Runge-Kutta solutions of stiff differential equations near stationary points

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Abstract. Runge-Kutta methods applied to stiff systems in singular perturbation form are shown to give accurate approximations of phase portraits near hyperbolic stationary points. Over arbitrarily long time intervals, Runge-Kutta solutions shadow solutions of the differential equation and vice versa. Sharp error bounds are derived. The proof uses attractive invariant manifolds to reduce the problem to the nonstiff case which was previously studied by Beyn.

Key words. Long-time error bounds, implicit Runge-Kutta method, stiff ODE, singular perturbation problem, hyperbolic equilibrium, shadowing, invariant manifold.

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1. Introduction

In the literature on the long-time behavior of numerical solutions of differential equations, there is a remarkable result of Beyn [2] which says that Runge-Kutta methods (and also other one-step methods and multistep methods) give accurate approximations of phase portraits near hyperbolic equilibria, such as saddle points. Stated in more detail: In a sufficiently small neighbourhood of the stationary point, every Runge-Kutta solution obtained with sufficiently small step size approximates some solution of the differential equation, and conversely, every solution in this neighbourhood is approximated by some Runge-Kutta solution, independently of the time interval which may be arbitrarily large. The approximation order is what one would expect for integration over bounded time intervals. The starting values of the solution and of its long-time approximant usually do not coincide. We also refer to the survey articles of Beyn [3] and Sanz-Serna and Larsson [17] which put this and related results into perspective. The result is meaningful in *nonstiff* situations: With increasing norm of the Jacobian, both the diameter of the neighbourhood and the maximum permitted stepsize shrink to zero in Beyn's result, and the approximation properties deteriorate.

In the present paper we study Runge-Kutta solutions near hyperbolic stationary points of stiff problems in singular perturbation form. We prove a Beyn type result which is valid in a neighbourhood of the equilibrium and for stepsizes that are not restricted by the small stiffness parameter ϵ, and which gives optimal-order error estimates. In Hairer, Lubich, and Roche [7] precise error bounds were obtained for Runge-Kutta approximations of "smooth" solutions of singularly perturbed problems over bounded time intervals. We will show the same approximation order as in [7] for the present problem. In Nipp and Stoffer [15], techniques of [14] and [7] were combined to study the existence and properties of an attractive invariant manifold for Runge-Kutta solutions of singularly perturbed problems. The invariant manifold results permit us to handle the initial rapid change of general solutions and the associated difficulty that in stiff problems the local error is not small in a whole neighbourhood of the stationary point.

The technique of proof used here aims at reducing the discrete and continuous systems to their invariant manifolds, on which the dynamics are described by nonstiff equations. These techniques permit to infer also other long-time properties of numerical solutions of stiff systems from known results for the nonstiff case. Typical examples are the persistence of hyperbolic periodic orbits and the approximation of attracting sets, which were studied in the nonstiff case by Eirola [5] (among others) and Kloeden and Lorenz [9], respectively. A related idea was recently used by Stoffer [18], where the results of [5] and [9] were extended from one-step methods to general linear methods with the aid of attractive invariant manifolds.

Also related to the present paper are the articles of Alouges and Debussche [1] and Larsson and Sanz-Serna [11]. They are concerned with the behavior near a hyperbolic stationary point of time and space discretizations of semilinear parabolic partial differential equations, which is another "stiff" problem. Larsson and Sanz-Serna [11] obtained sharp estimates for piecewise linear finite element space discretizations. Alouges and Debussche [1] gave a (sub-optimal) extension of Beyn's result for time discretization by the implicit Euler method. Their estimates can be improved to first-order error bounds by combining the techniques of [11] and [10]. However, better than first-order error estimates do not seem to be attainable for higher-order Runge-Kutta methods by using these arguments. One might expect that higher-order estimates require a study of existence and properties of (approximate) inertial manifolds, to be used in a way similar to the attractive invariant manifolds of the present paper.

The paper is organized as follows: In Section 2 we state our main result (Theorem 1) on the behavior of Runge-Kutta solutions of singularly perturbed problems near a hyperbolic equilibrium point. To prepare for the proof, we review the essentials of Beyn's result for the nonstiff case in Section 3. In Section 4 we discuss some aspects of attractive invariant manifolds for singularly perturbed problems. In Sections 5 and 6 we prove Theorem 1. To make the proof more transparent, we first derive a slightly weakened bound in Section 5, and we improve it in Section 6.

