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Invariant manifolds of numerical integration schemes applied to stiff systems of singular perturbation type – Part I: RK-methods

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Abstract

For implicit RK-methods applied to singularly perturbed systems of ODEs it is shown that the resulting discrete systems preserve the geometric properties of the underlying ODE. As an application of this invariant manifold result sharp bounds on the global error are derived.

Keywords: singular perturbation, attractive invariant manifold, stiff systems, global error, implicit RK-method

Subject Classification: 65L, 34C

Invariant manifolds of numerical integration schemes applied to stiff systems of singular perturbation type – Part I: RK-methods

Singularly perturbed systems of ODEs are a model class for so-called stiff systems which are difficult to treat numerically. The smaller the perturbation parameter ϵ the stiffer the system. Under usual assumptions a singularly perturbed system has an important geometric property: It admits a highly attractive smooth invariant manifold. In Section 1 we state the invariant manifold result for singularly perturbed ODEs proved in Nipp [3].

A numerical method applied to a system of ODEs defines a map in phase space. We deal with the question whether such a map preserves the geometric property of the underlying singularly perturbed ODE. In general, this geometric property carries over to the discrete system if the step size h is of the same order as the perturbation parameter ϵ. In this case the numerical integration is very inefficient, however. For explicit methods the step size h has to be of order ϵ due to their poor stability properties. This has been shown in Kirchgraber, Nipp [2] for the explicit Euler method. We show that for implicit RK-methods the step size h may be chosen such that h is independent of ϵ. For h fixed and for all ϵ small enough such stiff discrete systems admit an attractive invariant manifold close to the manifold of the ODE. This geometric result for stiff RK-methods is derived in Section 2.

The invariant manifold result of Section 2 is obtained by considering one step of the RK-map, only. In order to numerically approximate the solution of an ODE many steps have to be performed. Therefore, one is interested in bounds on the global error of the integration method. As for nonstiff systems this is an easy task it is a difficult problem for stiff systems. This problem was first solved by Hairer, Lubich, Roche [1] in 1988 for stiff systems of singular perturbation type. In Section 3 we give a new derivation for the bounds of the global error of RK-methods applied to singularly perturbed systems. By means of the invariant manifold result of Section 2 the RK-map is reduced to a map on the manifold. The discrete system restricted to the manifold is no longer stiff as $\epsilon \to 0$. This allows to derive bounds on the global error in a comparatively easy and transparent way.

In Part II which is in preparation multistep methods applied to stiff systems of singular perturbation type are investigated.

1. An invariant manifold result for singularly perturbed ODEs

We consider the singularly perturbed autonomous system

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

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

We make the following

Hypothesis H_{DE}

1) $r \geq 3$.

2) $f \in C_b^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $g \in C_b^r(\mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)$ and f and g are bounded.

3) 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 $x \in \mathbb{R}^m$.

4) There is a positive constant b_0 such that all eigenvalues of the Jacobian $B(x) := g_y(x, s^0(x))$ 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) has a smooth attractive invariant manifold M_ϵ which is $O(\epsilon)$-close to the so-called *reduced manifold* $M_0 := \{(x,y) \mid x \in \mathbb{R}^m,\ y = s^0(x)\}$. The precise result given below is proved in Nipp [3].

Theorem 1 *For every $\beta \in (0, b_0)$ there are positive constants ϵ^*, δ, K and a function $s \in C_b^r(\mathbb{R}^m \times (0, \epsilon^*), \mathbb{R}^n)$ such that the following assertions hold for $\epsilon \in (0, \epsilon^*)$.*

i) Invariance. *The set $M_\epsilon = \{(x,y) \mid x \in \mathbb{R}^m,\ y = s(x,\epsilon)\} \subset \mathbb{R}^m \times \mathbb{R}^n$ is invariant under Eq.(1), i.e., if $(x^0, y^0) \in M_\epsilon$ then also $(x(t),\ y(t)) \in M_\epsilon$ for all $t \in \mathbb{R}$, $(x(t),\ y(t))$ being the solution of Eq.(1) with $(x(0),\ y(0)) = (x^0, y^0)$. More precisely, $P_t(M_\epsilon) = M_\epsilon$, $t \in \mathbb{R}$, for the map $P_t : (x^0, y^0) \longmapsto (x(t), y(t))$.*

ii) Attractivity. *Every solution $(x(t),\ y(t))$ of Eq.(1) with $|y(0) - s^0(x(0))| \leq \delta$ satisfies*

$$|y(t) - s(x(t),\epsilon)| \leq K\, e^{-\beta t/\epsilon}\, |y(0) - s(x(0),\epsilon)|$$

for all $t \geq 0$.

iii) "Asymptotic phase". *For every solution $(x(t),\, y(t))$ of Eq.(1) with initial conditions (x^0, y^0) at $t = 0$ satisfying $|y^0 - s^0(x^0)| \;\le \delta$ there is $(\tilde{x}^0, \tilde{y}^0) \in M_\epsilon$ such that for $(\tilde{x}(t),\, \tilde{y}(t))$ being the solution of Eq.(1) with $(\tilde{x}(0),\, \tilde{y}(0)) = (\tilde{x}^0, \tilde{y}^0)$*

$$| \, x(t) - \tilde{x}(t) \, | \le K \, e^{-\beta t/\epsilon} \, | \, y^0 - s(x^0, \epsilon) \, |$$

$$| \, y(t) - \tilde{y}(t) \, | \le K \, e^{-\beta t/\epsilon} \, | \, y^0 - s(x^0, \epsilon) \, |$$

holds for $t \ge 0$.

iv) Closeness to M_0.

$$| \, s(x, \epsilon) - s^0(x) \, | \le K \, \epsilon \quad \text{for } \; x \in \mathbb{R}^m \, .$$

v) Maximality. *Every solution $(x(t),\, y(t))$ of Eq.(1) satisfying $| \, y(t) - s^0(x(t)) \, | \le \delta$ for all $t \in \mathbb{R}$ lies in M_ϵ, i.e., $y(t) = s(x(t), \epsilon)$ for all t.*

2. The invariant manifold result for the RK-map

In this section we investigate the geometric behaviour of RK-methods applied to Eq.(1). Since Eq.(1) is stiff for small ϵ, stiff RK-methods are needed to integrate such a system. In this case, the step size h of the integration method usually is much larger than the perturbation parameter ϵ.

