity in ii) given for x in (19) and for y as $|\bar{y} - \sigma_0(\bar{x}, h)| \,\le\, |R(\infty)|\,|y - \sigma_0(x, h)|$. The stable foliation (for σ_0) is still vertical but the y-part of the 'asymptotic phase' orbit satisfies $|\hat{y}_j - y_j| \,\le\, |R(\infty)|^j\,|y_0 - \sigma_0(x, h)|$, $j \ge 1$, in iii). Since $H(x, \Delta, h)$ in $(17)^*$ is of the form $R(\infty)\Delta + O(h)$ it follows that $\Delta_0(x, h) = O(h)$. A closer look yields the improved estimate $\Delta_0(x, h) = O(h^q)$.

Thus, we have shown that also in the nonstiffly accurate case where $a_{si} = b_i$, $i = 1, \ldots, s$, does not hold the picture of Fig. 7 is still true but the invariant manifold $\overline{M}_{h,0}$ of the RKM-map $(\overline{\mathrm{I}})_{\mathrm{h},0}$ is the intersection of $G(x) = h\Delta_0(x,h)$ with $M_{h,0}$ where $h\Delta_0(x,h)$ is $O(h^{q+1})$. The attractivity rate in x and in y is $|R(\infty)|$.

b) LMMs. For LMMs applied to Eq. $(\overline{\mathrm{I}})_0$ we have (cf. [4])

$$\begin{aligned} \sum_{i=0}^{k} \alpha_i \, x_i &= h \sum_{i=0}^{k} \beta_i \, f(x_i, y_i) \\ 0 &= G(x_k) \end{aligned} \tag{20}$$

with $\sum_{i=0}^{k} \alpha_i = 0$, $\alpha_k = 1$, $\beta_k \neq 0$ by Hypothesis $\mathrm{H}_{\mathrm{LMM}}$. 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. (21)) and thus obtain the existence of a solution of Eq. (20) for x_i-values in an h-dependent neighbourhood of $G(x) = 0$.

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

There are positive constants h_1, δ_1, d, K such that if $|\Delta| \leq \delta_1$ then for $h \leq h_1$ and for $|y_i - s_0(x_i)| \leq d$, $i = 0, \ldots, k-1$, the nonlinear system

$$\begin{aligned} \sum_{i=0}^{k} \alpha_i \, x_i &= h \sum_{i=0}^{k} \beta_i \, f(x_i, y_i) \\ G(x_k) &= -\sum_{i=0}^{k-1} \alpha_i \, G(x_i) - h\Delta(x_0, \ldots, x_{k-1}; h) \end{aligned} \tag{21}$$

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

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

Proof: The second equation of (21) is equivalent to

$$0 = \sum_{i=0}^{k-1} \alpha_i [G(x_k) - G(x_i)] - h\Delta \tag{22}$$

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

$$\sum_{i=0}^{k-1} \alpha_i [G(x_k) - G(x_i)] = \sum_{i=0}^{k-1} \alpha_i \int_0^1 G_x(x_i + \tau(x_k - x_1)) d\tau \cdot (x_k - x_i) \,.$$

Moreover, multiplying the first equation of (21) 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 (22) and dividing by h we thus obtain

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

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 (21) and by our assumption on $|x_i - x_\ell|$. We therefore conclude that the function Q is of the form $Q = -\Delta + O(h)$. It remains to show that the nonlinear system

$$\begin{aligned} x_k \;&=\; -\sum_{i=0}^{k-1} \alpha_i \, x_i + h \sum_{i=0}^{k} \beta_i \, f(x_i, y_i) \\ \beta_k \, G_x(x_k) \, f(x_k, y_k) \;&=\; -\sum_{i=0}^{k-1} \beta_i \, G_x(x_i) \, f(x_i, y_i) + Q(x_0, \ldots, x_k; h) \end{aligned} \tag{23}$$

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 $|z_i| \leq d$, $i = 0, \ldots, k-1$. Since, by Hypothesis $\overline{\mathrm{H}}_0$, $G_x(x) f(x, s_0(x)) = 0$ 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, $|\Delta|$ 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 $|x_k + \sum_{i=0}^{k-1} \alpha_i \, x_i| \leq const \cdot h$, $|z_k| \leq const \cdot (h + |\Delta| + |\beta| d)$ (cf. [9]). The smoothness follows from the implicit function theorem.
$\perp$

Remark 10): i) For x_i, $i = 0, \ldots, k-1$, such that $-\sum_{i=0}^{k-1} \alpha_i G(x_i) = O(h^2)$, i.e., $\Delta = O(h)$, 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

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

as in [4]. For BDF-like methods, i.e., $\beta = 0$ in Eq. (20), 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. (20)) are considered. Lemma 5 yields a solution (x_k, y_k) of such a method for x-starting values x_i such that $-\sum_{i=0}^{k-1}(\alpha_i - \frac{\beta_i}{\beta_k})G(x_i) = h\Delta$, $|\Delta|$ sufficiently small. $\dashv$

In the linear case, it is again easy to verify that the maps $(\mathrm{I})_{\mathrm{h},0}$ and $(\bar{\mathrm{I}})_{\mathrm{h},0}$ create the same orbit if $G(x_i) = 0$, $i = 0, \ldots, k-1$, implying the existence of the y-attractive invariant manifold $\overline{M}_0 = \{(x,y) \,|\, G(x) = 0,\ y = s_0(x)\}$ (for $\beta = 0$ *and* $\beta \neq 0$) with the properties already derived in Paragraph 3.1 for $(\mathrm{I})_{\mathrm{h},0}$.