2. Statement of the result

We consider the singularly perturbed problem

$$\begin{aligned} \frac{dy}{dt} &= f(y,z) \\ \epsilon\frac{dz}{dt} &= g(y,z)\,, \qquad 0<\epsilon\ll 1\,, \end{aligned} \tag{2.1}$$

in the neighbourhood of a stationary point, which we may assume to be situated at the origin. Thus $f(0,0)=0$ and $g(0,0)=0$. The functions f and g are assumed to be sufficiently differentiable. As usual in singular perturbation theory, we impose the following condition for Eq.(2.1):

$$\text{All eigenvalues of } g_z(0,0) \text{ have negative real part.} \tag{2.2}$$

Further we assume that for small ϵ the stationary point is *hyperbolic*, that is, the Jacobian of the system (2.1) at the stationary point, $\begin{pmatrix} f_y & f_z \\ \epsilon^{-1}g_y & \epsilon^{-1}g_z \end{pmatrix}(0,0)$, has no eigenvalues on the imaginary axis. A similarity transformation with the matrix $\begin{pmatrix} I & \epsilon B \\ 0 & I \end{pmatrix}$, where $B = f_z g_z^{-1}(0,0)$, shows that for small ϵ the hyperbolicity condition is equivalent to the following condition:

$$(f_y - f_z g_z^{-1} g_y)(0,0) \ \text{ has no eigenvalues on the imaginary axis.} \tag{2.3}$$

We are interested in the behavior of Runge-Kutta methods applied to (2.1) with step size $h \geq \epsilon$:

$$y_{n+1} = y_n + h \sum_{j=1}^{s} b_j Y'_{nj} \ , \quad z_{n+1} = z_n + h \sum_{j=1}^{s} b_j Z'_{nj} \ , \tag{2.4a}$$

with internal stages ($i = 1, \ldots, s$)

$$Y_{ni} = y_n + h \sum_{j=1}^{s} a_{ij} Y'_{nj} \ , \quad Z_{ni} = z_n + h \sum_{j=1}^{s} a_{ij} Z'_{nj} \tag{2.4b}$$

satisfying relations of the form of (2.1):

$$\begin{aligned} Y'_{ni} &= f(Y_{ni}, Z_{ni}) \\ \epsilon Z'_{ni} &= g(Y_{ni}, Z_{ni}) \ . \end{aligned} \tag{2.4c}$$

We will make the method assumptions of [7]: The Runge-Kutta method is *A-stable*, i.e., the stability function

$$R(w) = 1 + w b^T (I - w\mathcal{Q})^{-1} 1\!\!1 \ , \tag{2.5}$$

(where $b^T = (b_1, \ldots, b_s)$, $\mathcal{Q} = (a_{ij})_{i,j=1}^s$, $1\!\!1 = (1, \ldots, 1)^T$) satisfies

$$|R(w)| \leq 1 \qquad \text{for } \ \text{Re}\, w \leq 0 \ . \tag{2.6}$$

We further assume that all eigenvalues of the Runge-Kutta matrix $\mathcal{Q} = (a_{ij})_{i,j=1}^s$ have positive real part, and that $R(\infty) = 1 - b^T \mathcal{Q}^{-1} 1\!\!1$ satisfies

$$|R(\infty)| < 1 \ . \tag{2.7}$$

If one restricts the attention to $\epsilon \ll h$, then only the invertibility of $\mathcal{Q}$ and condition (2.7) are needed. The method has *stage order* q, if

$$\sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \qquad \text{for } \ k = 1, \ldots, q \quad \text{and all } i \ . \tag{2.8}$$

Here c_i is defined by (2.8) with $k = 1$. We assume that the *order* p of the method when applied to nonstiff ordinary differential equations satisfies $p \geq q + 1$. (If $p = q$, this is achieved by reducing q by 1.)

We will show the following result in this article.

Theorem 1. *Under the above assumptions, there are positive constants r and h_0 such that the following holds for $0 < \epsilon \leq h \leq h_0$.*
First assertion: For every Runge-Kutta solution (2.4) with $\|(y_n, z_n)\| \leq r$ for $0 \leq n \leq N$, there exists a solution $(y(t), z(t))$ of (2.1) for $0 \leq t \leq T = Nh$, such that for $0 \leq n \leq N$

$$
\begin{aligned}
\|y_n - y(nh)\| \quad &\leq C \cdot (h^p + \epsilon h^{q+1} + \epsilon \rho^n) \\
\|z_n - z(nh)\| \quad &\leq \begin{cases} C \cdot (h^p + \epsilon h^q + \rho^n) & \text{if } a_{sj} = b_j \text{ for } j = 1, \dots, s \ , \\ C \cdot (h^{q+1} + \rho^n) & \text{else .} \end{cases}
\end{aligned}
\tag{2.9}
$$

Here $\rho < 1$ and C depend only on f, g, r and h_0, and in particular are independent of ϵ, h, and N. Moreover, for $\epsilon \ll h$ we have $\rho = |R(\infty)| + O(\epsilon/h)$.
Second assertion: Conversely, for every solution of (2.1) with $\|(y(t), z(t))\| \leq r$ for $0 \leq t \leq T = Nh$, there exists a Runge-Kutta solution (y_n, z_n), $0 \leq n \leq N$, satisfying (2.9) with $\rho = e^{-\kappa h/\epsilon}$, with C and $\kappa > 0$ independent of ϵ, h, and N.

