

Ecole polytechnique fédérale de Zurich Politecnico federale di Zurigo Swiss Federal Institute of Technology Zurich

Invariant manifolds and global error estimates of numerical integration schemes applied to stiff systems of singular perturbation type – Part II: Linear multistep methods

K. Nipp and D. Stoffer

Research Report No. 95-03 February 1995

Seminar für Angewandte Mathematik Eidgenössische Technische Hochschule CH-8092 Zürich Switzerland Invariant manifolds and global error estimates of numerical integration schemes applied to stiff systems of singular perturbation type – Part II: Linear multistep methods

> K. Nipp and D. Stoffer Seminar für Angewandte Mathematik Eidgenössische Technische Hochschule CH-8092 Zürich Switzerland

Research Report No. 95-03

February 1995

Abstract

It is shown that appropriate linear multi-step methods (LMMs) applied to singularly perturbed systems of ODEs preserve the geometric properties of the underlying ODE. If the ODE admits an attractive invariant manifold so does the LMM. The continuous as well as the discrete dynamical system restricted to their invariant manifolds are no longer stiff and the dynamics of the full systems is essentially described by the dynamics of the systems reduced to the manifolds. These results may be used to transfer properties of the reduced system to the full system. As an example global error bounds of LMM-approximations to singularly perturbed ODEs are derived.

Keywords: singular perturbation, attractive invariant manifold, stiff system, global error, BDF-method

Subject Classification: 65L, 34C

1 Introduction

As in Part I [12] we consider the singularly perturbed system of ODEs (1) below admitting a highly attractive invariant manifold M_{ϵ} . In Part I we have shown that appropriate RKmethods applied to Eq.(1) preserve this strong geometric property, i.e., they admit an attractive invariant manifold close to M_{ϵ} . Linear multistep methods (LMMs), however, cannot be considered as a map from phase space into itself. They are best described by a map in some high dimensional space. We show that in the high dimensional space the LMM-map admits an attractive invariant manifold $S_{h,\epsilon}$ of the same dimension as M_{ϵ} . This invariant manifold $S_{h,\epsilon}$ may be projected onto a manifold $M_{h,\epsilon}$ close to M_{ϵ} . On $S_{h,\epsilon}$ the LMM-map may be viewed as a one-step method acting on $M_{h,\epsilon}$. This means that also for appropriate LMMs the strong geometric property of the ODE (1) is preserved. These geometric results are worked out in Section 2 for BDF-like methods and in Section 4 for general stiff LMMs.

The dynamical systems restricted to the invariant manifolds M_{ϵ} and $M_{h,\epsilon}$, respectively, are no longer stiff as $\epsilon \to 0$. The dynamics of the full continuous system (1) is essentially described by the dynamics of the system reduced to M_{ϵ} . Analogously, the dynamics of the full discrete system defined by the LMM is essentially described by the reduced dynamics on $M_{h,\epsilon}$. Since the manifolds M_{ϵ} and $M_{h,\epsilon}$ are close to each other the discrete system on $M_{h,\epsilon}$ approximates the continuous system on M_{ϵ} . Due to the attractivity of the manifolds M_{ϵ} and $M_{h,\epsilon}$ the full discrete system approximates the full continuous system. This allows to introduce the following concept. The LMM applied to the stiff system (1) is reduced to a one-step method on $M_{h,\epsilon}$ approximating the reduced nonstiff continuous system on M_{ϵ} . Certain properties of the nonstiff continuous system are preserved under onestep discretisation. Moreover, bounds for the one-step approximation may be derived. Examples are: Global error bounds, existence of hyperbolic invariant curves (cf. Beyn [1], Eirola [3]), existence of attracting sets (cf. Kloeden, Lorenz [6]), behaviour near a hyperbolic equilibrium (cf. Beyn [2]). It is often possible to transfer these properties with the corresponding error bounds to the full systems.

This concept works for the above examples. In Sections 3 and 4 we carry out this procedure to derive global error bounds for LMMs applied to Eq.(1). Such error bounds were first obtained by Lubich [7] using completely different methods. Our results slightly generalize and slightly improve the results in [7] (cf. Remark 5) below).

The general concept of transferring properties of the reduced system on an attractive invariant manifold to the full system has been used in the following related situations: In Part I [12] to derive global error bounds for implicit RK-methods applied to Eq.(1); in Lubich, Nipp, Stoffer [8] to describe the behaviour of RK-solutions near a hyperbolic equilibrium of Eq.(1); to show the existence of hyperbolic invariant curves (in the nonstiff case) for general linear methods in Stoffer [14] and for variable step-size one-step methods in Stoffer, Nipp [16].

We consider the singularly perturbed autonomous system

(1)
$$\begin{aligned} \frac{dx}{dt} &= f(x,y)\\ \epsilon \frac{dy}{dt} &= g(x,y) \end{aligned}$$

where $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ and $\epsilon \in (0, \epsilon_0)$. We denote by C_b^r spaces of functions of class C^r with bounded derivatives.

We make the following

Hypothesis H_{DE}

- 1) f and g are bounded and there is r with $3 \le r < \infty$ 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 $B_0(x) := g_u(x, s_0(x))$ have real parts smaller than $-b_0$ for all $x \in \mathbb{R}^m$.

Under the above assumptions it can be shown that for all $\epsilon > 0$ small enough Eq.(1) admits an attractive invariant manifold $M_{\epsilon} = \{(x, y) | x \in \mathbb{R}^m, y = s(x, \epsilon)\}$ which is $O(\epsilon)$ -close to the so-called *reduced manifold* $M_0 := \{(x, y) | x \in \mathbb{R}^m, y = s_0(x)\}$. The precise result is proved in Nipp [9], [10] and summarized in Part I [12].

In this paper we investigate the geometric behaviour of the discrete system generated by a LMM applied to Eq.(1). A LMM of k steps applied to the differential equation dw/dt = F(w) is defined by

$$\sum_{j=0}^{k} \alpha_{j} w_{j} = h \sum_{j=0}^{k} \beta_{j} F(w_{j}), \quad \alpha_{k} = 1,$$

where $w_0, ..., w_{k-1}$ are given starting values approximating the solution w(t) at t = 0, h, ..., (k-1)h. For a general discussion of LMMs, see Hairer, Norsett, Wanner [4]. We make the following assumptions on the LMM which are appropriate to integrate stiff systems.

Hypothesis H_{LMM}

- 1) The LMM is an irreducible k-step method of order $p \ge 1$.
- 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 $\sigma_1 < 1$.

Notation: It is convenient to introduce the vectors $\alpha := (\alpha_0, ..., \alpha_{k-1})^T$ and $\beta := (\beta_0, ..., \beta_{k-1})^T$.

Remarks:

- 1) A LMM is called irreducible if the polynomials ρ and σ have no common zero. In the case $\beta = 0$ (BDF-like methods) this implies $\alpha_0 \neq 0$.
- 2) Our Hypothesis H_{LMM} is sufficient to show the results below for $\epsilon \ll h$ which is the important case for approximating solutions of Eq.(1) near the invariant manifold M_{ϵ} . The same results also hold for $\epsilon \leq ch$, c > 0, under the following additional assumptions (used in Lubich [7]):
 - i) There is $\alpha \in (0, \pi/2)$ such that all eigenvalues λ of $g_y(x, s_0(x))$ lie in the open sector $|\arg \lambda \pi| < \alpha$.

 \neg

ii) The LMM is $A(\alpha)$ -stable.

We apply a LMM satisfying Hypothesis H_{LMM} with p < r to Eq.(1):

(2)
$$\sum_{j=0}^{k} \alpha_j x_j = h \sum_{j=0}^{k} \beta_j f(x_j, y_j) , \quad \alpha_k = 1 .$$
$$\sum_{j=0}^{k} \alpha_j y_j = \frac{h}{\epsilon} \sum_{j=0}^{k} \beta_j g(x_j, y_j)$$

We show that for given starting values (x_j, y_j) , j = 0, ..., k - 1, Eq.(2) has a unique solution (x_k, y_k) in a neighbourhood of the invariant manifold M_{ϵ} . We introduce the new coordinate z measuring the difference to the manifold M_{ϵ} by the change of coordinates

$$y = s(x, \epsilon) + z \; .$$

Notation: In functions depending on h and/or ϵ we shall mostly suppress these arguments, for short. E.g., we shall write s(x) instead of $s(x, \epsilon)$.

We choose starting values with $|z_j| \leq d$, $0 \leq j < k$, where d will be determined later. In the y-equation of Eq.(2) we expand $g(x_k, s(x_k) + z_k)$ about $z_k = 0$ and obtain

$$\sum_{j=0}^{k} \alpha_j(s(x_j) + z_j) = \frac{h}{\epsilon} \beta_k[g(x_k, s(x_k)) + (B(x_k) + \hat{B}(x_k, z_k))z_k] \\ + \frac{h}{\epsilon} \sum_{j=0}^{k-1} \beta_j g(x_j, s(x_j) + z_j)$$

with $B(x_j) := g_y(x_j, s(x_j)) = B_0(x_j) + O(\epsilon)$ and $\hat{B}(x_j, z_j) = O(|z_j|)$. Collecting the terms in z_k (and using $\alpha_k = 1$) yields

$$z_{k} = C(x_{k}, z_{k})^{-1} \Big\{ \beta_{k} g(x_{k}, s(x_{k})) - \frac{\epsilon}{h} s(x_{k}) \\ + \sum_{j=0}^{k-1} \beta_{j} g(x_{j}, s(x_{j}) + z_{j}) - \frac{\epsilon}{h} \sum_{j=0}^{k-1} \alpha_{j}(s(x_{j}) + z_{j}) \Big\}$$

with

$$C(x_k, z_k) := -\beta_k (B(x_k) + \hat{B}(x_k, z_k)) + \frac{\epsilon}{h} I_n$$

where we have suppressed the dependence on ϵ and ϵ/h in C. Note that the matrix C is invertible for $|z_k| \leq d_k$ small enough. Eq.(2) now may be written as

(3)

$$x_{k} = -\sum_{j=0}^{k-1} [\alpha_{j} x_{j} - h \beta_{j} f(x_{j}, s(x_{j}) + z_{j})] + h \beta_{k} f(x_{k}, s(x_{k}) + z_{k})$$

$$z_{k} = C(x_{k}, z_{k})^{-1} \Big\{ \sum_{j=0}^{k-1} [\beta_{j} g(x_{j}, s(x_{j}) + z_{j}) - \frac{\epsilon}{h} \alpha_{j}(s(x_{j}) + z_{j})] + \beta_{k} g(x_{k}, s(x_{k})) - \frac{\epsilon}{h} s(x_{k}) \Big\}.$$

Using the Newton-Kantorovich theorem (cf., e.g., Ortega, Rheinboldt [13]) it can be shown that for h, ϵ/h and $|\beta|d$ sufficiently small Eq.(3) has a solution (x_k, z_k) in a ball $\mathcal{B}_{\mu_1}(x_k^0, 0)$, with $x_k^0 := -\sum_{j=0}^{k-1} \alpha_j x_j$, $\mu_1 = O(h + \epsilon/h + |\beta|d)$, and this solution is unique in $\mathbb{R}^m \times \{|z_k| \leq d_k\} \cap \mathcal{B}_{\mu_2}(x_k^0, 0)$, with $\mu_2 = O(1/(h + \epsilon/h + |\beta|d))$. From the implicit function theorem it follows that for small h, ϵ/h , $|\beta|d$ this solution is smooth with bounded derivatives.