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

$$(24) \qquad \begin{aligned} \sum_{i=0}^{k} \alpha_i\, x_i \quad &= \quad h\beta_k\, f(x_k, y_k) \\ G(x_k) \quad &= \quad -\sum_{i=0}^{k-1} \alpha_i\, G(x_i)\,. \end{aligned}$$

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 $(x_k, z_k)(x_0, \ldots, x_{k-1}; h)$ of Eq. (24) satisfies

$$(25) \qquad \begin{aligned} x_k \quad &= \quad -\sum_{i=0}^{k-1} \alpha_i\, x_i + h\beta_k\, f(x_k, s_0(x_k) + z_k) \\ z_k \quad &= \quad \overline{Q}(x_0, \ldots, x_{k-1}; h) \end{aligned}$$

with $\overline{Q} = O(|Q|)$ (cf. Eq. (23) for $\beta = 0$). For every $x_0 \in \mathbb{R}^m$ and $\gamma > 0$ the function $\overline{Q}$ is $O(h)$ and of class C_b^r with respect to $x_0, \ldots, x_{k-1}$ if $|x_i - x_0| \le \gamma h$, $i = 1, \ldots, k-1$. We extend $\overline{Q}$ to all $\mathbb{R}^{km}$ by modifying it in the following way: Inside the tube $\Omega_{\gamma/2} = \{X_0 \in \mathbb{R}^{km} \,|\, x_0 \in \mathbb{R}^m,\ |x_i - x_0| \le \frac{\gamma}{2}\, h,\ i = 1, \ldots, k-1\}$ we put $\widehat{Q} := \overline{Q}$, outside the tube Ω_γ we put $\widehat{Q} = 0$ and, in between, $\widehat{Q}$ is taken such that it is C_b^r. The first equation of (25) may be considered for all $X_0 \in \mathbb{R}^{km}$. Hence, for d and h small enough we have a smooth map from $\mathbb{R}^{km} \times \{Z \in \mathbb{R}^{kn} \,|\, |Z|_\infty \le d\}$ into itself of the form

$$(26) \qquad \begin{aligned} X_1 \quad &= \quad ((R - L_\alpha) \otimes I_m)\, X_0 + (e_k \otimes \widehat{P}(X_0; h)) \\ Z_1 \quad &= \quad (R \otimes I_n) Z_0 + (e_k \otimes \widehat{Q}(X_0; h)) \end{aligned}$$

with $\widehat{P} = O(h)$ and $\widehat{Q} = O(h)$. As done in [9] we apply the invariant manifold theory of [7] and the analogous construction yields the existence of an m-dimensional attractive invariant manifold for the modified map (26) (in the x, y-variables)

$$M_{h,0} = \{(x,y) \,|\, x \in \mathbb{R}^m,\ y = \sigma_0(x,h)\}$$

if started appropriately, i.e., $x_i = \Phi^i(x_0, h), i = 0, \ldots, k-1$. The closeness to M_0 is $\sigma_0(x,h) - s_0(x) = O(|\widehat{Q}|) = O(|Q|)$, the attractivity in y-direction is $y_j - \sigma_0(x_j, h) = z_j + \sigma_0(x_j, h) - s_0(x_j) = O(|\widehat{Q}|)$ for $j \ge k$ and $\chi_{h,0}^k = 0$ if $x_i = \Phi^i(x_0, h)$, $i = 0, \ldots, k-1$, and $M_{h,0}$ has a vertical stable foliation ($L_{12}^{h,0} = 0$, since the $O(h)$-terms in Eq. (26) 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 (25).

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. $(\overline{1})_0$ with $x(0) = x_0$ satisfies

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

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

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

that

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

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

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

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 $Q = O(h^p)$.

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. (24) 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 $(\overline{\mathrm{I}})_{\mathrm{h},0}$:

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

- Closeness to M_0:

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

- Infinite attractivity in x-direction: There is $\delta > 0$ such that

$$|-\sum_{i=0}^{k-1} \alpha_i \, G(x_i)| \leq \delta h \quad \text{implies} \quad G(x_j) = 0 \;\text{ for }\; j \geq k \, .$$

- Attractivity in y-direction:

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

in any case,

$$|y_j - \sigma_0(x_j,h)| \le K h^p \text{ for } j \ge k\,.$$

- 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

$$|y_j - y(jh)| \le |\sigma_0(x_j,h) - s_0(x_j)| + K\,|x_j - x(jh)|\,.$$

$\dashv$

In the case of general LMMs (i.e., $\beta \neq 0$ in Eq. (20) and Hypothesis $\mathrm{H}_{\mathrm{LMM}}$) the same invariant manifold result holds as in the BDF-like case (cf. also [9]). The attractivity in y-direction is $|y_j - \sigma(x_j,h)| \le K\,\chi_{h,0}^{j}\,\max_{0\le i<k}\{|y_i - \sigma_0(x_i,h)|\}$ for $j \ge k$ 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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