This extends Theorem 3.1 of Beyn [2] to the stiff case. Apart from the rapidly changing initial phase, the approximation order is the same as that established by Hairer, Lubich, and Roche [7] for Runge-Kutta approximations of "smooth" solutions of (2.1) on bounded time intervals. An essential aspect of Theorem 1 is the fact that the estimates remain uniform as the integration interval becomes large. It is again possible to infer the existence of stable and unstable manifolds of the Runge-Kutta scheme which are close to those of the differential equation, similarly to Beyn [2] for the nonstiff case, cf. also Nipp and Stoffer [14].

3. A review of the nonstiff case

Consider the (nonstiff) differential equation

$$\frac{dx}{dt} = f(x) \ , \tag{3.1}$$

with $x = 0$ being a hyperbolic equilibrium. Beyn [2], Thm. 3.1, has shown the following for numerical solutions obtained by applying a Runge-Kutta method of order p to Eq. (3.1): For every RK-solution (x_n), $0 \leq n \leq N$, which stays in a sufficiently small neighbourhood U of the stationary point, there is a solution $x(t)$ of Eq. (3.1) satisfying $\|x_n - x(nh)\| \leq Ch^p$. Conversely, for every solution $x(t)$ in U, $0 \leq t \leq T = Nh$, there is a RK-solution (x_n) with $\|x_n - x(nh)\| \leq Ch^p$. The constant C is independent of h and N.

This result of Beyn can be viewed as a consequence of the stability lemma stated below. Lemma 2 will also be used in the proof of Theorem 1.

Let A be a square matrix which has no eigenvalues on the imaginary axis. We blockdiagonalize

$$A = V \begin{pmatrix} A^+ & 0 \\ 0 & A^- \end{pmatrix} V^{-1} \tag{3.2}$$

where all eigenvalues of A^+ (A^-) have positive (negative) real part. We use the corresponding spectral projections

$$P^+ = V\Pi^+ V^{-1} , \quad P^- = V\Pi^- V^{-1} , \tag{3.3}$$

where

$$\Pi^+ v = \begin{pmatrix} v^+ \\ 0 \end{pmatrix} , \; \Pi^- v = \begin{pmatrix} 0 \\ v^- \end{pmatrix} \quad \text{for} \quad v = \begin{pmatrix} v^+ \\ v^- \end{pmatrix} .$$

A Runge-Kutta method applied to the differential equation $dx/dt = Ax + \varphi(x)$ gives a recursion

$$x_{n+1} = R(hA)x_n + h\phi(x_n) , \tag{3.4}$$

where $R(w)$ is the stability function (2.5), and ϕ is some h-dependent function related to φ, with Lipschitz constant $L_\phi = \left(\sum_{i=1}^s |b_i| + O(h)\right) L_\varphi$. We also consider a perturbed variant

$$\tilde{x}_{n+1} = R(hA)\tilde{x}_n + h\phi(\tilde{x}_n) + h\delta_n . \tag{3.5}$$

Note that if we take $\tilde{x}_n = x(nh)$, where $x(t)$ is a solution of $dx/dt = Ax + \varphi(x)$, then $h\delta_n$ is the local error, which is $O(h^{p+1})$ uniformly in bounded neighbourhoods of the stationary point.

Lemma 2. *Assume $\phi(0) = 0$ and $\|\phi'(x)\| \le \ell$ for $\|x\| \le 2r$. Let $(\tilde{x}_n)$ with $\|\tilde{x}_n\| \le r$ for $0 \le n \le N$ satisfy (3.5). Let δ and β denote bounds*

$$\|\delta_n\| \le \delta \quad \text{for } 0 \le n \le N$$

$$\|P^-(x_0 - \tilde{x}_0)\| + \|P^+(x_N - \tilde{x}_N)\| \le \beta .$$

If ℓ, δ, β, and h are sufficiently small, then equation (3.4) has a unique solution (x_n) with prescribed boundary values $P^- x_0$ and $P^+ x_N$, which satisfies

$$\|x_n - \tilde{x}_n\| \le C \cdot (\beta + \delta) \quad \text{for} \;\; 0 \le n \le N .$$

The constant C is independent of h and N.