It is useful to describe the LMM in the high dimensional space $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ with 'coordinates' (X, Y) for Eq.(2) and with 'coordinates' (X, Z) for Eq.(3), respectively. The 'components' of (X, Z) in $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ are $[X]_j \in \mathbb{R}^m$, j = 0, ..., k - 1, and $[Z]_j \in \mathbb{R}^n$, j = 0, ..., k - 1. Thus, in (X, Z)-coordinates the starting values $(x_j, z_j), j = 0, ..., k - 1$, may be dscribed as (X_0, Z_0) with $[X_0]_j = x_j$, $[Z_0]_j = z_j$, j = 0, ..., k - 1. We also introduce the vectors

$$X_{i} := \begin{pmatrix} x_{i} \\ \vdots \\ x_{i+k-1} \end{pmatrix}, \quad Z_{i} := \begin{pmatrix} z_{i} \\ \vdots \\ z_{i+k-1} \end{pmatrix}, \quad i \ge 0,$$

$$s(X) := \begin{pmatrix} s([X]_{0}) \\ \vdots \\ s([X]_{k-1}) \end{pmatrix}, \quad g(X, s(X)) := \begin{pmatrix} f([X]_{0}, s([X]_{0})) \\ \vdots \\ f([X]_{k-1}, s([X]_{k-1})) \end{pmatrix}, \text{ etc. },$$

in \mathbb{R}^{km} and \mathbb{R}^{kn} , respectively, as well as the $(kn \times kn)$ -block diagonal matrix diag $[B(X) + \hat{B}(X, Z)]$ consisting of the $(n \times n)$ -blocks $B([X]_j) + \hat{B}([X]_j, [Z]_j)$, j = 0, ..., k - 1. We shall also need the $k \times k$ matrices

$$R := \begin{pmatrix} 0 & 1 & \cdots & 0 \\ 0 & \cdots & 1 \\ 0 & \cdots & 0 \end{pmatrix}, \ L_{\alpha} := e_k \alpha^T = \begin{pmatrix} 0 \\ \alpha_0 \cdots \alpha_{k-1} \end{pmatrix}, \ L_{\beta} := e_k \beta^T = \begin{pmatrix} 0 \\ \beta_0 \cdots \beta_{k-1} \end{pmatrix}$$

where $e_k = (0, ..., 1)^T$. Now the LMM may be regarded as a map from $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ into itself. Note that Y = s(X) + Z describes the coordinate change from (X, Y) to (X, Z). With the notation introduced this map is implicitly given by (cf. Eq.(3))

(4)
$$X_1 = \left((R - L_{\alpha}) \otimes I_m \right) X_0 + h(L_{\beta} \otimes I_m) f(X_0, s(X_0) + Z_0) + h \beta_k \left(e_k \otimes f(x_k, s(x_k) + z_k) \right)$$

$$Z_1 = D(X_0, Z_0, x_k, z_k) Z_0 - \frac{\epsilon}{h} \left(e_k \otimes C(x_k, z_k)^{-1} \right) E(x_k, X_0)$$

where

E

$$D(X_0, Z_0, x_k, z_k) := (R \otimes I_n) - \frac{\epsilon}{h} \left(L_\alpha \otimes C(x_k, z_k)^{-1} \right) \\ + \left(L_\beta \otimes C(x_k, z_k)^{-1} \right) \operatorname{diag}[B(X_0) + \hat{B}(X_0, Z_0)] \\ (x_k, X_0) := s(x_k) - \frac{h}{\epsilon} \beta_k g(x_k, s(x_k)) + (\alpha^T \otimes I_n) s(X_0) - \frac{h}{\epsilon} \left(\beta^T \otimes I_n \right) g(X_0, s(X_0)) .$$

We have again suppressed the dependence on ϵ and ϵ/h . Note that using the definition of $C(x_k, z_k)$ and the fact that $\sum_{j=0}^{k-1} \alpha_j = -1$ the term $(L_\beta \otimes C(x_k, z_k)^{-1}) \operatorname{diag}[B(X_0) + \hat{B}(X_0, Z_0)]$ may easily be estimated as $-\frac{1}{\beta_k}(L_\beta \otimes I_n) + |\beta|O(\max_{0 \le j < k}\{|x_j - x_0|\} + h + d + \epsilon/h)$. Eq.(4) is a formulation of the LMM equivalent to Eq.(3) and therefore has a unique solution. Hence, Eq.(4) defines a smooth map \tilde{P} of the form

(4)
$$\widetilde{P}: \begin{pmatrix} X_0 \\ Z_0 \end{pmatrix} \longmapsto \begin{pmatrix} X_1 \\ Z_1 \end{pmatrix} = \begin{pmatrix} ((R-L_{\alpha}) \otimes I_m) X_0 + \hat{F}(X_0, Z_0) \\ \overline{D}(X_0, Z_0) Z_0 + \hat{G}(X_0, Z_0) \end{pmatrix}$$

defined for $X_0 \in \mathbb{R}^{km}$, $Z_0 \in \mathbb{R}^{kn}$ with $|Z_0|_{\infty} \leq d$. The functions \overline{D} , \hat{F} , \hat{G} are of class C_b^r . Here we use the norm $|Z_0|_{\infty} := \max_{0 \leq j < k} \{|z_j|\}$ where $|\cdot|$ is an arbitrary norm in \mathbb{R}^n .

2 An invariant manifold result for BDF-like methods

In this section we investigate LMMs with $\beta = 0$ satisfying Hypothesis H_{LMM} (e.g., BDFmethods with $k \leq 6$). Methods with $\beta = 0$ are particularly well suited for integrating stiff systems since they are σ_1 -stiffly stable for σ_1 arbitrarily small. Although the choice $\sigma_1 = 0$ is not possible, σ_1 may be allowed to depend on ϵ and h.

For $\beta = 0$ the implicit form of the map \tilde{P} (cf. Eq.(4)) simplifies to

(5)
$$X_{1} = \left((R - L_{\alpha}) \otimes I_{m} \right) X_{0} + h \beta_{k} (e_{k} \otimes f(x_{k}, s(x_{k}) + z_{k}))$$
$$Z_{1} = \left\{ (R \otimes I_{n}) - \frac{\epsilon}{h} \left(L_{\alpha} \otimes C(x_{k}, z_{k})^{-1} \right) \right\} Z_{0} - \frac{\epsilon}{h} \left(e_{k} \otimes C(x_{k}, z_{k})^{-1} \right) E(x_{k}, X_{0})$$

with $E(x_k, X_0) = s(x_k) + (\alpha^T \otimes I_n) s(X_0) - \frac{h}{\epsilon} \beta_k g(x_k, s(x_k))$. The k-th component z_k of Z_1 is $O(\epsilon/h)$ whereas the first k-1 components are $O(|Z_0|_{\infty})$. Since the map \tilde{P} shifts the components of Z_0 one position upwards it maps the set $\mathbb{R}^{km} \times \{Z \in \mathbb{R}^{kn} \mid |Z|_{\infty} \leq d\}$ into itself for ϵ/h sufficiently small. Moreover, all Z-components of the k-th iterate of \tilde{P} are of order $O(\epsilon/h)$. It is therefore useful to investigate the map

(6)
$$\Psi: \begin{pmatrix} X_0 \\ Z_0 \end{pmatrix} \longmapsto \begin{pmatrix} X_k \\ Z_k \end{pmatrix} := \tilde{P}^k \begin{pmatrix} X_0 \\ Z_0 \end{pmatrix} =: \begin{pmatrix} A X_0 + \hat{U}(X_0, Z_0) \\ V(X_0, Z_0) \end{pmatrix}$$

where A is invertible since $\alpha_0 \neq 0$ (cf. Remark 1)). The map Ψ is given by an implicit equation of the form

(6)
$$X_{k} = A X_{0} + h \overline{U}(X_{k}, Z_{k})$$
$$Z_{k} = \frac{\epsilon}{h} \left[H(X_{k}, Z_{k}) Z_{0} + \overline{V}(X_{0}, X_{k}, Z_{k}) \right]$$

where the functions $H, \overline{U}, \overline{V}$ (also depending on h and ϵ/h) are bounded with bounded derivatives for $X_0, X_k \in \mathbb{R}^{km}, Z_k \in \mathbb{R}^{kn}$ with $|Z_k|_{\infty} \leq d$, h and ϵ/h sufficiently small.

We apply Theorem 5 of [11] to the map Ψ . Let $a := |A^{-1}|$ and let L_{ij} be the Lipschitz constants of the functions \hat{U} and V with respect to X_0 and Z_0 . The constants L_{ij} may be

estimated as follows. Taking the derivatives with respect to X_0 and Z_0 in Eq.(6) yields

$$\frac{\partial X_k}{\partial X_0} = A + O(h) \frac{\partial X_k}{\partial X_0} + O(h) \frac{\partial Z_k}{\partial X_0}
\frac{\partial Z_k}{\partial X_0} = O\left(\frac{\epsilon}{h}\right) + O\left(\frac{\epsilon}{h}\right) \frac{\partial X_k}{\partial X_0} + O\left(\frac{\epsilon}{h}\right) \frac{\partial Z_k}{\partial X_0}
\frac{\partial X_k}{\partial Z_0} = O(h) \frac{\partial X_k}{\partial Z_0} + O(h) \frac{\partial Z_k}{\partial Z_0}
\frac{\partial Z_k}{\partial Z_0} = O\left(\frac{\epsilon}{h}\right) + O\left(\frac{\epsilon}{h}\right) \frac{\partial X_k}{\partial Z_0} + O\left(\frac{\epsilon}{h}\right) \frac{\partial Z_k}{\partial Z_0}.$$

Solving for the partial derivatives one gets for h and ϵ/h small enough

$$\frac{\partial X_k}{\partial X_0} = A + O(h), \quad \frac{\partial X_k}{\partial Z_0} = O(\epsilon),$$
$$\frac{\partial Z_k}{\partial X_0} = O\left(\frac{\epsilon}{h}\right), \quad \frac{\partial Z_k}{\partial Z_0} = O\left(\frac{\epsilon}{h}\right).$$

It follows that the Lipschitz constants L_{ij} satisfy

$$L_{11} = O(h) , \quad L_{12} = O(\epsilon) ,$$

$$L_{21} = O\left(\frac{\epsilon}{h}\right) , \quad L_{22} = O\left(\frac{\epsilon}{h}\right) .$$

Theorem 5 of [11] implies the existence of an invariant C_b^r -manifold $\tilde{N}_{h,\epsilon}$ for the map Ψ if the conditions