For our approach it is essential that a RK-method is considered as a map in phase space. The RK-method applied to the differential equation $\dot{w} = F(w), \; w \in \mathbb{R}^\ell$, is a map which takes $w \in \mathbb{R}^\ell$ to

$$\overline{w} \;\; = \;\; w + h \sum_{j=1}^{s} b_j \, F(W_j)$$

where the W_i are defined by

$$W_i \;\; = \;\; w + h \sum_{j=1}^{s} a_{ij} \, F(W_j), \quad i = 1, ..., s \, .$$

It is convenient to introduce the following vectors in $\mathbb{R}^{s\ell}$

$$W := \begin{pmatrix} W_1 \\ \cdot \\ \cdot \\ \cdot \\ W_s \end{pmatrix} , \quad F(W) := \begin{pmatrix} F(W_1) \\ \cdot \\ \cdot \\ \cdot \\ F(W_s) \end{pmatrix} , \quad \mathbf{w} = \begin{pmatrix} w \\ \cdot \\ \cdot \\ \cdot \\ w \end{pmatrix} .$$

In this notation the RK-map may be written as

$$\begin{aligned} \overline{w} \;&=\; w + h \, (b^T \otimes I_\ell) \, F(W) \\ W \;&=\; \mathbf{w} + h \, (A \otimes I_\ell) \, F(W) \, . \end{aligned}$$

We make the following assumptions on the RK-method which are appropriate to integrate stiff systems.

Hypothesis H_{RK}

1) The RK-method has order p and stage order $1 \le q < p$.
2) The RK-matrix A is invertible.
3) The stability function $R(z) := 1 + z\, b^T (I_s - zA)^{-1} 1\!\!1,\ z \in \mathbb{C}$, where $1\!\!1 = (1, ..., 1)^T \in \mathbb{R}^s$, satisfies $|R(\infty)| < 1$.

Remarks:

1) If $q = p$ then for $p > 1$ one may redefine $q = p - 1$ for Hypothesis H_{RK} 1) to hold. In this way, the results are not weakened. For $p = 1$ see Remark 7).

2) Usually, the matrix A of stiff RK-methods has eigenvalues with positive real parts. This implies Hypothesis H_{RK} 2). In our case where $\epsilon << h$ we do not need this stronger assumption.

3) Since A is invertible $R(\infty)$ may be written as $R(\infty) = 1 - b^T A^{-1} 1\!\!1$. $\dashv$

We now apply a RK-method satisfying Hypothesis H_{RK} to Eq.(1) and assume $p < r$. This defines a map

$$P: \ \mathbb{R}^m \times \mathbb{R}^n \ni \begin{pmatrix} x \\ y \end{pmatrix} \longmapsto \begin{pmatrix} \overline{x} \\ \overline{y} \end{pmatrix} \in \mathbb{R}^m \times \mathbb{R}^n \tag{2}$$

of the form

$$\begin{aligned} \overline{x} &= x + h(b^T \otimes I_m)\, f(X, Y) \\ \overline{y} &= y + \frac{h}{\epsilon}(b^T \otimes I_n)\, g(X, Y) \end{aligned}$$

where X and Y are given by

$$\begin{aligned} X &= \mathbf{x} + h(A \otimes I_m)\, f(X, Y) \\ Y &= \mathbf{y} + \frac{h}{\epsilon}(A \otimes I_n)\, g(X, Y)\ . \end{aligned}$$

We introduce the new variables z, Z measuring the difference to the manifold M_ϵ of the differential equation (1). Writing $s(x)$ instead of $s(x, \epsilon)$, for short, we define

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

We expand the function g about $z = 0$ and have

$$g(x,\, s(x) + z) = g(x,\, s(x)) + (B(x) + \hat{B}(x, z))\, z$$

with $\hat{B}(x,z) = O(|z|)$. In the new variables the y-component of the RK-map P takes the form

$$(3) \qquad s(\overline{x}) + \overline{z} = s(x) + z + \frac{h}{\epsilon}\,(b^T \otimes I_n)\Big\{g(X,\, s(X)\big) + \text{diag}\,\Big[B(X) + \hat{B}(X,Z)\Big]\,Z\Big\}$$

$$(4) \quad s(X) + Z = s(\mathbf{x}) + \mathbf{z} + \frac{h}{\epsilon}\,(A \otimes I_n)\Big\{g(X,\, s(X)\big) + \text{diag}\,\Big[B(X) + \hat{B}(X,Z)\Big]\,Z\Big\}$$

where, e.g., diag$[B(X)]$ denotes the $sn \times sn$ block diagonal matrix with $n \times n$ blocks $B(X_1), ..., B(X_s)$. We denote the RK-map in the new variables by $\widetilde{P}$ and we consider this map in the space $\mathbb{R}^m \times D_d$, $D_d := \{z \mid z \in \mathbb{R}^n,\ |z| \leq d\}$, where d will be determined later. We here suppose that $Z \in [D_d]^s$. It will be shown that Eq.(4) indeed has a unique solution in $[D_d]^s$. Collecting the linear terms in Z in Eq.(4) yields

$$Z = \frac{\epsilon}{h}\, C(X,Z)^{-1}(\mathbf{z} - E)$$

with

$$(5) \qquad C(X,Z) := -(A \otimes I_n)\ \text{diag}\,\Big[B(X) + \hat{B}(X,Z)\Big] + \frac{\epsilon}{h}\,(I_s \otimes I_n)$$

and

$$(6) \qquad E := s(X) - s(\mathbf{x}) - \frac{h}{\epsilon}\,(A \otimes I_n)\ g(X,\, s(X))\ .$$

Note that due to H_{DE} 4) and H_{RK} 2) the matrix C is invertible for d and ϵ/h small enough. Inserting the expression obtained for Z into Eq.(3) we find

$$\overline{z} = z - e + (b^T \otimes I_n)\ \text{diag}\Big[B(X) + \hat{B}(X,Z)\Big]\,C(X,Z)^{-1}\,(\mathbf{z} - E)$$

where

$$(7) \qquad e := s(\overline{x}) - s(x) - \frac{h}{\epsilon}\,(b^T \otimes I_n)\,g(X,\, s(X))\ .$$