Proof. Since $R(w)$ is an approximation of the exponential function, we have the bounds

$$\|R(hA^-)^n\| \le C \cdot e^{-\alpha h n} , \quad \|R(hA^+)^{-n}\| \le C \cdot e^{-\alpha h n} , \qquad n \ge 0 ,$$

with some $\alpha > 0$ which depends on A and the maximum permitted step size h_0. Using the discrete variation of constants formula forwards and backwards, we have with $x_n = V\begin{pmatrix} x_n^+ \\ x_n^- \end{pmatrix}$ and $\phi = V\begin{pmatrix} \phi^+ \\ \phi^- \end{pmatrix}$

$$x_n^- = R(hA^-)^n x_0^- + h\sum_{j=0}^{n-1} R(hA^-)^{n-j-1}\phi^-(x_j) ,$$

$$x_n^+ = R(hA^+)^{n-N} x_N^+ - h\sum_{j=n}^{N-1} R(hA^+)^{n-j-1}\phi^+(x_j) ,$$

and similarly for $\tilde{x}_n$. As the Lipschitz constant of ϕ can be kept as small as we please, the result follows from the Banach contraction principle (cf. also [11]). □

4. Attractive invariant manifolds

One difficulty in extending Beyn's result to the stiff problem (2.1), is that the local error is not small for *arbitrary* starting values near the stationary point. The reason is that general solutions of (2.1) undergo rapid initial changes as is shown in the so-called Tikhonov-Levinson theory of singularly perturbed systems. A description of this theory may be found e.g. in the text-books [19], [16] and also [8]. As is known from [4], [6], [12], [13], there is a smooth *attractive invariant manifold* $M_\epsilon = \{(y,z) |\ z = s_\epsilon(y)\}$ (locally near the stationary point, which itself is on M_ϵ). Solutions of (2.1) starting on M_ϵ remain on M_ϵ and are *"smooth"* in the sense that arbitrarily many derivatives are bounded independently of ϵ. An arbitrary solution $(y(t), z(t))$ of (2.1) near $(0,0)$ quickly approaches a solution on M_ϵ: There is a solution $(\tilde{y}(t), \tilde{z}(t))$ on M_ϵ such that

$$\|y(t) - \tilde{y}(t)\| + \epsilon \cdot \|z(t) - \tilde{z}(t)\| \le C \cdot \epsilon e^{-\kappa t/\epsilon} , \quad 0 \le t \le T , \tag{4.1}$$

with some constants C and $\kappa > 0$ which do not depend on ϵ and T ("property of asymptotic phase"). If $(y(t), z(t)) = (y(t), s_\epsilon(y(t)))$ is a solution of Eq. (2.1) on M_ϵ then $y(t)$ is a solution of the (nonstiff) differential equation

$$\frac{dy}{dt} = f(y, s_\epsilon(y)) , \tag{4.2}$$

which has $y = 0$ as an equilibrium. The function s_ϵ depends smoothly on $\epsilon \ge 0$. For $\epsilon = 0$ we denote by $s_0(y) = z$ the locally unique solution of the "reduced system" $0 = g(y,z)$. In particular, we have $s_\epsilon'(0) = s_0'(0) + O(\epsilon) = -(g_z^{-1}g_y)(0,0) + O(\epsilon)$. Hence, the Jacobian of Eq. (4.2) at $y = 0$ is

$$(f_y - f_z g_z^{-1} g_y)(0,0) + O(\epsilon) .$$

By condition (2.3), this matrix has no eigenvalues on the imaginary axis for small ϵ.

Not only the continuous system (2.1), but also its RK-discretisation admits an invariant manifold. This was recently studied by Nipp and Stoffer [15]. Let us summarize their findings: For $0 < \epsilon \le h \le h_0$, there is a local attractive invariant manifold $M_{\epsilon,h} = \{(y,z)|\ z = s_{\epsilon,h}(y)\}$ for the Runge-Kutta solutions (2.4). $M_{\epsilon,h}$ is close to M_ϵ:

$$\|s_{\epsilon,h}(y) - s_\epsilon(y)\| \le \begin{cases} C\,\epsilon\, h^q & \text{if } b_i = a_{si} \text{ for all } i\,, \\ C\,h^{q+1} & \text{else}\,. \end{cases} \tag{4.3}$$

Again, the property of asymptotic phase states that for every (y_0, z_0) in an h- and ϵ-independent neighbourhood of $M_{\epsilon,h}$, there exists $(\tilde{y}_0, \tilde{z}_0) \in M_{\epsilon,h}$ such that the corresponding Runge-Kutta solutions satisfy

$$\|y_n - \tilde{y}_n\| + \epsilon \cdot \|z_n - \tilde{z}_n\| \le C \cdot \epsilon\rho^n\ , \quad 0 \le n \le N\ , \tag{4.4}$$

where $\rho < 1$ and C do not depend on ϵ, h, and N. For $\epsilon \ll h$ we have $\rho = |R(\infty)| + O(\epsilon/h)$.

Remark. The result in [15] is formulated for $\epsilon \ll h$, but it extends to $\epsilon \le h$ under the stronger method assumptions that we have imposed. This can be shown using the estimates in Section 5 of [7].