(7)

$$2\sqrt{L_{12} L_{21}} < \frac{1}{a} - L_{11} - L_{22} ,$$

$$L_{22} + L_{12} \lambda < \left(\frac{1}{a} - L_{11} - L_{12} \lambda\right)^{2}$$

with

$$\lambda = \frac{2L_{21}}{1/a - L_{11} - L_{22} + \sqrt{(1/a - L_{11} - L_{22})^2 - 4L_{12}L_{21}}}$$

hold. Using the estimates for L_{ij} above we find that for h and ϵ/h small enough $\lambda = O(\epsilon/h)$ and the two conditions are satisfied. (Note that the larger r the smaller ϵ/h has to be taken.) The invariant manifold $\tilde{N}_{h,\epsilon}$ is the graph of a smooth function $\tilde{\Sigma}$, i.e., $\tilde{N}_{h,\epsilon} = \{(X,Z)) \mid X \in \mathbb{R}^{km}, Z = \tilde{\Sigma}(X,h,\epsilon)\}$, and has the following properties.

a) $\tilde{\Sigma}$ is of order $O(\epsilon/h)$, λ -Lipschitz and is of class C_b^r with respect to X.

b) $\widetilde{N}_{h,\epsilon}$ is uniformly attractive for the map Ψ with attractivity constant $\chi(h,\epsilon) = O(\epsilon/h) < 1$, i.e., for every (X_0, Z_0) with $|Z_0|_{\infty} \leq d$

(8)
$$|Z_k - \widetilde{\Sigma}(X_k, h, \epsilon)|_{\infty} \le \chi(h, \epsilon) |Z_0 - \widetilde{\Sigma}(X_0, h, \epsilon)|_{\infty}$$

where $(X_k, Z_k) := \Psi(X_0, Z_0).$

c) $\widetilde{N}_{h,\epsilon}$ has the "property of asymptotic phase", i.e., for every (X_0, Z_0) with $|Z_0|_{\infty} \leq d$ there is $(\widetilde{X}_0, \widetilde{Z}_0) \in \widetilde{N}_{h,\epsilon}$ such that for $(X_{jk}, Z_{jk}) := \Psi^j(X_0, Z_0), (\widetilde{X}_{jk}, \widetilde{Z}_{jk}) := \Psi^j(\widetilde{X}_0, \widetilde{Z}_0)$

$$\begin{aligned} |\tilde{X}_{jk} - X_{jk}|_{\infty} &\leq c \,\chi(h,\epsilon)^j \,|\, Z_0 - \tilde{\Sigma}(X_0,h,\epsilon)|_{\infty} \\ |\tilde{Z}_{jk} - Z_{jk}|_{\infty} &\leq (1+\lambda c) \,\chi(h,\epsilon)^j \,|Z_0 - \tilde{\Sigma}(X_0,h,\epsilon)|_{\infty} \end{aligned} , \ j \geq 0 , \end{aligned}$$

holds with $c = O(\epsilon)$.

The manifold $\tilde{N}_{h,\epsilon}$ is also invariant for the map \tilde{P} given by Eq.(5) (cf. [11]). We transform $\tilde{N}_{h,\epsilon}$ and \tilde{P} back to the original coordinates (X, Y). In (X, Y)-coordinates the LMM generates a map

(9)
$$P: \begin{pmatrix} X_0 \\ Y_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ \vdots \\ x_{k-1} \\ y_0 \\ \vdots \\ y_{k-1} \end{pmatrix} \mapsto \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_k \\ y_1 \\ \vdots \\ y_k \end{pmatrix}$$

defined for $X_0 \in \mathbb{R}^{km}$, $Y_0 \in \mathbb{R}^{kn}$ with $|Y_0 - s(X_0)|_{\infty} \leq d$ admitting the invariant manifold $N_{h,\epsilon} := \{(X,Y) \mid X \in \mathbb{R}^{km}, Y = \Sigma(X,h,\epsilon) := s(X,\epsilon) + \tilde{\Sigma}(X,h,\epsilon)\}$ with the properties given in

Proposition 1 Let the differential equation (1) satisfy Hypothesis H_{DE} . Apply a LMM with $\beta = 0$ satisfying Hypothesis H_{LMM} to Eq.(1) and assume p < r.

Then there are constants h_0, δ_0, d, K and a function $\Sigma : \Omega_{h_0,\delta_0} \to \mathbb{R}^{kn}, \Omega_{h_0,\delta_0} := \{(X, h, \epsilon) | X \in \mathbb{R}^{km}, h \in (0, h_0), \epsilon \in (0, h\delta_0)\}, \Sigma \text{ of class } C_b^r \text{ with respect to } X, \text{ such that for all } h \leq h_0, \epsilon/h \leq \delta_0 \text{ the following assertions hold.}$

i) The set $N_{h,\epsilon} := \{(X,Y) \mid X \in \mathbb{R}^{km}, Y = \Sigma(X,h,\epsilon)\}$ is invariant under the map P, i.e., $P(N_{h,\epsilon}) = N_{h,\epsilon}$. ii) The manifold $N_{h,\epsilon}$ is attractive for the map P in the following sense: For all (X_0, Y_0) with $|Y_0 - s(X_0, \epsilon)|_{\infty} \leq d$ the estimates

$$|Y_{\ell} - \Sigma(X_{\ell}, h, \epsilon)|_{\infty} \leq (1 + K\epsilon) |Y_0 - \Sigma(X_0, h, \epsilon)|_{\infty}, \quad 0 \leq \ell < k,$$

$$|Y_k - \Sigma(X_k, h, \epsilon)|_{\infty} \leq \chi(h, \epsilon) |Y_0 - \Sigma(X_0, h, \epsilon)|_{\infty}$$

hold with $\chi(h, \epsilon) = K\epsilon/h < 1$.

iii) The "property of asymptotic phase" holds, i.e., for every (X_0, Y_0) with $|Y_0 - s(X_0, \epsilon)|_{\infty} \leq d$ there is $(\widetilde{X}_0, \widetilde{Y}_0) \in N_{h,\epsilon}$ such that for $(X_i, Y_i) := P^i(X_0, Y_0)$, $(\widetilde{X}_i, \widetilde{Y}_i) := P^i(\widetilde{X}_0, \widetilde{Y}_0), i \geq 0$, the estimates

$$\begin{aligned} |\tilde{X}_{jk+\ell} - X_{jk+\ell}|_{\infty} &\leq K \epsilon \, \chi(h,\epsilon)^j \, |Y_0 - \Sigma(X_0,h,\epsilon)|_{\infty} \\ |\tilde{Y}_{jk+\ell} - Y_{jk+\ell}|_{\infty} &\leq (1+K \epsilon) \, \chi(h,\epsilon)^j \, |Y_0 - \Sigma(X_0,h,\epsilon)|_{\infty} \end{aligned}$$

hold for $j \in \mathbb{N}_0$, $0 \leq \ell < k$.

iv) The function Σ satisfies the estimate

$$|\Sigma(X,h,\epsilon) - s(X,\epsilon)|_{\infty} \le K \frac{\epsilon}{h}$$
.

Proof: ii) It suffices to verify the first estimate for $\ell = 1$ (cf. Eq.(8)). We show the estimate in the (X, Z)-coordinates:

$$|Z_1 - \widetilde{\Sigma}(X_1)|_{\infty} \le (1 + K \epsilon) |Z_0 - \widetilde{\Sigma}(X_0)|_{\infty}.$$

Let $(\overline{X}_j, \overline{Z}_j) := \widetilde{P}^j(X_0, \widetilde{\Sigma}(X_0)), \ j \ge 0$. For the components of $X_1, \overline{X}_1, Z_1, \overline{Z}_1 = \widetilde{\Sigma}(\overline{X}_1)$ we have

(10)
$$\begin{aligned} [X_{1}]_{i} &= x_{i+1} &= [X_{0}]_{i+1} , \ 0 \leq i < k-1 ,\\ [\overline{X}_{1}]_{i} &= x_{i+1} &= [X_{0}]_{i+1} , \ 0 \leq i < k-1 ,\\ [X_{1}]_{k-1} &= x_{k} &= [X_{k}]_{0} \\ [\overline{X}_{1}]_{k-1} &= [\overline{X}_{k}]_{0} \end{aligned}$$

and

(11)
$$\begin{bmatrix} Z_1]_i &= z_{i+1} &= [Z_0]_{i+1} &, \ 0 \le i < k-1 , \\ [\tilde{\Sigma}(\overline{X}_1)]_i &= [\overline{Z}_1]_i &= [\overline{Z}_0]_{i+1} = [\tilde{\Sigma}(X_0)]_{i+1}, \\ [Z_1]_{k-1} &= z_k &= [Z_k]_0 \\ [\tilde{\Sigma}(\overline{X}_1)]_{k-1} &= [\overline{Z}_k]_0 &= [\tilde{\Sigma}(\overline{X}_k)]_0 .$$

Note that $(X_k, Z_k) = \Psi(X_0, Z_0), (\overline{X}_k, \overline{Z}_k) = \Psi(X_0, \widetilde{\Sigma}(X_0))$ for the map Ψ given in Eq.(6). We estimate

(12)
$$|Z_1 - \widetilde{\Sigma}(X_1)|_{\infty} \le |Z_1 - \widetilde{\Sigma}(\overline{X}_1)|_{\infty} + |\widetilde{\Sigma}(\overline{X}_1) - \widetilde{\Sigma}(X_1)|_{\infty}.$$

For the second term on the right-hand side we have $|\tilde{\Sigma}(\overline{X}_1) - \tilde{\Sigma}(X_1)|_{\infty} \leq \lambda |\overline{X}_1 - X_1|_{\infty}$. Eq.(10) implies

$$|X_1 - \overline{X}_1|_{\infty} = |[X_k - \overline{X}_k]_0| \le |X_k - \overline{X}_k|_{\infty}.$$

From Eq.(6) we know that

(13)
$$\begin{aligned} |X_k - \overline{X}_k|_{\infty} &\leq |\hat{U}(X_0, Z_0) - \hat{U}(X_0, \widetilde{\Sigma}(X_0))|_{\infty} \\ &\leq L_{12} |Z_0 - \widetilde{\Sigma}(X_0)|_{\infty} . \end{aligned}$$

Since $L_{12} = O(\epsilon)$ we have

$$|\widetilde{\Sigma}(\overline{X}_1) - \widetilde{\Sigma}(X_1)|_{\infty} \le \operatorname{const} \lambda \epsilon |Z_0 - \widetilde{\Sigma}(X_0)|_{\infty}.$$

For the first term on the right-hand side in (12) Eq.(11) implies

$$[Z_1 - \widetilde{\Sigma}(\overline{X}_1)]_{\infty} = \max\{\max_{0 \le i < k-1} \{ |[Z_0 - \widetilde{\Sigma}(X_0)]_{i+1}| \}, |[Z_k - \widetilde{\Sigma}(\overline{X}_k)]_0| \}$$

$$\leq \max\{ |Z_0 - \widetilde{\Sigma}(X_0)|_{\infty}, |Z_k - \widetilde{\Sigma}(\overline{X}_k)|_{\infty} \}.$$