Note that E and e are of order $O(h)$. This is due to the fact that $g(X, s^0(X)) = 0$ and $s(X) - s^0(X) = O(\epsilon)$ and that $X - \mathbf{x}$ and $\overline{x} - x$ are $O(h)$. By means of Eq.(5) we may replace diag$\Big[B(X) + \hat{B}(X,Z)\Big]$ by $(A^{-1} \otimes I_n)\Big(\frac{\epsilon}{h}\,(I_s \otimes I_n) - C(X,Z)\Big)$. Hence, we have

$$\overline{z} = z - e + (b^T A^{-1} \otimes I_n)\Big(\frac{\epsilon}{h}\,C(X,Z)^{-1} - (I_s \otimes I_n)\Big)(\mathbf{z} - E)$$

or

$$\overline{z} = \Big((1 - b^T A^{-1}\mathbb{1})\,I_n + \frac{\epsilon}{h}\,\Delta(\mathbb{1} \otimes I_n)\Big)\,z + \Big((b^T A^{-1} \otimes I_n) - \frac{\epsilon}{h}\,\Delta\Big)\,E - e$$

where

$$\Delta := (b^T A^{-1} \otimes I_n)\ C(X,Z)^{-1}\ .$$

Thus, we have shown that the map $\widetilde{P}$ may be written in the form

$$\begin{aligned} \overline{x} &= x + h(b^T \otimes I_m) f(X, s(X) + Z) \\ \overline{z} &= \Big(R(\infty)\, I_n + \frac{\epsilon}{h}\, \Delta(1\!\!1 \otimes I_n)\Big)\, z + \Big((b^T A^{-1} \otimes I_n) - \frac{\epsilon}{h}\, \Delta\Big)\, E - e \end{aligned} \tag{8}$$

with X, Z defined by

$$\begin{aligned} \Phi(X, Z) &:= X - \mathbf{x} - h(A \otimes I_m) f(X, s(X) + Z) = 0 \\ \Psi(X, Z) &:= Z - \frac{\epsilon}{h}\, C(X, Z)^{-1}\, (\mathbf{z} - E) = 0\,. \end{aligned} \tag{9}$$

This form is appropriate to show that the map $\widetilde{P}$ is well defined and that it admits a highly attractive invariant manifold.

We first show that Eq.(9) has a unique solution $(X(x, z, h, \epsilon), Z(x, z, h, \epsilon))$ in some large neighborhood of $X = \mathbf{x}$ and $Z = 0$ in $\Big[\mathbb{R}^m\Big]^s \times \Big[D_d\Big]^s$. This is done by using the Newton-Kantorovich theorem (cf., e.g., Ortega, Rheinboldt [5]). The Jacobian J of (9) satisfies

$$J(X, Z) := \frac{\partial(\Phi, \Psi)}{\partial(X, Z)} = \begin{pmatrix} (I_s \otimes I_m) + O(h) & O(h) \\ O\big(\frac{\epsilon}{h}\big) & (I_s \otimes I_n) + O\big(\frac{\epsilon}{h}\big) \end{pmatrix}$$

for $(X, Z) \in \Big[\mathbb{R}^m\Big]^s \times \Big[D_d\Big]^s$. This implies that J has Lipschitz constant $\gamma = O(h) + O(\epsilon/h)$. Moreover, $|J^{-1}(\mathbf{x}, 0)|$ is bounded by $\beta = 2$ and $\Big|J^{-1}(\mathbf{x}, 0)\begin{pmatrix} \Phi(\mathbf{x}, 0) \\ \Psi(\mathbf{x}, 0) \end{pmatrix}\Big|$ is bounded by $\alpha = O(h) + O(\epsilon/h)$ for h and ϵ/h small enough. The quantity $H := \alpha\beta\gamma$ is of order $O\Big((h + \epsilon/h)^2\Big)$ and for $r_{1,2} := \alpha(1 \mp \sqrt{1 - 2H})/H$ we have $r_1 = O(h + \epsilon/h)$ and $r_2 = O\Big(\frac{1}{h + \epsilon/h}\Big)$. Hence, the Newton-Kantorovich theorem implies the existence of a solution of (9) in the ball $S_{r_1}(\mathbf{x}, 0)$ and the solution is unique in $\Big[\mathbb{R}^m\Big]^s \times \Big[D_d\Big]^s \cap S_{r_2}(\mathbf{x}, 0)$. From the implicit function theorem it follows that this solution is smooth. Since the Jacobian J is near the identity for small h and ϵ/h the derivatives are bounded. Therefore, the map $\widetilde{P}$ given in Eq.(8) is well defined and is of the form

$$\widetilde{P} : \begin{pmatrix} x \\ z \end{pmatrix} \longmapsto \begin{pmatrix} \overline{x} \\ \overline{z} \end{pmatrix} = \begin{pmatrix} x + \hat{F}(x, z, h, \epsilon) \\ G(x, z, h, \epsilon) \end{pmatrix}$$

where $\hat{F}$ and G are of class C_b^r.

We now apply the invariant manifold result of Nipp, Stoffer [4]. The cylinder $\mathbb{R}^m \times D_d$ is mapped into itself by the map $\widetilde{P}$ if d, h and ϵ/h are sufficiently small. The functions $\hat{F}$ and G have the following Lipschitz constants with respect to x and z:

$$\begin{aligned} L_{11} &= O(h)\,, & L_{12} &= O(\epsilon)\,, \\ L_{21} &= O(h) + O\Big(\frac{\epsilon}{h}\Big)\,, & L_{22} &= R(\infty) + O\Big(\frac{\epsilon}{h}\Big)\,. \end{aligned}$$

We have to verify the two conditions

$$\begin{aligned} 2\sqrt{L_{12}\,L_{21}} &< 1 - L_{11} - L_{22} \\ L_{22} + L_{12}\,\lambda &< (1 - L_{11} - L_{12}\,\lambda)^r \end{aligned}$$

where

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

These two conditions are satisfied if h and ϵ/h are sufficiently small. Now, Theorem 5 of Nipp, Stoffer [4] implies the existence of a smooth attractive invariant manifold $\widetilde{M}_{h,\epsilon}$ of the map $\widetilde{P}$. More precisely: Let Ω_{h^*,δ^*} be the domain $\{(x,h,\epsilon)|\; x \in \mathbb{R}^m,\; h \in (0,h^*),\; \epsilon \in (0, h\delta^*)\}$.