5. Proof of Theorem 1 (slightly weakened estimate)

The basic idea is to reduce the stiff case to the nonstiff case by means of the invariant manifolds $M_{\epsilon,h}$ and M_ϵ. Reducing the discrete and continuous systems to the corresponding invariant manifolds, the dynamics only depend on the nonstiff y-equation. More precisely, we proceed as follows to prove the first assertion of Theorem 1: Let (y_n, z_n), $0 \le n \le N$, be a given RK-solution of Eq.(2.1) staying in an r-neighbourhood of $(0,0)$, r sufficiently small. We first take the RK-solution $(\tilde{y}_n, \tilde{z}_n)$ on $M_{\epsilon,h}$ with the same "asymptotic phase" (see (4.4)). Then, using M_ϵ we construct a RK-solution (η_n) of the nonstiff system (4.2) "shadowing" $(\tilde{y}_n)$. In a third step, we apply Beyn's result to Eq.(4.2) in order to establish the claimed solution $(y(t), z(t)) = (y(t), s_\epsilon(y(t))$, $0 \le t \le T = Nh$, of Eq.(2.1). Conversely, for the second assertion of Theorem 1: Given a solution $(y(t), z(t))$ of Eq.(2.1), we first take the solution $(\tilde{y}(t), \tilde{z}(t))$ on M_ϵ with the same "asymptotic phase" (see (4.1)). Then, by means of Beyn's result there is a RK-solution (η_n) of Eq.(4.2) staying close to $(\tilde{y}(nh))$. Finally, we construct a RK-solution $(y_n, z_n) = (y_n, s_{\epsilon,h}(y_n))$ of Eq.(2.1) on $M_{\epsilon,h}$ "shadowing" $(\eta_n, s_\epsilon(\eta_n))$. Hence, in both cases the shadowing solutions lie on the (continuous or discrete) attractive invariant manifolds. We remark that accurate approximation of the rapid initial transient is not possible with step sizes $h \gg \epsilon$, as can be seen already from the example $\epsilon z' = -z$.

Proof of the first assertion: We estimate

$$\|y_n - y(nh)\| \le \|y_n - \tilde{y}_n\| + \|\tilde{y}_n - \eta_n\| + \|\eta_n - y(nh)\| \tag{5.1}$$

in three steps.

1) By the bound (4.4) we have $\|y_n - \tilde{y}_n\| \le C\epsilon\rho^n$ for $0 \le n \le N$.

2) To simplify this step we show first that $\tilde{y}_n - \eta_n = O(\epsilon h^q)$. The stronger estimate $O(\epsilon h^{q+1})$ will be obtained in the following section.

In order to apply Lemma 2 we need the estimate given in the following lemma.

Lemma 3. *Let y_0 be in an r-neighbourhood of 0. Apply one step of the RK-method to Eq. (4.2) taking $\eta_0 = y_0$ to η_1. Let (y_1, z_1) denote the result of one step of the RK-method applied to Eq. (2.1) with starting value $(y_0, z_0) = (y_0, s_{\epsilon,h}(y_0)) \in M_{\epsilon,h}$. Then*

$$y_1 - \eta_1 \;=\; O(\epsilon h^{q+1})$$

holds for $0 < \epsilon \le h \le h_0$, uniformly for $\|y_0\| \le r$.

Proof. (a) Let $\widehat{Y}_i$ $(i = 1, \ldots, s)$ denote the internal stages of the RK-method applied to Eq. (4.2). Putting

$$\widehat{Z}_i = s_\epsilon(\widehat{Y}_i) \ ,$$

we then have

$$\eta_1 = \eta_0 + h \sum_{j=1}^{s} b_j f(\widehat{Y}_j, \widehat{Z}_j) \ , \quad \widehat{Y}_i = \eta_0 + h \sum_{j=1}^{s} a_{ij} f(\widehat{Y}_j, \widehat{Z}_j) \ .$$

We will show in part (b) of the proof that we have, with $\zeta_0 = s_\epsilon(\eta_0)$,

$$\epsilon(\widehat{Z}_i - \zeta_0) = h \sum_{j=1}^{s} a_{ij} g(\widehat{Y}_j, \widehat{Z}_j) + O(\epsilon h^{q+1}) \ . \tag{5.2}$$

On the other hand, the internal stages Y_i, Z_i of the RK-method applied to Eq. (2.1) satisfy (2.4). The starting values are $\eta_0 = y_0$, and $\zeta_0 = z_0 + O(h^{q+1})$ by (4.3). We next apply Lemma 6 of [7]. This perturbation lemma says that the difference between the internal stages Y_i, Z_i $(i = 1, \ldots, m)$ and those of a perturbed scheme

$$\widehat{Y}_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(\widehat{Y}_j, \widehat{Z}_j) + h\delta_i \ , \qquad \epsilon(\widehat{Z}_i - z_0) = h \sum_{j=1}^{s} a_{ij} g(\widehat{Y}_j, \widehat{Z}_j) + h\theta_i$$

are bounded by $\|\widehat{Y}_i - Y_i\| \le Ch(\|\delta\| + \|\theta\|)$, $\|\widehat{Z}_i - Z_i\| \le C(h\|\delta\| + \|\theta\|)$. In the present situation, we have defects $\delta_i = 0$ and $h\theta_i = O(\epsilon h^{q+1})$. This gives us the bounds

$$\widehat{Y}_i - Y_i = O(\epsilon h^{q+1}) \ , \quad \widehat{Z}_i - Z_i = O(\epsilon h^q) \ .$$