Using Eqs.(8), (13) we find

$$|Z_k - \widetilde{\Sigma}(\overline{X}_k)|_{\infty} \leq |Z_k - \widetilde{\Sigma}(X_k)|_{\infty} + |\widetilde{\Sigma}(X_k) - \widetilde{\Sigma}(\overline{X}_k)|_{\infty}$$

$$\leq (\chi(h, \epsilon) + \operatorname{const} \lambda \epsilon) |Z_0 - \widetilde{\Sigma}(X_0)|_{\infty}$$

and hence $|Z_1 - \tilde{\Sigma}(\overline{X}_1)|_{\infty} \leq |Z_0 - \tilde{\Sigma}(X_0)|_{\infty}$ for ϵ sufficiently small. Inserting the estimates obtained into Eq.(12) we conclude

$$|Z_1 - \widetilde{\Sigma}(X_1)|_{\infty} \le (1 + \operatorname{const} \lambda \,\epsilon) \, |Z_0 - \widetilde{\Sigma}(X_0)|_{\infty} \, .$$

iii) From the property of asymptotic phase of the map Ψ we know that there is $c \leq \text{const } \epsilon$ such that for $j \in \mathbb{N}_0, 0 \leq \ell < k$,

$$\begin{aligned} |\tilde{X}_{jk+\ell} - X_{jk+\ell}|_{\infty} &\leq c \,\chi^j |Z_\ell - \tilde{\Sigma}(X_\ell)|_{\infty} \\ |\tilde{Z}_{jk+\ell} - Z_{jk+\ell}|_{\infty} &\leq (1+\lambda c) \,\chi^j |Z_\ell - \tilde{\Sigma}(X_\ell)|_{\infty} \end{aligned}$$

Here we have viewed (X_{ℓ}, Z_{ℓ}) as starting point of the map Ψ . Now ii) implies the estimates claimed. \bot

Proposition 1 implies that the dynamics of the LMM is essentially described by its dynamics restricted to the manifold $N_{h,\epsilon}$. Y_0 is entirely determined by X_0 for any point $(X_0, Y_0) \in N_{h,\epsilon}$, i.e., $Y_0 = \Sigma(X_0, h, \epsilon)$. The LMM-map P is then determined by the map

(14)
$$P_X: X_0 = \begin{pmatrix} x_0 \\ \vdots \\ x_{k-1} \end{pmatrix} \longmapsto X_1 = \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix}$$

where X_1 is given by the implicit equation

(14)
$$X_1 = \left((R - L_\alpha) \right) \otimes I_m \right) X_0 + h\beta_k \left(e_k \otimes f(x_k, [\Sigma(X_1, h, \epsilon)]_{k-1}) \right)$$

Thus, restricting the LMM to the manifold $N_{h,\epsilon}$ reduces the original stiff problem to a nonstiff one. Therefore the nonstiff theory may be applied. As shown in Kirchgraber [5], Stoffer [15] there is an invariant manifold in \mathbb{R}^{km} of dimension m on which the map P_X is equivalent to a one-step method Φ . The existence of this manifold is established as follows. Hypothesis H_{LMM} 2) implies that the matrix $R - L_{\alpha}$ has 1 as a simple eigenvalue and all other eigenvalues have modulus smaller than $\rho_1 < 1$. Introducing new coordinates (x^*, X_a^*) by

$$X = (T \otimes I_m) \left(\begin{array}{c} x^* \\ X_a^* \end{array}\right)$$

with an appropriate choice of T it may be achieved that

$$T^{-1}(R-L_{\alpha})T = \begin{pmatrix} 1 & 0\\ 0 & Q_a \end{pmatrix}$$
 with $|Q_a|_{\infty} < \rho_1$.

In the new coordinates the map is contracting in the X_a^* -part. This allows to prove the existence of an invariant manifold being the graph of some function $\xi^*(x^*, h, \epsilon)$. In the original coordinates this manifold may be described as the graph of a function $\xi(x, h, \epsilon)$ or by a one-step method Φ (Φ^i denotes the *i*-th iterate of Φ):

(15)
$$\left\{X = \begin{pmatrix} x\\ \xi(x,h,\epsilon) \end{pmatrix} \mid x \in \mathbb{R}^m, \ [X]_i = \Phi^i(x,h,\epsilon), \ i = 0, ..., k-1\right\}.$$

Projecting this manifold into the manifold $N_{h,\epsilon}$ one obtains an *m*-dimensional invariant manifold $S_{h,\epsilon}$ in the space $\mathbb{R}^{km} \times \mathbb{R}^{kn}$ with the following properties.

Theorem 2 Let the differential equation (1) satisfy Hypothesis H_{DE} . Apply a LMM with $\beta = 0$ satisfying Hypothesis H_{LMM} to Eq.(1) and assume p < r.

Then there are constants h_0, δ_0, d, K and functions $\Phi : D_{h_0,\delta_0} \to \mathbb{R}^m, \sigma : D_{h_0,\delta_0} \to \mathbb{R}^n,$ $D_{h_0,\delta_0} := \{(x,h,\epsilon) \mid x \in \mathbb{R}^m, h \in (0,h_0), \epsilon \in (0,h\delta_0)\}, \sigma \text{ of class } C_b^r \text{ with respect to } x,$ such that with

$$\begin{array}{llll} \Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) & := & \max_{1 \le i < k} & |x_i - \Phi^i(x_0, h, \epsilon)| \\ \Delta_y(x_0, \dots, x_{k-1}, y_0, \dots, y_{k-1}, h, \epsilon) & := & \max_{0 \le i < k} & |y_i - \sigma(x_i, h, \epsilon)| \end{array}$$

the following assertions hold for all $h \leq h_0$, $\epsilon/h \leq \delta_0$.

- i) The set $S_{h,\epsilon} := \{(x_0, ..., x_{k-1}, y_0, ..., y_{k-1}) \mid x_0 \in \mathbb{R}^m, x_i = \Phi^i(x_0, h, \epsilon), y_i = \sigma(x_i, h, \epsilon), i = 0, ..., k-1\}$ is invariant under the map P, i.e., $P(S_{h,\epsilon}) = S_{h,\epsilon}$.
- ii) The manifold $S_{h,\epsilon}$ is attractive for the map P in the following sense: For all starting values $(x_i, y_i), i = 0, ..., k 1$, with $|y_i s(x_i, \epsilon)| \leq d$ the estimates

$$\begin{aligned} |x_{jk+\ell+1} - \Phi(x_{jk+\ell}, h, \epsilon)| &\leq K \kappa(h)^{jk+\ell} \Big(\Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) \\ &+ \epsilon \Delta_y(x_0, \dots, y_{k-1}, h, \epsilon) \Big) \\ |y_{jk+\ell} - \sigma(x_{jk+\ell}, h, \epsilon)| &\leq K \kappa(h)^{jk+\ell} \Big(\Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) \\ &+ \epsilon \Delta_y(x_0, \dots, y_{k-1}, h, \epsilon) \Big) \\ &+ (1 + K\epsilon) \chi(h, \epsilon)^j \Delta_y(x_0, \dots, y_{k-1}, h, \epsilon) \end{aligned}$$

hold for all $j \ge 0$, $0 \le \ell < k$, with $\kappa(h) = \rho_1 + Kh < 1$ and $\chi(h, \epsilon) = K\epsilon/h < 1$.

iii) The "property of asymptotic phase" holds, i.e., for all starting values (x_i, y_i) , i = 0, ..., k - 1, with $|y_i - s(x_i, \epsilon)| \leq d$ there is \hat{x}_0 such that for $\hat{x}_i := \Phi^i(\hat{x}_0, h, \epsilon)$, $\hat{y}_i := \sigma(\hat{x}_i, h, \epsilon), i \geq 0$, the estimates

$$\begin{aligned} |\hat{x}_{jk+\ell} - x_{jk+\ell}| &\leq K \,\kappa(h)^{jk+\ell} \Big(\Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) + \epsilon \,\Delta y(x_0, \dots, y_{k-1}, h, \epsilon) \Big) \\ |\hat{y}_{jk+\ell} - y_{jk+\ell}| &\leq K \,\kappa(h)^{jk+\ell} \Big(\Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) + \epsilon \,\Delta y(x_0, \dots, y_{k-1}, h, \epsilon) \Big) \\ &+ (1 + K\epsilon) \,\chi(h, \epsilon)^j \,\Delta_y(x_0, \dots, y_{k-1}, h, \epsilon) \end{aligned}$$

hold for $j \ge 0, 0 \le \ell < k$.

iv) The function σ satisfies the estimate

$$|\sigma(x,h,\epsilon) - s(x,\epsilon)| \le K\epsilon h^p$$
.

v) The function Φ is a one-step method of order p for the differential equation $\dot{x} = f(x, s(x, \epsilon)), i.e.,$

$$\Phi(x, h, \epsilon) - \varphi^h(x, \epsilon) = O(h^{p+1})$$

where $\varphi^t(x,\epsilon)$ is the solution of $\dot{x} = f(x, s(x,\epsilon))$ with $\varphi^0(x,\epsilon) = x$.

The situation concerning the manifolds $N_{h,\epsilon}$ and $S_{h,\epsilon}$ as given in Proposition 1 and Theorem 2, respectively, is sketched in Fig. 1.



Fig. 1: The invariant manifolds $N_{h,\epsilon}$ and $S_{h,\epsilon}$

Proof of Theorem 2: i) We have already shown that the map P generated by the LMM has an invariant manifold $S_{h,\epsilon}$. In (X, Z)-coordinates this invariant manifold is denoted by $\tilde{S}_{h,\epsilon}$. We already know that

$$\widetilde{S}_{h,\epsilon} = \{ (X,Z) \mid x \in \mathbb{R}^m, \ [X]_i = \Phi^i(x), \ i = 0, ..., k - 1, \ Z = \widetilde{\Sigma}(X) \} .$$

For $x_i = \Phi^i(x_0)$ we have

$$[\tilde{\Sigma}(x_0, ..., x_{k-1})]_i = \left[\tilde{\Sigma}\left(\Phi^{-i}(x_i), ..., \Phi^{k-1-i}(x_i)\right)\right]_i, \quad i = 0, ..., k-1,$$

and hence we may define

$$\widetilde{\sigma}_i(x) := \left[\widetilde{\Sigma}\left(\Phi^{-i}(x), ..., \Phi^{k-1-i}(x)\right)\right]_i, \quad i = 0, ..., k-1.$$

The map \tilde{P} shifts the components of X_0 , Z_0 one position upwards (cf. Eq.(11)). Hence for $(X_0, Z_0) \in \tilde{S}_{h,\epsilon}$

$$z_i = [\tilde{\Sigma}(x_0, ..., x_{k-1})]_i = [\tilde{\Sigma}(x_1, ..., x_k)]_{i-1}, \quad i = 1, ..., k-1$$

holds. Using the definition of $\tilde{\sigma}_i$ we obtain

$$z_i = \widetilde{\sigma}_i(x_i) = \widetilde{\sigma}_{i-1}(x_i), \quad i = 1, \dots, k-1 ,$$

implying $\tilde{\sigma}_0 = \tilde{\sigma}_1 = ... = \tilde{\sigma}_{k-1} =: \tilde{\sigma}$. It follows that in the (X, Y)-coordinates the manifold $S_{h,\epsilon}$ is described by the functions $\Phi(x)$ and $\sigma(x) := s(x) + \tilde{\sigma}(x)$.

iii) We know from Proposition 1 iii) that for given $(X_0, Y_0) \in \mathbb{R}^{km} \times \mathbb{R}^{kn}$ with $|Y_0 - s(X_0)|_{\infty} \leq d$ there is $(\tilde{X}_0, \tilde{Y}_0) \in N_{h,\epsilon}$ such that the orbits $\{(X_i, Y_i)\}_{i\geq 0} := \{P^i(X_0, Y_0)\}_{i\geq 0}$, $\{(\tilde{X}_i, \tilde{Y}_i)\}_{i\geq 0} := \{P^i(\tilde{X}_0, \tilde{Y}_0)\}_{i\geq 0}$ tend exponentially together. On the other hand, it follows from [5], [15] that there is $\hat{X}_0 = (\hat{x}_0, \xi(\hat{x}_0)) = (\hat{x}_0, \Phi(\hat{x}_0), ..., \Phi^{k-1}(\hat{x}_0)) \in S_{h,\epsilon}$ such that for $\hat{X}_i := P_X^i(\hat{X}_0)$ (P_X defined in Eq.(14); note that $\tilde{X}_i = P_X^i(\tilde{X}_0)$) the following estimate holds

$$|\hat{X}_i - \tilde{X}_i|_{\infty} \le \operatorname{const} \kappa^i \Delta_x(\tilde{X}_0)$$
.