There is a λ-Lipschitz function $\widetilde{\sigma} : \Omega_{h^*,\delta^*} \longrightarrow D_d \subset \mathbb{R}^n$ of class C_b^r with respect to x, $\lambda = O(h) + O(\epsilon/h)$, such that the following assertions hold.

i) *$\widetilde{M}_{h,\epsilon} = \{(x,z)\,|\; x \in \mathbb{R}^m,\;\; z = \widetilde{\sigma}(x,h,\epsilon)\}$ is an invariant set of the map $\widetilde{P}$, i.e., $\widetilde{P}(\widetilde{M}_{h,\epsilon}) = \widetilde{M}_{h,\epsilon}$.*

ii) *$\widetilde{M}_{h,\epsilon}$ is uniformly attractive for $\widetilde{P}$ with attractivity constant $\chi(\lambda) = L_{22} + L_{12}\,\lambda = R(\infty) + O(\epsilon/h) < 1$.*

iii) *The "property of asymptotic phase" holds.*

iv) *According to Eq.(8) the function $G(x,z,h,\epsilon)$ has the form $G(x,z,h,\epsilon) = H(x,z,h,\epsilon)z + \hat{G}(x,z,h,\epsilon)$ with $|H(x,z,h,\epsilon)| = |R(\infty)| + O(\epsilon/h) \le \rho < 1$. Thus, $\widetilde{\sigma}$ may be estimated by*

$$|\widetilde{\sigma}(x,h,\epsilon)| \le \frac{1}{1-\rho} \sup_{x \in \mathbb{R}^m} |\hat{G}(x, \widetilde{\sigma}(x,h,\epsilon), h, \epsilon)| \,.$$

v) *Every invariant set Ω of $\widetilde{P}$ is contained in $\widetilde{M}_{h,\epsilon}$.*

From Eq.(8) we have $\hat{G} = ((b^T A^{-1} \otimes I_n) - \frac{\epsilon}{h}\,\Delta)\,E - e$. Since the expressions E and e are of order $O(h)$ as noted above the function $\hat{G}$ is of order $O(h)$. It therefore follows from iv) that $\widetilde{\sigma}$ is of order $O(h)$ as well. This estimate may be improved, however.

Claim *$\widetilde{\sigma}$ is of order $O(h^{q+1})$. Moreover, if the method is stiffly accurate, i.e., if $b_i = a_{si}$, then $\widetilde{\sigma} = O(\epsilon\, h^q)$.*

To prove this claim we need some preparations. We consider solutions (u(t),v(t)) of Eq.(1) on the manifold M_ϵ established in Theorem 1. These solutions satisfy the differential equation

$$
\begin{aligned}
\dot{u} &= f(u, s(u)) \\
\dot{v} &= \frac{1}{\epsilon}\, g(u, s(u)) = s'(u) f(u, s(u))\ .
\end{aligned}
\tag{10}
$$

Here, $s(u)$ is the function defining the manifold M_ϵ (for simplicity we again drop the parameter ϵ in $s(u,\epsilon)$). The identity $g(u, s(u)) = \epsilon s'(u) f(u, s(u))$ follows from $v(t) = s(u(t))$. s' denotes the derivative of $s(u)$ with respect to u. Applying a RK-method to Eq.(10) we obtain

$$
\begin{aligned}
\overline{u} &= u + h(b^T \otimes I_m)\, f(U, s(U)) \\
\overline{v} &= v + h(b^T \otimes I_n)\, \mathrm{diag}\,[s'(U)]\, f(U, s(U))
\end{aligned}
\tag{11}
$$

with

$$
\begin{aligned}
U &= \mathbf{u} + h(A \otimes I_m)\, f(U, s(U)) \\
V &= \mathbf{v} + h(A \otimes I_n)\, \mathrm{diag}\,[s'(U)]\, f(U, s(U))\ .
\end{aligned}
\tag{12}
$$

Since the method is of order p and has stage order q and since f, g are of class C_b^r with $r > p$ we conclude that

$$
\begin{aligned}
O(h^{p+1}) &= \overline{v} - v(h) &&= \overline{v} - s(u(h)) &&= \overline{v} - s(\overline{u}) + O(h^{p+1}) \\
O(h^{q+1}) &= V - \mathbf{v}(c_i h) &&= V - s(\mathbf{u}(c_i h)) &&= V - s(U) + O(h^{q+1})
\end{aligned}
$$

where $c_i = \sum_{j=1}^{s} a_{ij}$ and $\mathbf{v}(c_i h) := \Big(v(c_1 h)^T, ..., v(c_s h)^T\Big)^T$. It follows that

$$
\begin{aligned}
s(\overline{u}) &= s(u) + h(b^T \otimes I_n)\, \mathrm{diag}\,[s'(U)]\, f(U, s(U)) + O(h^{p+1}) \\
s(U) &= s(\mathbf{u}) + h(A \otimes I_n)\ \mathrm{diag}\,[s'(U)]\, f(U, s(U)) + O(h^{q+1})\ .
\end{aligned}
\tag{13}
$$

Next we improve the estimates for e and E using the following

Lemma 2 *Let* $(x, z) \in \widetilde{M}_{h,\epsilon}$. *Then* $e = O(h^j)$ *and* $E = O(h^j)$ *implies* $e = O(h^{j+1}) + O(h^{p+1})$ *and* $E = O(h^{j+1}) + O(h^{q+1})$.