Using $\eta_0 = y_0$ and the Lipschitz boundedness of f in the equation defining η_1, we thus get the estimate stated in Lemma 3.

(b) The key to proving (5.2) is the identity

$$\epsilon s_\epsilon'(y) f(y, s_\epsilon(y)) = g(y, s_\epsilon(y)) \quad \text{for all } y \text{ (near 0)},$$

which is obtained from the second equation in (2.1) restricted to the invariant manifold $M_\epsilon : z = s_\epsilon(y)$.
Let $y(t)$ be the solution of Eq. (4.2) with starting value $y(0) = \eta_0$, and let $z(t) = s_\epsilon(y(t))$. Since the stage order is q, we have

$$\widehat{Y}_i - y(c_i h) = O(h^{q+1}) \ , \quad \widehat{Z}_i - z(c_i h) = O(h^{q+1}) \ .$$

Hence,

$$h \sum_{j=1}^s a_{ij}\, g(\widehat{Y}_j, \widehat{Z}_j) = \epsilon h \sum_{j=1}^s a_{ij}\, s_\epsilon'(\widehat{Y}_j) f(\widehat{Y}_j, s_\epsilon(\widehat{Y}_j))$$

$$= \epsilon \left(\int_0^{c_i h} s_\epsilon'(y(t))\, f(y(t), s_\epsilon(y(t)))\, dt + O(h^{q+1}) \right) = \epsilon \left(\int_0^{c_i h} \tfrac{dz}{dt}(t)\, dt + O(h^{q+1}) \right)$$

$$= \epsilon \Big(z(c_i h) - z(0) + O(h^{q+1}) \Big) = \epsilon \left(\widehat{Z}_i - \zeta_0 + O(h^{q+1}) \right) \ ,$$

which gives the desired relation (5.2). □

As shown in Section 4, Eq.(4.2) may be written as

$$\frac{dy}{dt} = Ay \,+\, \varphi(y)$$

where $A = (f_y - f_z g_z^{-1} g_y)(0,0)$ is hyperbolic and φ has Lipschitz constant $O(r) + O(\epsilon) = O(r)$ (assuming $\epsilon < r$). Hence, applying the RK-method to Eq.(4.2) yields a recursion of the form

$$\eta_{n+1} = R(hA)\eta_n + h\phi(\eta_n) \ , \tag{5.3}$$

where the Lipschitz constant of ϕ is again $O(r)$. We now use Lemma 3 with $\widetilde{y}_n$ in the role of $\eta_0 = y_0$. The result of a RK-step for Eq. (4.2) starting from $\widetilde{y}_n$ is $R(hA)\widetilde{y}_n + h\phi(\widetilde{y}_n)$, and hence Lemma 3 shows that the RK-solution $(\widetilde{y}_n, \widetilde{z}_n) = (\widetilde{y}_n, s_{\epsilon,h}(\widetilde{y}_n)) \in M_{\epsilon,h}$ of the singularly perturbed system (2.1) satisfies

$$\widetilde{y}_{n+1} = R(hA)\widetilde{y}_n + h\phi(\widetilde{y}_n) + O(\epsilon h^{q+1}) \ .$$

We may thus apply Lemma 2 with η_n in the role of x_n, with $\widetilde{y}_n$ in the role of $\widetilde{x}_n$ and with $h\delta_n = O(\epsilon h^{q+1})$. With boundary values chosen as

$$P^- \eta_0 = P^- \widetilde{y}_0 \ , \qquad P^+ \eta_N = P^+ \widetilde{y}_N \ ,$$

Lemma 2 gives us a RK-solution (η_n) of Eq.(4.2) which satisfies

$$\|\widetilde{y}_n - \eta_n\| \le C\, \epsilon\, h^q \quad \text{for } \ 0 \le n \le N \ . \tag{5.4}$$

3) Beyn's result applied to Eq. (4.2) now yields: There is a solution $y(t)$ satisfying

$$\|\eta_n - y(nh)\| \le C\, h^p \qquad \text{for } \ 0 \le n \le N \ .$$

The constant C is again independent of ϵ, because the right-hand side of Eq. (4.2) depends smoothly on $\epsilon \geq 0$.