From Proposition 1 iii) we get

$$\begin{aligned} \Delta_x(X_0) &\leq \quad \Delta_x(X_0) + \operatorname{Lip}(\Delta_x) |X_0 - X_0|_{\infty} \\ &\leq \quad \Delta_x(X_0) + \operatorname{const} \epsilon |Y_0 - \Sigma(X_0))|_{\infty} . \end{aligned}$$

Combining these estimates with the first estimate of Proposition 1 iii) and using $\chi^j \leq \text{const } \kappa^{jk+\ell}$ we find for $j \geq 0, 0 \leq \ell < k$,

$$|\hat{X}_{jk+\ell} - X_{jk+\ell}|_{\infty} \le \operatorname{const} \kappa^{jk+\ell} \left(\Delta_x(X_0) + \epsilon |Y_0 - \Sigma(X_0)|_{\infty}) \right).$$

Setting $\hat{Y}_i := \Sigma(\hat{X}_i)$ we get from Proposition 1 iii) that

$$\begin{aligned} |\hat{Y}_{jk+\ell} - Y_{jk+\ell}|_{\infty} &\leq |\hat{Y}_{jk+\ell} - \tilde{Y}_{jk+\ell}|_{\infty} + |\tilde{Y}_{jk+\ell} - Y_{jk+\ell}|_{\infty} \\ &= |\Sigma(\hat{X}_{jk+\ell}) - \Sigma(\tilde{X}_{jk+\ell})|_{\infty} + |\tilde{Y}_{jk+\ell} - Y_{jk+\ell}|_{\infty} \\ &\leq \operatorname{const} \kappa^{jk+\ell} \Big(\Delta_x(X_0) + \operatorname{const} \epsilon |Y_0 - \Sigma(X_0)|_{\infty} \Big) \\ &+ (1 + \operatorname{const} \epsilon) \chi^j |Y_0 - \Sigma(X_0)|_{\infty} \,. \end{aligned}$$

Estimating $Y_0 - \Sigma(X_0)$ as

$$|Y_0 - \Sigma(X_0)|_{\infty} \leq |Y_0 - \Sigma(x_0, \xi(x_0))|_{\infty} + |\Sigma(x_0, \xi(x_0)) - \Sigma(X_0)|_{\infty}$$

$$\leq \Delta_y(X_0, Y_0) + \operatorname{Lip}(\Sigma) \Delta_x(X_0)$$

we have shown that for (X_0, Y_0) with $|Y_0 - s(X_0)|_{\infty} \leq d$ there is $(\hat{X}_0, \hat{Y}_0) \in S_{h,\epsilon}$ such that for $(X_i, Y_i) := P^i(X_0, Y_0), (\hat{X}_i, \hat{Y}_i) := P^i(\hat{X}_0, \hat{Y}_0) \in S_{h,\epsilon}, i \geq 0$, the estimates

$$\begin{aligned} |\hat{X}_{jk+\ell} - X_{jk+\ell}|_{\infty} &\leq \operatorname{const} \kappa^{jk+\ell} \Big(\Delta_x(X_0) + \epsilon \, \Delta_y(X_0, Y_0) \Big) \\ |\hat{Y}_{jk+\ell} - Y_{jk+\ell}|_{\infty} &\leq \operatorname{const} \kappa^{jk+\ell} \Big(\Delta_x(X_0) + \epsilon \, \Delta_y(X_0, Y_0) \Big) \\ &+ (1 + \operatorname{const} \epsilon) \, \chi^j \Big(\operatorname{const} \Delta_x(X_0) + \Delta_y(X_0, Y_0) \Big) \end{aligned}$$

hold for $j \ge 0, 0 \le \ell < k$. This proves assertion iii).

ii) is a consequence of iii). We estimate

$$\begin{aligned} |x_{jk+\ell+1} - \Phi(x_{jk+\ell})| &\leq |x_{jk+\ell+1} - \hat{x}_{jk+\ell+1}| + |\Phi(\hat{x}_{jk+\ell}) - \Phi(x_{jk+\ell})| \\ &\leq \operatorname{const} \kappa^{jk+\ell} \left(\Delta_x(x_0, ..., x_{k-1}) + \epsilon \Delta_y(x_0, ..., y_{k-1}) \right) \\ |y_{jk+\ell} - \sigma(x_{jk+\ell})| &\leq |y_{jk+\ell} - \hat{y}_{jk+\ell}| + |\sigma(\hat{x}_{jk+\ell}) - \sigma(x_{jk+\ell})| \\ &\leq \operatorname{const} \kappa^{jk+\ell} \left(\Delta_x(x_0, ..., x_{k-1}) + \epsilon \Delta_y(x_0, ..., y_{k-1}) \right) \\ &+ (1 + \operatorname{const} \epsilon) \chi^j \Delta_y(x_0, ..., y_{k-1}) . \end{aligned}$$

iv) We apply the LMM to Eq.(1) with initial condition (x(0), y(0)), taking starting values $x_0 = x(0), y_0 = y(0)$ and $(X_0, Y_0) \in S_{h,\epsilon}$. In (X, Z)-coordinates the LMM is described by the map \tilde{P} given in Eq.(5). In order to estimate $|\sigma - s|$ we derive a better estimate for $E(x_k, X_0)$. We consider solutions (u(t), v(t)) of Eq.(1) on the manifold M_{ϵ} with u(0) = x(0). These solutions satisfy the differential equation

(16)
$$\dot{u} = f(u, s(u))$$
$$\dot{v} = \frac{1}{\epsilon} g(u, s(u)) = s'(u) f(u, s(u))$$

The identity $g(u, s(u)) = \epsilon s'(u) f(u, s(u))$ follows from v(t) = s(u(t)). We apply the LMM to Eq.(16) with starting values

(17)
$$u_i = u(ih) \\ v_i = v(ih) = s(u(ih)) , \quad i = 0, ..., k - 1.$$

We obtain

(18)
$$U_{1} = \left((R - L_{\alpha}) \otimes I_{m} \right) U_{0} + h \beta_{k} (e_{k} \otimes f(u_{k}, s(u_{k})))$$
$$V_{1} = \left((R - L_{\alpha}) \otimes I_{n} \right) V_{0} + \frac{h}{\epsilon} \beta_{k} (e_{k} \otimes g(u_{k}, s(u_{k}))) .$$

We first estimate $E(u_k, U_0)$. By our choice of starting values we have $V_0 = s(U_0)$. Using the last component of the second equation of (18) we find

$$E(u_k, U_0) = s(u_k) + (\alpha^T \otimes I_n) s(U_0) - \frac{h}{\epsilon} \beta_k g(u_k, s(u_k))$$

= $s(u_k) - v_k$.

Since the LMM is of order p and since f, g and s are of class C_b^r with r > p we have

$$O(h^{p+1}) = v_k - v(kh) = v_k - s(u(kh)) = v_k - s(u_k) + O(h^{p+1})$$

implying $E(u_k, U_0) = O(h^{p+1}).$

We next estimate $E(x_k, X_0) - E(u_k, U_0)$. Taking the difference of the first equations in Eqs. (5), (18) we obtain

(19)
$$x_k - u_k = O(1)(X_0 - U_0) + O(h)z_k .$$

From the second equation of (5) we find

$$z_k = O(1) Z_0 + O\left(\frac{\epsilon}{h}\right) E(x_k, X_0)$$

= $O(1) Z_0 + O\left(\frac{\epsilon}{h}\right) \left(E(x_k, X_0) - E(u_k, U_0)\right) + O(\epsilon h^p)$

Inserting this expression for z_k into Eq.(19) and using $E(x_k, X_0) - E(u_k, U_0) = O(1)(x_k - u_k) + O(1)(X_0 - U_0)$ we get

$$E(x_k, X_0) - E(u_k, U_0) = O(1)(X_0 - U_0) + O(h) Z_0 + O(\epsilon h^{p+1}) + O(\epsilon) (E(x_k, X_0) - E(u_k, U_0)).$$

We solve for $E(x_k, X_0) - E(u_k, U_0)$ and find with $E(u_k, U_0) = O(h^{p+1})$ that

$$E(x_k, X_0) = O(1)(X_0 - U_0) + O(h) Z_0 + O(h^{p+1}).$$

From Eq.(5) we obtain

$$Z_1 = \left[(R \otimes I_n) - \frac{\epsilon}{h} \left(L_\alpha \otimes C(x_k, z_k)^{-1} \right) + O(\epsilon) \right] Z_0 + O\left(\frac{\epsilon}{h}\right) (X_0 - U_0) + O(\epsilon h^p) .$$

Since the initial values (X_0, Z_0) are in $\tilde{S}_{h,\epsilon}$ we obtain for the last component

$$\tilde{\sigma}(x_k) = O\left(\frac{\epsilon}{h}\right) \begin{pmatrix} \tilde{\sigma}(x_0) \\ \vdots \\ \tilde{\sigma}(x_{k-1}) \end{pmatrix} + O\left(\frac{\epsilon}{h}\right) (X_0 - U_0) + O(\epsilon h^p)$$

This implies

$$|\tilde{\sigma}| \leq \operatorname{const}\left[\frac{\epsilon}{h} |\tilde{\sigma}| + \frac{\epsilon}{h} |X_0 - U_0|_{\infty} + \epsilon h^p\right]$$

and therefore

(20)
$$|\tilde{\sigma}| \leq \operatorname{const} \left[\frac{\epsilon}{h} |X_0 - U_0|_{\infty} + \epsilon h^p\right].$$

We apply the LMM to $\dot{u} = f(u, s(u))$. This LMM-map is given by the U-equation of Eq.(18). We know from [15] that this map admits an invariant manifold $\{(u_0, \eta(u_0, h))\}$ and that our starting values U_0 are $O(h^{p+1})$ -close to this manifold. Since (X_0, Z_0) in $\tilde{S}_{h,\epsilon}$ we have $z_i = \tilde{\sigma}(x_i), i = 0, ..., k$ (cf. proof of i)). Inserting these relations into the X-equation of Eq.(5) we obtain