Proof: We are looking for estimates for $\overline{x} - \overline{u}$ and $X - U$ where $\overline{x}$ and X are defined by Eqs.(8), (9) and $\overline{u}$, U by Eqs.(11), (12). For $u = x$ we have

$$
\begin{aligned}
\overline{x} - \overline{u} &= h(b^T \otimes I_m)\Big(f(X, s(X) + Z) - (f(U, s(U))\Big) \\
X - U &= h(A \otimes I_m)\ \Big(f(X, s(X) + Z) - (f(U, s(U))\Big)
\end{aligned}
$$

or

$$
\begin{aligned}
\overline{x} - \overline{u} &= h\, O(|X - U|) + h\, O(|Z|) \\
\Big((I_s \otimes I_m) + O(h)\Big)(X - U) &= h\, O(|Z|)
\end{aligned}
$$

implying

$$\begin{aligned} \overline{x} - \overline{u} &= O(h\,|Z|) \\ X - U &= O(h\,|Z|)\ . \end{aligned} \tag{14}$$

For $e, E = O(h^j)$ the property iv) of $\widetilde{M}_{h,\epsilon}$ implies $z = \widetilde{\sigma} = O(h^j)$. Now Eq.(9) gives $Z = O(\epsilon\, h^{j-1})$. Inserting this estimate into Eq.(14) we obtain $\overline{x} - \overline{u} = O(\epsilon\, h^j)$ and $X - U = O(\epsilon\, h^j)$. Replacing $\overline{u}$ and U, respectively, by $\overline{x} + O(\epsilon\, h^j)$ and $X + O(\epsilon\, h^j)$, respectively, in Eq.(13) and introducing the estimates obtained into Eqs.(6) and (7) we get

$$\begin{aligned} e &= O(h^{j+1}) + O(h^{p+1}) \\ E &= O(h^{j+1}) + O(h^{q+1})\ . \end{aligned}$$

Here, we have used the identity $\epsilon s'(u) f(u, s(u)) = g(u, s(u))$ and the fact that ϵ/h is small. This completes the proof of Lemma 2. $\perp$

We know that $e = O(h)$, $E = O(h)$ holds. Using Lemma 2 successively it follows that $e = O(h^{q+1})$, $E = O(h^{q+1})$. Hence, the function $\hat{G}$ in property iv) of $\widetilde{M}_{h,\epsilon}$ is of order $O(h^{q+1})$ implying $\widetilde{\sigma} = O(h^{q+1})$. With these estimates for E and $\widetilde{\sigma}$ it follows fom Eq.(9) that

$$Z = O(\epsilon\, h^q)\ . \tag{15}$$

Since for $b_i = a_{si}$ one has $\overline{z} = Z_s$ it follows that $\widetilde{\sigma} = O(\epsilon\, h^q)$ in this special case. Thus, we have proved the above claim.

Expressing the results above in the original variables x, y and defining $\sigma(x, h, \epsilon) := s(x, \epsilon) + \widetilde{\sigma}(x, h, \epsilon)$ we have shown

Theorem 3 *Let the differential equation (1) satisfy Hypothesis H_{DE}. Apply a RK-method with Hypothesis H_{RK} to Eq.(1) and assume $p < r$.*

Then there are constants h_0, δ_0, d, c, K and a function $\sigma : \Omega_{h_0,\delta_0} \longrightarrow \mathbb{R}^n$, $\Omega_{h_0,\delta_0} := \{(x, h, \epsilon) |\, x \in \mathbb{R}^m,\ h \in (0, h_0),\ \epsilon \in (0, h\delta_0)\}$, σ of class C_b^r with respect to x, such that for all h, ϵ with $h \le h_0$, $\epsilon \le \delta_0 h$ the following assertions hold.

i) Invariance. *The set $M_{h,\epsilon} = \{(x, y) \,|\, x \in \mathbb{R}^m,\ y = \sigma(x, h, \epsilon)\}$ is an invariant set of the map P given in Eq.(2), i.e., $P(M_{h,\epsilon}) = M_{h,\epsilon}$.*

ii) Attractivity. *The manifold $M_{h,\epsilon}$ is uniformly attractive for P with attractivity constant $\chi(h, \epsilon) = R(\infty) + c\,\epsilon/h < 1$, i.e., for all (x, y) with $|y - s(x, \epsilon)\,| \le d$ the inequality*

$$|\overline{y} - \sigma(\overline{x}, h, \epsilon)| \;\le\; \chi(h, \epsilon)\, |y - \sigma(x, h, \epsilon)|$$

holds.

iii) "Asymptotic phase". *For every* (x_0, y_0) *with* $|y_0 - s(x_0, \epsilon)| \leq d$ *there is* $(\tilde{x}_0, \tilde{y}_0) \in M_{h,\epsilon}$ *such that for* $(x_j, y_j) := P^j(x_0, y_0)$ *and* $(\tilde{x}_j, \tilde{y}_j) := P^j(\tilde{x}_o, \tilde{y}_0) \in M_{h,\epsilon}$, $j \in \mathbb{N}_0$,

$$\begin{aligned} |x_j - \tilde{x}_j| &\leq K\, \chi(h, \epsilon)^j \mid y_0 - \sigma(x_0, h, \epsilon)| \\ |y_j - \tilde{y}_j| &\leq K\, \chi(h, \epsilon)^j \mid y_0 - \sigma(x_0, h, \epsilon)| \;. \end{aligned}$$

iv) Closeness to M_ϵ.

$$|\sigma(x, h, \epsilon) - s(x, \epsilon)| \leq K\, h^{q+1} \quad \textit{for } x \in \mathbb{R}^m \;.$$

If the RK-method satisfies $b_i = a_{si}$ *then*

$$|\sigma(x, h, \epsilon) - s(x, \epsilon)| \leq K\, \epsilon\, h^q \quad \textit{for } x \in \mathbb{R}^m \;.$$

v) Maximality. *Every invariant set* Ω *of* P *is contained in* $M_{h,\epsilon}$, *i.e.,* $P(\Omega) = \Omega$ *implies* $\Omega \subset M_{h,\epsilon}$.

Remarks:

4) Under Hypothesis H_{DE} the singularly perturbed differential equation (1) admits an attractive invariant manifold. Theorem 3 states that under Hypothesis H_{RK} the RK-map (2) inherits this geometric property.

5) The invariant manifold of the differential equation is highly attractive, i.e., the manifold M_ϵ of the time-h map of Eq.(1) has attractivity $O(e^{-\beta h/\epsilon})$. The invariant manifold $M_{h,\epsilon}$ of the RK-map (2) has attractivity $R(\infty) + O(\epsilon/h)$. Hence, the attractivity property of the manifold M_ϵ is poorly reproduced by the attractivity of $M_{h,\epsilon}$ unless $R(\infty) = 0$.