¿From the steps 1), 2) and 3) it follows with (5.1) that

$$\|y_n - y(nh)\| \leq C(\epsilon\, \rho^n + \epsilon\, h^q + h^p)\ .$$

It remains to estimate the z-components. We have

$$\|z_n - z(nh)\| \leq \|z_n - \tilde{z}_n\| + \|\tilde{z}_n - z(nh)\|\ , \qquad 0 \leq n \leq N\ ,$$

where $(\tilde{y}_n, \tilde{z}_n) \in M_{\epsilon,h}$, $(y(t), z(t)) \in M_\epsilon$. We thus get

$$\|z_n - z(nh)\| \leq \|z_n - \tilde{z}_n\| + \|s_{\epsilon,h}(\tilde{y}_n) - s_{\epsilon,h}(y(nh))\| + \|s_{\epsilon,h}(y(nh)) - s_\epsilon(y(nh))\|\ .$$

The property of asymptotic phase (4.4) yields $\|z_n - \tilde{z}_n\| \leq C\,\rho^n$; steps 2), 3) imply $\|s_{\epsilon,h}(\tilde{y}_n) - s_{\epsilon,h}(y(nh))\| \leq C(\epsilon\, h^q + h^p)$, and the last term is bounded by (4.3). Combining these estimates we obtain

$$\|z_n - z(nh)\| \leq \begin{cases} C\,(\rho^n + \epsilon\, h^q + h^p) & \text{if } b_i = a_{si}\ , \\ C\,(\rho^n + h^{q+1}) & \text{else}\,. \end{cases}$$

This completes the proof of the first assertion of Theorem 1, except that the $O(\epsilon h^q)$ term in the error estimate of the y-component is not yet optimal. This term will be improved to $O(\epsilon h^{q+1})$ in the following section.

Proof of the second assertion: The three steps to construct a RK-solution (y_n, z_n) on $M_{\epsilon,h}$ are sketched in the beginning of Section 5. We do not give the details, since they are almost the same as in the proof of the first assertion.

6. Proof of Theorem 1 (refined estimate)

To complete the proof of Theorem 1, we show that the difference between the sequences $(\tilde{y}_n)$ and (η_n) constructed in Section 5 is $O(\epsilon h^{q+1})$. From (5.4) we know already that the difference is $O(\epsilon h^q)$. To improve this estimate, we need a refined version of Lemma 3. In the situation of Lemma 3, we would of course have $y_1 = \eta_1$ if the function f were independent of z, i.e., if $f_z \equiv 0$. For $f_z(y_0, s_\epsilon(y_0)) = O(h)$, tracing the proof of Lemma 3 shows that we still have $y_1 - \eta_1 = O(\epsilon h^{q+2})$ which improves the estimate of Lemma 3 by the missing factor h. The idea for improving the estimate in the general case now consists in transforming variables

$$u = y - \epsilon B z\ , \quad v = z$$

where the constant matrix B is chosen such that Eq. (2.1) written in the variables (u, v),

$$\begin{aligned} \frac{du}{dt} &= f(u+\epsilon Bv, v) - Bg(u+\epsilon Bv, v) \qquad &=: F(u,v) \\ \epsilon \frac{dv}{dt} &= g(u+\epsilon Bv, v) &=: G(u,v) \end{aligned} \tag{6.1}$$

has a small derivative F_v. Since $F_v = f_z - Bg_z + O(\epsilon)$, we choose B close to $(f_z g_z^{-1})(y, z)$. This procedure leads to the following.

Lemma 4. *Let the situation of Lemma 3 be given, except that the initial condition $y_0 = \eta_0$ is replaced by*

$$y_0 - \epsilon B s_{\epsilon,h}(y_0) = \eta_0 - \epsilon B s_\epsilon(\eta_0) ,$$

with $B = (f_z g_z^{-1})(y_0, z_0) + O(h)$. Then,

$$y_1 - \epsilon B s_{\epsilon,h}(y_1) = \eta_1 - \epsilon B s_\epsilon(\eta_1) + O(\epsilon h^{q+2}) + O(h^{p+1}) .$$

Proof. Since the RK-method is invariant under linear transformations of variables, we have that $(u_1, v_1) := (y_1 - \epsilon B z_1, z_1)$ is the result of one step of the RK-method applied to Eq. (6.1) with starting value $(u_0, v_0) := (y_0 - \epsilon B z_0, z_0)$.