(21)
$$X_1 = \left((R - L_\alpha) \otimes I_m \right) X_0 + h \,\beta_k (e_k \otimes f \left(x_k, s(x_k) + \tilde{\sigma}(x_k) \right) \,.$$

We already know that the map $P_X : X_0 \mapsto X_1$ admits the invariant manifold $\{(x_0, \xi(x_0, h, \epsilon))\}$ (cf. Eq.(15)). Moreover, this map is a perturbation of the map $U_0 \mapsto U_1$. Therefore Corollary 4 of [11] implies

$$\xi - \eta = O(h|\widetilde{\sigma}|) = O(\epsilon |X_0 - U_0|_{\infty} + \epsilon h^{p+1}) .$$

Since $X_0 - U_0 = [(x_0, \xi(x_0, h, \epsilon)) - (u_0, \eta(u_0, h))] + [(u_0, \eta(u_0, h)) - U_0] = O(|\xi - \eta|) + O(h^{p+1})$ we get $\xi - \eta = O(\epsilon h^{p+1})$ and therefore $X_0 - U_0 = O(h^{p+1})$. From Eq.(20) we find

$$\sigma - s = \tilde{\sigma} = O(\epsilon h^p) \; .$$

v) Let us denote the solution of $\dot{x} = f(x, s(x, \epsilon) + \tilde{\sigma}(x, h, \epsilon))$ with initial value x by $\varphi_1^t(x, h, \epsilon)$. The LMM applied to this differential equation has the form of Eq.(21). According to [5], [15] this LMM-map admits the invariant manifold (15) where the function Φ is a one-step method of order p, i.e., it satisfies $\Phi(x, h, \epsilon) - \varphi_1^h(x, h, \epsilon) = O(h^{p+1})$. From $\varphi_1^h(x, h, \epsilon) - \varphi^h(x, \epsilon) = O(h|\tilde{\sigma}|) = O(\epsilon h^{p+1})$ it follows that

$$\begin{aligned} |\Phi(x,h,\epsilon) - \varphi^h(x,\epsilon)| &\leq |\Phi(x,h,\epsilon) - \varphi^h_1(x,h,\epsilon)| + |\varphi^h_1(x,h,\epsilon)| - \varphi^h(x,\epsilon)| \\ &\leq \operatorname{const} \left(h^{p+1} + \epsilon h^{p+1}\right). \end{aligned}$$

We stress the geometric aspects of a LMM applied to Eq.(1) in a corollary. The differential equation (1) admits a highly attractive invariant manifold $M_{\epsilon} = \{(x, y) | x \in \mathbb{R}^m, y = s(x, \epsilon)\}$. From Theorem 2 we conclude that the discrete system generated by the LMM admits a manifold $M_{h,\epsilon} = \{(x, y) | x \in \mathbb{R}^m, y = \sigma(x, h, \epsilon)\}$ close to M_{ϵ} (cf. Fig. 2).



Fig. 2: The invariant manifolds $S_{h,\epsilon}$, $M_{h,\epsilon}$ and M_{ϵ}

Corollary 3 Let the assumptions of Theorem 2 hold.

Then for the constants h_0, δ_0, d, K and the functions $\Phi, \sigma, \Delta_x, \Delta_y$ of Theorem 2 the following assertions hold for $h \leq h_0, \epsilon/h \leq \delta_0$.

- i) The set $M_{h,\epsilon} := \{(x,y) \mid x \in \mathbb{R}^m, y = \sigma(x,h,\epsilon)\}$ is invariant under the LMM in the following sense: If the starting values $(x_i, y_i) \in M_{h,\epsilon}$, i = 0, ..., k - 1, satisfy $\Delta_x(x_0, ..., x_{k-1}, h, \epsilon) = 0$ then $(x_i, y_i) \in M_{h,\epsilon}$ for all $i \ge 0$.
- ii) The manifold $M_{h,\epsilon}$ is attractive, i.e.,

$$|y_i - \sigma(x_i, h, \epsilon)| \leq K \kappa(h)^i \left(\Delta_x(x_0, ..., x_{k-1}, h, \epsilon) + \epsilon \Delta_y(x_0, ..., y_{k-1}, h, \epsilon) \right) + (1 + K\epsilon) \chi(h, \epsilon)^{[i/k]} \Delta_y(x_0, ..., y_{k-1}, h, \epsilon)$$

holds for all $i \ge 0$ with $\kappa(h) = \rho_1 + Kh < 1$, $\chi(h, \epsilon) = K\epsilon/h < 1$.

- iii) The manifold $M_{h,\epsilon}$ has the "property of asymptotic phase" stated in Theorem 2 iii).
- iv) The manifold $M_{h,\epsilon}$ is $O(\epsilon h^p)$ -close to M_{ϵ} .

3 Global error bounds for BDF-like methods

The geometric results of Section 2 allow to reduce the original stiff problem to a nonstiff one. This fact may be used to transfer general properties of nonstiff problems to stiff problems. Examples are the existence of invariant curves, the behaviour near a hyperbolic equilibrium, the existence of attracting sets. In this section this general principle is used to derive bounds of the global error for BDF-like methods applied to singularly perturbed systems.

Theorem 4 Let the differential equation (1) satisfy Hypothesis H_{DE} and let (x(t), y(t))be a solution of Eq.(1). Let (x_i, y_i) be a LMM-approximation by a method with $\beta = 0$ satisfying Hypothesis H_{LMM} . Let T > 0 and assume p < r.

Then there are constants h_0, δ_0, d, K such that for all $h \leq h_0, \epsilon/h \leq \delta_0$ the following assertion holds. If the initial values $x_0 = x(0), x_1, ..., x_{k-1}, y_0 = y(0), y_1, ..., y_{k-1}$ satisfy $|y_{\ell} - s(x_{\ell}, \epsilon)| \leq d, 0 \leq \ell < k$, then for $ih \leq T$

$$\begin{aligned} |x_i - x(ih)| &\leq K \Big[\max_{0 \leq \ell < k} \{ |x_\ell - x(\ell h)| \} + \epsilon \Big(\max_{0 \leq \ell < k} \{ |y_\ell - y(\ell h)| \} + |y_0 - s(x_0, \epsilon)| \Big) + h^p \Big] \\ |y_i - y(ih)| &\leq K \Big[\max_{0 \leq \ell < k} \{ |x_\ell - x(\ell h)| \} \\ &+ (\epsilon + \chi(h, \epsilon)^{[i/k]}) \Big(\max_{0 \leq \ell < k} \{ |y_\ell - y(\ell h)| \} + |y_0 - s(x_0, \epsilon)| \Big) + h^p \Big] \end{aligned}$$

where $\chi(h,\epsilon) = K \epsilon/h < 1$.

Remarks:

3) If the LMM is started by a stiff RK-method of order p and stage order q then it follows from Part I [12] that

$$\begin{aligned} |x_i - x(ih)| &\leq \text{ const } [h^p + \epsilon h^{q+1} + \epsilon |y_0 - s(x_0, \epsilon)|] \\ |y_i - y(ih)| &\leq \text{ const} [h^p + (\epsilon + \chi(h, \epsilon)^{[i/k]})(h^{q+1} + |y_0 - s(x_0, \epsilon)|)] \end{aligned}$$

4) For arbitrary starting values $x_0, ..., x_{k-1}, y_0, ..., y_{k-1}$ the LMM approximates a certain solution $(\xi(t), \eta(t))$ of Eq.(1) with a global error $O(h^p)$: Let (\hat{x}_i, \hat{y}_i) be the "asymptotic phase orbit" in $S_{h,\epsilon}$ of the LMM-orbit (x_i, y_i) and let $\xi(0) = \hat{x}_0, \eta(0) = s(\hat{x}_0, \epsilon)$. Then by Theorem 2 iii), iv), v) we find

$$\begin{aligned} |x_i - \xi(ih)| &\leq |x_i - \hat{x}_i| + |\hat{x}_i - \xi(ih)| \\ &\leq \operatorname{const} \kappa(h)^i \left(\Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) + \epsilon \Delta_y(x_0, \dots, y_{k-1}, h, \epsilon) \right) + \operatorname{const} h^p \\ |y_i - \eta(ih)| &\leq |y_i - \hat{y}_i| + |\sigma(\hat{x}_i) - s(\hat{x}_i)| + |s(\hat{x}_i) - s(\xi(ih))| \\ &\leq \operatorname{const} \kappa(h)^i \left(\Delta_x + \epsilon \Delta_y \right) + (1 + \operatorname{const} \epsilon) \chi(h, \epsilon)^{[i/k]} \Delta_y + \operatorname{const} h^p . \end{aligned}$$

5) The global error estimates of Theorem 4 generalize the results given in Lubich [7]. In [7] results are derived only for solutions of Eq.(1) starting on the invariant manifold M_{ϵ} . The additional term $|y_0 - s(x_0, \epsilon)|$ in our estimates is the initial distance of the solution to the manifold M_{ϵ} . Moreover, our estimates slightly improve the ones in [7] in two respects. In [7] there is a number $\rho < 1$ independent of ϵ and h instead of the small damping factor $\chi(h, \epsilon)^{1/k} \leq (K\epsilon/h)^{1/k}$ in Theorem 4. Second, the x- and the y-estimates in [7] are the same, as in our result the term $\chi(h, \epsilon)^{[i/k]}(\max\{|y_{\ell} - y(\ell h)|\} + |y_0 - s(x_0, \epsilon)|)$ does not appear in the x-estimate. \dashv

Proof of Theorem 4: We first estimate $x_i - x(ih)$, $ih \leq T$. Let u(t) be the solution of the reduced differential equation

$$\dot{u} = f(u, s(u))$$

with $u(0) = x_0$ and let (u_i) be its LMM-approximation with starting values $u_i = x_i$, i = 0, ..., k - 1. According to the property of asymptotic phase of M_{ϵ} for Eq.(1) (cf. Part I [12]) there is a solution $(\tilde{x}(t), s(\tilde{x}(t)))$ of Eq.(1) in M_{ϵ} with

(23)
$$|\widetilde{x}(t) - x(t)| \le \operatorname{const} \epsilon \, e^{-\beta t/\epsilon} \, |y_0 - s(x_0)| \, .$$

Note that $\tilde{x}(t)$ satisfies Eq.(22). We estimate

(24)
$$|x_i - x(ih)| \le |x_i - u_i| + |u_i - u(ih)| + |u(ih) - \tilde{x}(ih)| + |\tilde{x}(ih) - x(ih)|$$
.