6) In general, the distance between the manifolds M_ϵ and $M_{h,\epsilon}$ is $O(h^{q+1})$. If $|y - s(x, \epsilon)| = O(h^{q+1})$ then Eq.(9) shows that $Z = O(\epsilon\, h^q)$. This means that in this case all the information to step forward the numerical method is taken $O(\epsilon\, h^q)$-close to M_ϵ. ⊣

3. Global error bounds for stiff RK-methods

Our main result in Section 2 was obtained by investigating one step of the RK-method, only. One step corresponds to the local error. Integrating an ODE one is mainly interested in the global error, however, i.e., the error at time $T = Nh$. Since the invariant manifold result in fact is a global result it is very helpful to derive bounds on the global error of the RK-method. The flow of Eq.(1) close to the manifold M_ϵ is essentially described by the m-dimentional system $\dot{x} = f(x, s(x,\epsilon))$ which is no longer stiff with $\epsilon \to 0$. Similarly, the dynamics of the RK-map (2) near the manifold $M_{h,\epsilon}$ is essentially described by an m-dimensional map (the x-part of (2) on $M_{h,\epsilon}$). Thus, our approach reduces the stiff problem to a nonstiff one.

Let us consider a solution $(x(t),\, y(t))$ of Eq.(1) on M_ϵ and its RK-approximation $(x^k, y^k),\ k = 0, 1, 2, ...,$ given by

$$\begin{pmatrix} x^{k+1} \\ y^{k+1} \end{pmatrix} := P \begin{pmatrix} x^k \\ y^k \end{pmatrix}, \quad \begin{pmatrix} x^0 \\ y^0 \end{pmatrix} := \begin{pmatrix} x(0) \\ s(x(0),\epsilon) \end{pmatrix}$$

where P denotes the RK-map (2). We want to find bounds for $x^k - x(kh)$, $y^k - y(kh)$, $kh \leq T$.

Theorem 4 *Let the differential equation (1) satisfy Hypothesis H_{DE}. Apply a RK-method with Hypothesis H_{RK} to Eq. (1) and assume $p < r$. Moreover, assume that the initial conditions satisfy $y(0) = s(x(0),\epsilon)$, $x^0 = x(0)$, $y^0 - y(0) = O(h^{q+1})$.*

Then the following error bounds hold for $kh \leq T$.

$$\begin{aligned} x^k - x(kh) &= O(h^p) + O(\epsilon\, h^{q+1}) \\ y^k - y(kh) &= O(h^{q+1})\ . \end{aligned}$$

Moreover, if $b_i = a_{si}$ the estimate

$$y^k - y(kh) = O(h^p) + O(\epsilon\, h^q)$$

holds.

Remark:

7) If $q = p = 1$ then $x^k - x(kh) = O(h)$, $y^k - y(kh) = O(h)$. See also Remark 1). ⊣

The proof of Theorem 4 is done in two steps. In Lemma 5 we first derive a weaker bound. This preliminary bound then simplifies the proof of Theorem 4.

As in Section 2 we compare x^k with the RK-solution u^k of the differential equation $\dot{u} = f(u,\, s(u))$. (We again write $s(u)$ instead of $s(u,\epsilon)$.) We set $u(0) = x(0)$. Note that this implies $u(t) = x(t)$ for all t. The RK-solution of the full system satisfies

$$(16) \qquad \begin{aligned} x^{k+1} &= x^k + h(b^T \otimes I_m)\, X'^k \\ y^{k+1} &= y^k + h(b^T \otimes I_n)\, Y'^k \end{aligned}$$

$$
(17)\qquad \begin{array}{rclrcl} X^k &=& \mathbf{x}^k + h(A\otimes I_m)\,X'^k & X'^k &=& f(X^k,Y^k) \\ Y^k &=& \mathbf{y}^k + h(A\otimes I_n)\,Y'^k\,, & \epsilon\,Y'^k &=& g(X^k,Y^k) \end{array}
$$

and the RK-solution of the simplified system satisfies

$$
(18)\qquad u^{k+1} = u^k + h(b^T \otimes I_m)\; U'^k
$$

$$
(19)\qquad U^k = \mathbf{u}^k + h(A\otimes I_m)\,U'^k\,, \qquad U'^k = f(U^k,\, s(U^k))\;.
$$

Lemma 5 *Under the assumptions of Theorem 4 the bounds*

$$
x^k - u^k = O(\epsilon\, h^q)\,, \qquad X^k - U^k = O(\epsilon\, h^q)
$$

hold for $k\,h \le T$.

Proof: In addition to the variables u^k, U^k we define variables for the simplified system which correspond to y:

$$
\begin{array}{rcl} v^k &:=& s(u^k) \\ V^k &:=& s(U^k)\,, \qquad \epsilon V'^k = g(U^k,\, s(U^k))\;. \end{array}
$$

Noting that $\epsilon s'(u) f(u, s(u)) = g(u, s(u))$ (cf. Eq.(10)) we get from Eq.(13) that

$$
(20)\qquad \begin{array}{rcl} v^{k+1} &=& v^k + h(b^T\otimes I_n)\; V'^k \;+\; O(h^{p+1}) \\ V^k &=& \mathbf{v}^k + h(A\otimes I_n)\; V'^k \;+\; O(h^{q+1})\;. \end{array}
$$

We introduce the differences

$$
\begin{array}{rcl} \Delta x^k &=& x^k - u^k \\ \Delta y^k &=& y^k - v^k\,, \end{array}
$$

$$
\begin{array}{rclrcl} \Delta X^k &=& X^k - U^k & \Delta X'^k &=& X'^k - U'^k \\ \Delta Y^k &=& Y^k - V^k\,, & \Delta Y'^k &=& Y'^k - V'^k\;. \end{array}
$$

From Eqs.(16) - (20) we conclude that

$$
(21)\qquad \begin{array}{rclcl} \Delta x^{k+1} &=& \Delta x^k &+& h(b^T\otimes I_m)\,\Delta X'^k \\ \Delta y^{k+1} &=& \Delta y^k &+& h(b^T\otimes I_n)\;\Delta Y'^k + O(h^{p+1}) \\ \Delta X^k &=& \boldsymbol{\Delta}\mathbf{x}^k &+& h(A\otimes I_m)\;\Delta X'^k \\ \Delta Y^k &=& \boldsymbol{\Delta}\mathbf{y}^k &+& h(A\otimes I_n)\;\;\Delta Y'^k + O(h^{q+1})\;. \end{array}
$$