By the continuous dependence on initial conditions we have $|u(ih) - \tilde{x}(ih)| \le \text{const} |x(0) - \tilde{x}(0)|$ for $ih \le T$ and by Eq.(23)

(25)
$$|u(ih) - \tilde{x}(ih)| \le \operatorname{const} \epsilon |y_0 - s(x_0)|.$$

Since Eq.(22) is nonstiff the global error bound

(26)
$$|u_i - u(ih)| \le \operatorname{const}(h^p + \Delta_x(x_0, ..., x_{k-1}))$$

holds for $ih \leq T$ where Δ_x is as in Theorem 2. It remains to estimate $|x_i - u_i|$. We choose a norm $\|\cdot\| \in \mathbb{R}^{km}$ for which the induced matrix norm satisfies $\|(R - L_{\alpha}) \otimes I_m\| = 1$. From the first equation of Eqs.(5) and (18) we get for some constant c

$$||X_{i+1} - U_{i+1}|| \le (1 + ch) ||X_i - U_i|| + ch |z_{i+k}|.$$

Since $U_0 = X_0$, a simple induction argument leads to

$$||X_i - U_i|| \le ch \left[|z_{i-1+k}| + (1+ch)|z_{i-2+k}| + \dots + (1+ch)^{i-1}|z_k| \right].$$

Using Theorem 2 iv) we estimate

$$|z_j| = |y_j - s(x_j)| \le |y_j - \sigma(x_j)| + |\sigma(x_j) - s(x_j)| \le |y_j - \sigma(x_j)| + \operatorname{const} \epsilon h^p$$

This yields

$$||X_i - U_i|| \leq ch [|y_{i-1+k} - \sigma(x_{i-1+k})| + \dots + (1+ch)^{i-1}|y_k - \sigma(x_k)|] + ch \operatorname{const} \epsilon h^p [1 + (1+ch) + \dots + (1+ch)^{i-1}].$$

Since by Theorem 2 ii)

$$|y_j - \sigma(x_j)| \le \operatorname{const} \left[\kappa^j (\Delta_x + \epsilon \Delta_y) + \chi^{[j/k]} \Delta_y\right]$$

holds we get

(27)
$$||X_i - U_i|| \le \operatorname{const} \left[h\Delta_x + \epsilon \Delta_y + \epsilon h^p\right], \quad ih \le T.$$

Using the estimates (27), (26), (25) and (23) in Eq.(24) yields

(28)
$$|x_i - x(ih)| \le \operatorname{const} \left[\Delta_x + \epsilon \Delta_y + \epsilon |y_0 - s(x_0)| + h^p\right].$$

In order to estimate $y_i - y(ih)$ we use the attractivity of the manifolds $M_{h,\epsilon}$ and M_{ϵ} , their closeness and the above estimate of the x-component:

$$|y_{i} - y(ih)| \leq |y_{i} - \sigma(x_{i})| + |\sigma(x_{i}) - s(x_{i})| + |s(x_{i}) - s(x(ih))| + |s(x(ih)) - y(ih)| \leq \operatorname{const} \left(\Delta_{x} + (\epsilon + \chi^{[i/k]}) \Delta_{y} + (\epsilon + e^{-\beta ih/\epsilon}) |y_{0} - s(x_{0})| + h^{p} \right).$$

We express the functions Δ_x and Δ_y in terms of $\max_{0 \le \ell < k} |x_\ell - x(\ell h)|$ and $\max_{0 \le \ell < k} |y_\ell - y(\ell h)|$. Using the estimates (23) and (25) and the fact that Φ is a method of order p we find

$$\begin{aligned} \Delta_x(x_0, \dots, x_{k-1}) &= \max_{0 \le \ell < k} \{ |x_\ell - \Phi^\ell(x_0)| \} \\ &\le \max_{0 \le \ell < k} \{ |x_\ell - x(\ell h)| \\ &+ |x(\ell h) - \widetilde{x}(\ell h)| + |\widetilde{x}(\ell h) - u(\ell h)| + |u(\ell h) - \Phi^\ell(u_0)| \} \\ &\le \max_{0 \le \ell < k} \{ |x_\ell - x(\ell h)| \} + \operatorname{const} \left(\epsilon |y_0 - s(x_0)| + h^{p+1} \right). \end{aligned}$$

Using the attractivity of M_{ϵ} and the distance of M_{ϵ} and $M_{h,\epsilon}$ (cf. Corollary 3 iv)) and Eq.(28) we get

$$\begin{aligned} \Delta_{y}(x_{0},...,y_{k-1}) &= \max_{0 \leq \ell < k} \{y_{\ell} - \sigma(x_{\ell})|\} \\ &\leq \max_{0 \leq \ell < k} \{|y_{\ell} - y(\ell h)| + |y(\ell h) - s(x(\ell h))| + |s(x(\ell h)) - \sigma(x(\ell h))| \\ &+ |\sigma(x(\ell h)) - \sigma(x_{\ell})|\} \\ &\leq \max_{0 \leq \ell < k} \{|y_{\ell} - y(\ell h)|\} + \operatorname{const}(|y_{0} - s(x_{0})| + \epsilon h^{p} + \Delta_{x} + \epsilon \Delta_{y} + h^{p}). \end{aligned}$$

We conclude

$$\Delta_y(x_0, ..., y_{k-1}) \leq (1 + \text{const}\,\epsilon) \max_{\substack{0 \le \ell < k}} \{|y_\ell - y(\ell h)|\} + \text{const} \max_{\substack{0 \le \ell < k}} \{|x_\ell - x(\ell h)|\} + \text{const}\,(|y_0 - s(x_0)| + h^p) \,.$$

Inserting the estimates for Δ_x and Δ_y into Eqs.(28), (29) completes the proof of Theorem 4.

4 General stiff LMMs

In this section we investigate LMMs satisfying Hypothesis H_{LMM} without requiring $\beta = 0$. In this general case the invariant manifold $N_{h,\epsilon}$ established in Proposition 1 for $\beta = 0$ typically does not exist since the attractivity in Y-direction might no be stronger than the attractivity in X-direction. The existence of the invariant manifold $S_{h,\epsilon}$ (cf. Theorem 2), however, can still be shown in the general case. This result as well as the global error estimate are derived by the same methods as in the case $\beta = 0$. We therefore do not go into all details.

For $\beta \neq 0$ we assume that the starting values x_i , 0 < i < k, satisfy $|x_i - x_0| \leq d$ for d small enough. In the (X, Z)-coordinates the LMM-map \tilde{P} is given by Eq.(4). Since the LMM is ρ_1 -strictly stable the matrix $R - L_{\alpha}$ has 1 as a simple eigenvalue and all

other eigenvalues have modulus smaller than $\rho_1 < 1$. We introduce the new coordinates (x^*, X_a^*) by

$$X = (T_x \otimes I_m) \left(\begin{array}{c} x^* \\ X_a^* \end{array}\right)$$

where T_x is a $k \times k$ -matrix such that

$$T_x^{-1} (R - L_\alpha) T_x = \begin{pmatrix} 1 & 0 \\ 0 & Q_a \end{pmatrix}$$
 with $|Q_a|_\infty \le \rho_1$.

Since the LMM is assumed to be σ_1 -stiffly stable the matrix $R - \frac{1}{\beta_k}L_\beta$ has eigenvalues with modulus smaller than $\sigma_1 < 1$. We need a form of the map \tilde{P} which is also contractive in the Z-variables. We therefore transform

$$Z = (T_z \otimes I_n) Z^*$$

where T_z is a $k \times k$ -matrix such that

$$T_z^{-1}(R - \frac{1}{\beta_k} L_\beta) T_z = H$$
 with $|H|_\infty \le \sigma_1$.

In the new coordinates the map \tilde{P} has the form (we suppress the dependence on h and ϵ)

$$P^*: \begin{pmatrix} x_0^* \\ X_{0a}^* \\ Z_0^* \end{pmatrix} \longmapsto \begin{pmatrix} x_1^* \\ X_{1a}^* \\ Z_1^* \end{pmatrix} = \begin{pmatrix} x_0^* + \hat{f}^*(x_0^*, X_{0a}^*, Z_0^*) \\ g^*(x_0^*, X_{0a}^*, Z_0^*) \end{pmatrix}$$
$$= \begin{pmatrix} x_0^* + \hat{f}^*(x_0^*, X_{0a}^*, Z_0^*) \\ (Q_a \otimes I_m) X_{0a}^* + \hat{F}_a^*(x_0^*, X_{0a}^*, Z_0^*) \\ \overline{D}^*(x_0^*, X_{0a}^*, Z_0^*) Z_0^* + \hat{G}^*(x_0^*, X_{0a}^*, Z_0^*) \end{pmatrix}$$

where $\hat{f}^* = O(h)$, $\hat{F}^*_a = O(h)$, $\overline{D}^* = H + |\beta| O(\max_{0 \le i \le k} |x_i^* - x_0^*| + h + d + \epsilon/h)$, $\hat{G}^* = O(\epsilon/h)$ (cf. Eq.(4)). We choose ϵ/h and $|\beta|(h+d)$ so small that $|\overline{D}^*|_{\infty}$ is smaller than or equal to some $d^* \in (\max\{\rho_1, \sigma_1\}, 1)$. It then follows that for h and ϵ/h small enough the cylinder $\{x^* \in \mathbb{R}^m\} \times \{|X_a^*|_{\infty} \le d^*\} \times \{|Z^*|_{\infty} \le d^*\}$ is invariant under the map P^* . Thus, since the functions \hat{f}^* and g^* have the Lipschitz constants

$$L_{11} = O(h), \quad L_{12} = O(h)$$

$$L_{21} = O(h) + O(\epsilon/h) + |\beta|O(d^2), \quad L_{22} = \max\{\rho_1, \sigma_1\} + O(h) + O(\epsilon/h) + |\beta|O(d)$$

with respect to x_0^* and (X_{0a}^*, Z_0^*) we are able to apply the invariant manifold result of Nipp, Stoffer [11] (the conditions (7) are satisfied). It implies the existence of a smooth attractive invariant manifold

$$S_{h,\epsilon}^* = \{ (x^*, X_a^*, Z^*) \mid x^* \in \mathbb{R}^m, \ X_a^* = \xi^* (x^*, h, \epsilon), \ Z^* = \zeta^* (x^*, h, \epsilon) \}$$

of the map P^* . The manifold $S_{h,\epsilon}^*$ is λ -Lipschitz with $\lambda = O(L_{21}) = O(h + \epsilon/h + |\beta|d^2)$ and it is attractive with attractivity constant $\gamma(h, \epsilon) := L_{22} + L_{12}\lambda = \max\{\rho_1, \sigma_1\} + O(h + \epsilon/h + |\beta|d) < 1$:

$$|(X_{1a}^*, Z_1^*) - (\xi^*(x_1^*, h, \epsilon), \zeta^*(x_1^*, h, \epsilon)| \le \gamma(h, \epsilon) |(X_{0a}^*, Z_0^*) - (\xi^*(x_0^*, h, \epsilon), \zeta^*(x_0^*, h, \epsilon))|.$$

Moreover, $S_{h,\epsilon}^*$ has the "property of asymptotic phase" and the functions ξ^* and ζ^* are of the size of the functions \hat{F}_a^* and \hat{G}^* , respectively.