From the definitions it follows that

$$\Delta X'^k = R_1(X^k, Y^k, U^k)\,\Delta X^k + R_2(X^k, Y^k, U^k)\,\Delta Y^k$$

where $R_1 = \mathrm{diag}[f_x(U^k, s(U^k))] + O(|\Delta X^k|) + O(|\Delta Y^k|)$ and $R_2 = \mathrm{diag}[f_y(U^k, s(U^k))] + O(|\Delta X^k|) + O(|\Delta Y^k|)$. We have

$$|\Delta Y^k| = |Y^k - s(U^k)| \leq |Y^k - s(X^k)| + |s(X^k) - s(U^k)|\ .$$

Since $Y^k - s(X^k) = O(\epsilon\, h^q)$ by Eq.(15) and since the function s is uniformly Lipschitz in x it follows that

$$\Delta Y^k = O(1)\Delta X^k + O(\epsilon\, h^q)\ . \tag{22}$$

Hence, we have

$$\begin{aligned} \Delta X'^k &= \Big\{\mathrm{diag}[f_x(U^k, s(U^k))] + O(|\Delta X^k|) + O(|\Delta Y^k|)\Big\}\,\Delta X^k \\ &+ \Big\{\mathrm{diag}[f_y(U^k, s(U^k))] + O(|\Delta X^k|) + O(|\Delta Y^k|)\Big\}\,\Delta Y^k \\ &= O(1)\,\Delta X^k + O(\epsilon\, h^q) \end{aligned} \tag{23}$$

and

$$\Delta X^k = \mathbf{\Delta x}^k + O(h)\,\Delta X^k + O(\epsilon\, h^{q+1})$$

which may be written as

$$\Big((I_s \otimes I_m) + O(h)\Big)\,\Delta X^k = \mathbf{\Delta x}^k + O(\epsilon\, h^{q+1})\ . \tag{24}$$

Inserting this estimate for ΔX^k into Eq.(23) we obtain from Eq.(21) that

$$\Delta x^{k+1} = \Big(I_m + O(h)\Big)\,\Delta x^k + O(\epsilon\, h^{q+1})\ . \tag{25}$$

We apply the following *Gronwall* type argument which is easily proved by induction: *For any sequence* (δ^k), $\delta^k \in \mathbb{R}^+$, *satisfying* $\delta^0 = 0$ *and*

$$\delta^{k+1} \leq (1 + c_0)\delta^k + c_1, \quad c_0 > 0, \quad for\ \ 0 \leq k < N$$

the estimate

$$\delta^k \leq \frac{c_1}{c_0}\Big[(1 + c_0)^k - 1\Big] \leq \frac{c_1}{c_0}\left[e^{k\,c_0} - 1\right]$$

holds for $k \leq N$.

Setting $\delta^k = |\Delta x^k|$, $c_0 = C_0 h$, $c_1 = C_1\,\epsilon\, h^{q+1}$ we get from Eq.(25)

$$|\Delta x^k| \ \leq\ \frac{C_1}{C_0}\,\epsilon\, h^q (e^{C_0 T} - 1) \qquad \text{for}\ \ k \leq N\ .$$

Inserting this estimate into Eq.(24) terminates the proof of Lemma 5. ⊥

Proof of Theorem 4: In order to improve the bound of Lemma 5 we investigate the $O(\epsilon\, h^{q+1})$-term of Eq.(25) more precisely. Using the estimates of Lemma 5 and of Eq.(22) in Eq.(23) and noting that $\epsilon h^q \leq h^2$ we obtain

(26) $$\Delta X'^k = \mathrm{diag}[f_x^k]\, \Delta X^k + \mathrm{diag}[f_y^k]\, \Delta Y^k + O(\epsilon\, h^{q+2})$$

where $\mathrm{diag}[f_x^k] := \mathrm{diag}[f_x(U^k, s(U^k))]$ and $\mathrm{diag}[f_y^k] := \mathrm{diag}[f_y(U^k, s(U^k))]$. Similarly, we get

(27) $$\epsilon \Delta Y'^k = \mathrm{diag}[g_x^k]\, \Delta X^k + \mathrm{diag}[g_y^k]\, \Delta Y^k + O(\epsilon\, h^{q+2}) \ .$$

Solving Eq.(27) for ΔY^k and inserting the expression obtained into Eq.(26) yields

$$\Delta X'^k = \Big\{\mathrm{diag}[f_x^k] - \mathrm{diag}\Big[f_y^k (g_y^k)^{-1}\, g_x^k\Big]\Big\}\, \Delta X^k \ + \ \epsilon\, \mathrm{diag}\Big[f_y^k (g_y^k)^{-1}\Big]\, \Delta Y'^k + O(\epsilon\, h^{q+2}).$$

Inserting this into Eq.(21) and using Eq.(24) and Lemma 5 we have

$$\begin{aligned}\Delta x^{k+1} \ &= \ \Delta x^k + h(b^T \otimes I_m)\mathrm{diag}\Big[f_x^k - f_y^k (g_y^k)^{-1}\, g_x^k\Big]\mathbf{\Delta x}^k \\ &\quad + \epsilon\, h(b^T \otimes I_m)\mathrm{diag}\Big[f_y^k (g_y^k)^{-1}\Big]\, \Delta Y'^k + O(\epsilon\, h^{q+2}) \ .\end{aligned}$$

Subtracting Δx^k on both sides, taking the sum from $k = 0$ to $k = j$ and then taking norms yields

(28) $$|\Delta x^{j+1}| \leq hC_0 \sum_{k=0}^{j} |\Delta x^k| + \Big|\epsilon\, h(b^T \otimes I_m) \sum_{k=0}^{j} \mathrm{diag}\Big[f_y^k (g_y^k)^{-1}\Big]\Delta Y'^k + O(\epsilon\, h^{q+1})\Big|$$

where C_0 is a bound for $h(b^T \otimes I_m)\mathrm{diag}\Big[f_x^k - f_y^k (g_y^k)^{-1}\, g_x^k\Big]$.

We again use a *Gronwall* type argument easily proved by induction:
For any sequence (δ^j), $\delta^j \in \mathbb{R}^+$, *satisfying* $\delta^0 = 0$ *and*

$$\delta^{j+1} \leq c_0 \sum_{k=0}^{j} \delta^k + c_1 \,, \quad c_0 > 0 \,, \quad \mathit{for}\ \ 0 \leq j < N$$

the estimate

$$\delta^{j+1} \leq c_1 (1 + c_0)^j \leq c_1 e^{j\, c_0}$$

holds for $j < N$.