We express the invariant manifold in the (X, Z)-coordinates:

$$\widetilde{S}_{h,\epsilon} = \left\{ (X,Z) \mid X = (T_x \otimes I_m) \begin{pmatrix} x^* \\ X_a^* \end{pmatrix} \text{ where } X_a^* = \xi^*(x^*,h,\epsilon) ; \\ Z = (T_z \otimes I_n) Z^* \text{ where } Z^* = \zeta^*(x^*,h,\epsilon) ; x^* \in \mathbb{R}^m \right\}.$$

As in Kirchgraber [5], Stoffer [15] for the X-part and in the proof of Theorem 2 i) for the Z-part it can be shown that the manifold $\tilde{S}_{h,\epsilon}$ may be described as

$$\widetilde{S}_{h,\epsilon} = \{ (X,Z) \mid x \in \mathbb{R}^m, \ [X]_i = \Phi^i(x,h,\epsilon), \ [Z]_i = \widetilde{\sigma}([X]_i,h,\epsilon), \ i = 0, ..., k-1 \}$$

where the function Φ is a one-step method for $\dot{x} = f(x, s(x, \epsilon))$. $\tilde{S}_{h,\epsilon}$ inherits the properties of attractivity and of asymptotic phase from $S_{h,\epsilon}^*$ and similarly as in the proof of Theorem 2 it can be shown that $\tilde{\sigma} = O(\epsilon h^p)$. The precise statements in the (X, Y)-coordinates are given in

Theorem 5 Let the differential equation (1) satisfy Hypothesis H_{DE} . Apply a LMM satisfying Hypothesis H_{LMM} to Eq.(1) and assume p < r.

Then there are constants h_0, δ_0, d, K and functions $\Phi : D_{h_0,\delta_0} \to \mathbb{R}^m, \sigma : D_{h_0,\delta_0} \to \mathbb{R}^n$, $D_{h_0,\delta_0} := \{(x,h,\epsilon) \mid x \in \mathbb{R}^m, h \in (0,h_0), \epsilon \in (0,h\delta_0)\}, \sigma \text{ of class } C_b^r \text{ with respect to } x,$ such that with

$$\Delta_x(x_0, ..., x_{k-1}, h, \epsilon) := \max_{\substack{0 \le i < k}} \{ |x_i - \Phi^i(x_0, h, \epsilon)| \}$$

$$\Delta_y(x_0, ..., x_{k-1}, y_0, ..., y_{k-1}, h, \epsilon) := \max_{\substack{0 \le i < k}} \{ |y_i - \sigma(x_i, h, \epsilon)| \}$$

the following assertions hold for all $h \leq h_0$, $\epsilon/h \leq \delta_0$.

i) The set $S_{h,\epsilon} := \{(x_0, ..., x_{k-1}, y_0, ..., y_{k-1}) | x_0 \in \mathbb{R}^m, x_i = \Phi^i(x_0, h, \epsilon), y_i = \sigma(x_i, h, \epsilon), i = 0, ..., k-1 \}$ is invariant under the LMM-map.

ii) The manifold $S_{h,\epsilon}$ is attractive, i.e., for all starting values (x_i, y_i) , i = 0, ..., k - 1, with $|x_i - x_0| \le d$ and $|y_i - s(x_i, \epsilon)| \le d$ the estimate

$$|x_{i+1} - \Phi(x_i, h, \epsilon)| + |y_i - \sigma(x_i, h, \epsilon)| \leq K \gamma(h, \epsilon)^i \left(\Delta_x(x_0, \dots, x_{k-1}, h, \epsilon) + \Delta_y(x_0, \dots, y_{k-1}, h, \epsilon) \right)$$

holds for all $i \ge 0$ with $\gamma(h, \epsilon) = \max\{\rho_1, \sigma_1\} + K(h + \epsilon/h + |\beta|d) < 1$.

iii) The "property of asymptotic phase holds", i.e., for all starting values (x_i, y_i) , i = 0, ..., k - 1, with $|x_i - x_0| \leq d$ and $|y_i - s(x_i, \epsilon)| \leq d$ there is \hat{x}_0 such that for $\hat{x}_i := \Phi^i(\hat{x}_0, h, \epsilon)$, $\hat{y}_i := \sigma(\hat{x}_i, h, \epsilon)$, $i \geq 0$, the estimate

$$|\hat{x}_i - x_i| + |\hat{y}_i - y_i| \le K \gamma(h, \epsilon)^i \left(\Delta_x(x_0, ..., x_{k-1}, h, \epsilon) + \Delta_y(x_0, ..., y_{k-1}, h, \epsilon) \right)$$

holds for $i \geq 0$.

iv) The function σ satisfies the estimate

$$|\sigma(x,h,\epsilon) - s(x,\epsilon)| \le K\epsilon h^p$$

v) The function Φ is a one-step method of order p for the differential equation $\dot{x} = f(x, s(x, \epsilon)).$

Remark:

6) As a consequence of Theorem 2 we stated Corollary 3 establishing the manifold $M_{h,\epsilon} := \{(x,y) | x \in \mathbb{R}^m, y = \sigma(x,h,\epsilon)\}$. For general stiff LMMs the manifold $M_{h,\epsilon}$ also exists and inherits the properties i), ii), iii) and iv) of Theorem 5 (see Fig. 2 at the end of Section 2).

As in Section 3 for BDF-like methods the geometric results of Theorem 5 allow to derive bounds of the global error for general stiff LMMs. The derivation is identical to the one in the proof of Theorem 4. Remark 5) above relating our results to the ones in Lubich [7] again holds for the general case in Theorem 6 except that our damping factor $\gamma(h, \epsilon)$ is now not smaller than the ρ in [7].

Theorem 6 Let the differential equation (1) satisfy Hypothesis H_{DE} and let (x(t), y(t))be a solution of Eq.(1). Let (x_i, y_i) be a LMM-approximation by a method satisfying Hypothesis H_{LMM} . Let T > 0 and assume p < r. Then there are constants h_0, δ_0, d, K such that for all $h \leq h_0, \epsilon/h \leq \delta_0$ the following assertion holds. If the initial values $x_0 = x(0), x_1, ..., x_{k-1}, y_0 = y(0), y_1, ..., y_{k-1}$ satisfy $|x_{\ell} - x_0| \leq d$ and $|y_{\ell} - s(x_{\ell}, \epsilon)| \leq d, 0 \leq \ell < k$, then for $ih \leq T$

$$\begin{aligned} |x_i - x(ih)| &\leq K \Big[\max_{0 \leq \ell < k} \{ |x_\ell - x(\ell h)| \} + h \Big(\max_{0 \leq \ell < k} \{ |y_\ell - y(\ell h)| \} + |y_0 - s(x_0, \epsilon)| \Big) + h^p \Big] \\ |y_i - y(ih)| &\leq K \Big[\max_{0 \leq \ell < k} \{ |x_\ell - x(\ell h)| \} \\ &+ (h + \gamma(h, \epsilon)^i) \Big(\max_{0 \leq \ell < k} \{ |y_\ell - y(\ell h)| \} + |y_0 - s(x_0, \epsilon)| \Big) + h^p \Big] \end{aligned}$$

where $\gamma(h, \epsilon) = \max\{\rho_1, \sigma_1\} + K(h + \epsilon/h + |\beta|d) < 1.$

References

- W.J. Beyn, On invariant closed curves for one-step methods, Numer. Math. 51 (1987), 103-122.
- W.J. Beyn, On the numerical approximation of phase portraits near stationary points, SIAM J. Numer. Anal. 24 (1987), 1095-1113.
- [3] T. Eirola, Invariant curves of one-step methods, BIT 28 (1988), 113-122.
- [4] E. Hairer, S. Nørsett, G. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems, Springer-Verlag, Berlin, 2nd Ed. 1993.
- [5] U. Kirchgraber, Multistep methods are essentially one-step methods, Numer. Math. 48, 85-90 (1986)
- [6] P.E. Kloeden, J. Lorenz, Stable attracting sets in dynamical systems and in their one-step discretizations, SIAM J. Numer. Anal. 23 (1986), 986-995.
- [7] Ch. Lubich, On the convergence of multistep methods for nonlinear stiff differential equations, Numer. Math. 58 (1991), 839-853.
- [8] Ch. Lubich, K. Nipp and D. Stoffer, *Runge-Kutta solutions of stiff differential equations near stationary points*, to appear in SIAM J. Num. Anal.
- K. Nipp, Invariant manifolds of singularly perturbed ordinary differential equations, ZAMP 36 (1985), 309-320.
- [10] K. Nipp, Smooth attractive invariant manifolds of singularly perturbed ODE's, Research Report No. 92-13, Seminar für Angewandte Mathematik, ETH Zürich (1992).

- [11] K. Nipp and D. Stoffer, Attractive invariant manifolds for maps: Existence, smoothness and continuous dependence on the map, Research Report No. 92-11, Seminar für Angewandte Mathematik, ETH Zürich (1992).
- [12] K. Nipp and D. Stoffer, Invariant manifolds and global error estimates of numerical integration schemes applied to stiff systems of singular perturbation type – Part I: RK-methods, to appear in Numer. Math.
- [13] J. Ortega and W. Rheinboldt, Iterative Solution of Nonlinear Equations in Several Variables, Academic Press, 1970.
- [14] D. Stoffer, General linear methods: connection to one-step methods and invariant curves, Numer. Math. 64 (1993), 395-408.
- [15] D. Stoffer, On the global error of linear multistep methods, in Geometric behaviour of numerical integration methods for ODEs, submitted as Habilitationsschrift, ETH Zürich (1994).
- [16] D. Stoffer and K. Nipp, Invariant curves for variable step size integrators, BIT 31 (1991), 169-180.

Research Reports

No.	Authors	Title
95-03	K. Nipp, D. Stoffer	Invariant manifolds and global error esti- mates of numerical integration schemes ap- plied to stiff systems of singular perturbation tune. Part II: Linear multistan methods
95-02	M.D. Buhmann, F. Der- rien, A. Le Méhauté	Spectral Properties and Knot Removal for In- terpolation by Pure Radial Sums
95-01	R. Jeltsch, R. Renaut, J.H. Smit	An Accuracy Barrier for Stable Three-Time- Level Difference Schemes for Hyperbolic Equations
94-13	J. Waldvogel	Circuits in Power Electronics
94-12	A. Williams, K. Burrage	A parallel implementation of a deflation algo- rithm for systems of linear equations
94-11	N. Botta, R. Jeltsch	A numerical method for unsteady flows
94-10	M. Rezny	Parallel Implementation of ADVISE on the Intel Paragon
94-09	M.D. Buhmann, A. Le Méhauté	Knot removal with radial function interpolation
94-08	M.D. Buhmann	Pre-wavelets on scattered knots and from ra- dial function spaces: A review
94-07	P. Klingenstein	Hyperbolic conservation laws with source terms: Errors of the shock location
94-06	M.D. Buhmann	Multiquadric Pre-Wavelets on Non-Equally Spaced Centres
94-05	K. Burrage, A. Williams, J. Erhel, B. Pohl	The implementation of a Generalized Cross Validation algorithm using deflation tech- niques for linear systems
94-04	J. Erhel, K. Burrage, B. Pohl	Restarted GMRES preconditioned by de- flation
94-03	L. Lau, M. Rezny, J. Belward, K. Burrage, B. Pohl	ADVISE - Agricultural Developmental Visu- alisation Interactive Software Environment
94-02	K. Burrage, J. Erhel, B. Pohl	A deflation technique for linear systems of equations
94-01	R. Sperb	An alternative to Ewald sums
93-07	R. Sperb	Isoperimetric Inequalities in a Boundary Value Problem in an Unbounded Domain
93-06	R. Sperb	Extension and simple Proof of Lekner's Summation Formula for Coulomb Forces
93-05	A. Frommer, B. Pohl	A Comparison Result for Multisplittings Based on Overlapping Blocks and its Appli- cation to Waveform Relaxation Methods