We set $\delta^j = |\Delta x^j|$, $c_0 = C_0\, h$ and introduce the bound $c_1(h, \epsilon)$ as follows:

$$\Big|\epsilon\, h(b^T \otimes I_m) \ \sum_{k=0}^{j} \mathit{diag}\Big[f_y^k (g_y^k)^{-1}\Big]\Delta Y'^k \ + \ O(\epsilon\, h^{q+1})\Big| \leq \ c_1(h, \epsilon) \ .$$

From Eq.(28) we get

$$|\Delta x^{j+1}| \le c_1(h,\epsilon)\, e^{C_0 T}\ . \tag{29}$$

We show that $c_1(h,\epsilon) = O(\epsilon\, h^{q+1})$. We have to estimate the terms

$$S^j := \epsilon\, h(b^T \otimes I_m) \sum_{k=0}^{j} \operatorname{diag}[f_y^k (g_y^k)^{-1}]\, \Delta Y'^k, \quad 0 \le j < N\ .$$

Note that, if the matrices $\operatorname{diag}[f_y^k (g_y^k)^{-1}]$ were omitted, Eq.(21) would imply $S^j = \epsilon\,(\Delta y^{j+1} - \Delta y^0 + O(h^p))$. We show that indeed a similar expression may be obtained with appropriate factors, however. We define for $0 \le k < N$

$$H(x^k) := f_y(x^k, s(x^k))\ g_y(x^k, s(x^k))^{-1}$$

and

$$\begin{aligned} Q^k &:= \epsilon\, h(b^T \otimes I_m)\{\operatorname{diag}[H(U^k)] - (I_s \otimes H(x^{k+1}))\}\, \Delta Y'^k \\ R^k &:= \epsilon\{H(x^k) - H(x^{k+1})\}\, \Delta y^k\ . \end{aligned}$$

From Eq.(21) we have

$$\Delta y^{k+1} = \Delta y^k + h(b^T \otimes I_n)\, \Delta Y'^k + T^k$$

with $T^k = O(h^{p+1})$. By induction it is now easily shown that

$$S^j = \epsilon\, H(x^{j+1})\, \Delta y^{j+1} - \epsilon\, H(x^0)\, \Delta y^0 + \sum_{k=0}^{j} \left(Q^k + R^k - \epsilon\, H(x^{k+1}) T^k\right)$$

holds. We estimate the first two terms of this expression. By assumption we have $\Delta y^0 = y^0 - s(x^0) = y^0 - y(0) = O(h^{q+1})$. From the properties ii), iv) of Theorem 3 and from Lemma 5 we conclude that

$$\begin{aligned} \Delta y^k &= y^k - s(u^k) = [y^k - \sigma(x^k,h,\epsilon)] + [\sigma(x^k,h,\epsilon) - s(x^k)] + [s(x^k) - s(u^k)] \\ &= \chi(h,\epsilon)^k\, O(|y^0 - \sigma(x^0,h,\epsilon)|) + O(h^{q+1}) \\ &= O(|\Delta y^0|) + O(|\sigma(x^0,h,\epsilon) - s(x^0)|) + O(h^{q+1}) = O(h^{q+1})\ . \end{aligned} \tag{30}$$

Hence, $S^j = \sum_{k=0}^{j} \left(Q^k + R^k - \epsilon\, H(x^{k+1}) T^k\right) + O(\epsilon\, h^{q+1})$. We estimate R^k and Q^k. Since $H(x^k) - H(x^{k+1}) = O(|x^{k+1} - x^k|) = O(h)$ we conclude using Eq.(30) that $R^k = O(\epsilon\, h^{q+2})$. Similarly, we have

$$\begin{aligned} \operatorname{diag}[H(U^k)] - (I_s \otimes H(x^{k+1})) &= O(|U^k - \mathbf{x}^{k+1}|) \\ &= O(|U^k - X^k|) + O(|X^k - \mathbf{x}^{k+1}|) \\ &= O(\epsilon\, h^q) + O(h) \end{aligned}$$

where we have used Lemma 5. Inserting the estimates of Eqs.(22), (24) and of Lemma 5 into Eq.(27) yields $\epsilon\,\Delta Y'^k = O(\epsilon\, h^q)$. Hence, we have shown that $Q^k = O(\epsilon\, h^{q+2})$. We conclude

$$\sum_{k=0}^{j}\Big(Q^k + R^k - \epsilon\, H(x^{k+1})T^k\Big) = \sum_{k=0}^{j}\Big(O(\epsilon\, h^{q+2}) + O(\epsilon\, h^{p+1})\Big) = O(\epsilon\, h^{q+1}) + O(\epsilon\, h^p)$$

implying $S^j = O(\epsilon\, h^{q+1})$ and thus $c_1(h,\epsilon) = O(\epsilon\, h^{q+1})$. From Eq.(29) we obtain

$$\Delta x^k = x^k - u^k = O(\epsilon\, h^{q+1}). \tag{31}$$

We now estimate

$$x^k - x(kh) = [x^k - u^k] + [u^k - u(kh)] = O(\epsilon\, h^{q+1}) + O(h^p)\ . \tag{32}$$

Here, we have used that $u^k - u(kh)$ is the global error of the differential equation $\dot{u} = f(u, s(u))$. Since this differential equation is not stiff with respect to ϵ the global error is $O(h^p)$. For the y component we find

$$\begin{aligned} y^k - y(kh) &= [y^k - s(u^k)] + [s(u^k) - s(x^k)] + [s(x^k) - y(kh)] \\ &= \Delta y^k + [s(u^k) - s(x^k)] + [s(x^k) - s(x(kh))] \\ &= \Delta y^k + O(|x^k - u^k|) + O(|x^k - x(kh)|)\ . \end{aligned}$$

By means of Eqs.(30), (31) and (32) we get $y^k - y(kh) = O(h^{q+1})$. It remains to consider the case $b_i = a_{si}$. By property iv) of Theorem 3 we have $\sigma(x^k, h, \epsilon) - s(x^k) = O(\epsilon\, h^q)$ and we conclude as in Eq.(30) that $\Delta y^k = O(\epsilon\, h^q)$ holds. It follows again with Eqs.(31) and (32) that

$$y^k - y(kh) = O(\epsilon\, h^q) + O(h^p)$$

which completes the proof of Theorem 4. $\perp$

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