The invariant manifold of the singularly perturbed system (6.1) is parametrized by $v = S_\epsilon(u)$ with S_ϵ defined by $S_\epsilon(u) = s_\epsilon(y)$ for $u = y - \epsilon B s_\epsilon(y)$. Let μ_1 denote the result of the RK-method applied to the differential equation (which is the u-version of Eq. (4.2))

$$\frac{du}{dt} = F(u, S_\epsilon(u)) \tag{6.2}$$

with starting value $\mu_0 = \eta_0 - \epsilon B s_\epsilon(\eta_0)$. By our assumptions, we have $u_0 = \mu_0$ and $F_v(u_0, v_0) = O(h)$. By the arguments in the beginning of this section we thus have

$$u_1 - \mu_1 = O(\epsilon h^{q+2}) .$$

Both μ_1 and $\eta_1 - \epsilon B s_\epsilon(\eta_1)$ approximate the solution $u(t) = y(t) - \epsilon B s_\epsilon(y(t))$ of Eq. (6.2) with initial value $u(0) = \mu_0$ at $t = h$ with an error of size $O(h^{p+1})$. Hence we have

$$\mu_1 = \eta_1 - \epsilon B s_\epsilon(\eta_1) + O(h^{p+1}) .$$

Since $u_1 = y_1 - \epsilon B s_{\epsilon,h}(y_1)$, the result follows. □

Remark. A more detailed study (using trees and elementary differentials) reveals that the difference between μ_1 and $\eta_1 - \epsilon B s_\epsilon(\eta_1)$ is actually $O(\epsilon h^{p+1})$. Hence the $O(h^{p+1})$ term in Lemma 4 can be omitted. We have not carried this out, because Lemma 4 as stated above is sufficient for our needs. □

Let $(\widetilde{y}_n)$ and (η_n) be the sequences constructed in Section 5. We put

$$B_n = (f_z g_z^{-1})(\eta_n, s_\epsilon(\eta_n))$$

and introduce

$$\widetilde{u}_n = \widetilde{y}_n - \epsilon B_n s_{\epsilon,h}(\widetilde{y}_n) \ , \quad \mu_n = \eta_n - \epsilon B_n s_\epsilon(\eta_n) \ . \tag{6.3}$$

We recall that by (5.4) and (4.3)

$$s_{\epsilon,h}(\widetilde{y}_n) - s_\epsilon(\eta_n) = O(h^{q+1}) \ . \tag{6.4}$$

We now formulate recursions for μ_n and $\widetilde{u}_n$. To this end, we set

$$\phi_n(\mu) = \phi(\eta) + h^{-1}\{R(hA) \cdot \epsilon B_n s_\epsilon(\eta) - \epsilon B_n s_\epsilon(\widehat{\eta})\}$$

where η is defined as a function of μ by $\mu = \eta - \epsilon B_n s_\epsilon(\eta)$ (as in (6.3)), and $\widehat{\eta} = R(hA)\eta + h\phi(\eta)$ is the result of an RK-step for Eq. (4.2) with starting value η. We note that ϕ_n has a Lipschitz constant of size $O(r) + O(\epsilon)$ uniformly for all n. Inserting the recursion (5.3) for η_n into (6.3), we get a recursion for μ_n:

$$\mu_{n+1} = R(hA)\mu_n + h\phi_n(\mu_n) + c_n \ ,$$

where $c_n = -\epsilon(B_{n+1} - B_n)s_\epsilon(\eta_{n+1})$. We define $\widetilde{\eta}_n$ by $\widetilde{u}_n = \widetilde{\eta}_n - \epsilon B_n s_\epsilon(\widetilde{\eta}_n)$ and let $\widehat{\eta}_{n+1} = R(hA)\widetilde{\eta}_n + h\phi(\widetilde{\eta}_n)$. Lemma 4 applied with $\widetilde{y}_n$ and $\widetilde{\eta}_n$ in the roles of y_0 and η_0 now gives

$$\begin{aligned} \widetilde{y}_{n+1} - \epsilon B_n s_{\epsilon,h}(\widetilde{y}_{n+1}) &= \widehat{\eta}_{n+1} - \epsilon B_n s_\epsilon(\widehat{\eta}_{n+1}) + O(\epsilon h^{q+2}) + O(h^{p+1}) \\ &= R(hA)\widetilde{u}_n + h\phi_n(\widetilde{u}_n) + O(\epsilon h^{q+2}) + O(h^{p+1}) \ . \end{aligned}$$

Together with the estimate $\epsilon(B_{n+1} - B_n)(s_{\epsilon,h}(\widetilde{y}_{n+1}) - s_\epsilon(\eta_{n+1})) = O(\epsilon h^{q+2})$, see (6.4), this yields

$$\widetilde{u}_{n+1} = R(hA)\widetilde{u}_n + h\phi_n(\widetilde{u}_n) + c_n + O(\epsilon h^{q+2}) + O(h^{p+1}) \ .$$

Moreover, the boundary values satisfy

$$P^-\widetilde{u}_0 - P^-\mu_0 = -\,P^-\,\epsilon B_0\Big(s_{\epsilon,h}(\widetilde{y}_0) - s_\epsilon(\eta_0)\Big) = O(\epsilon h^{q+1})$$

where we used again (6.4), and similarly also

$$P^+\widetilde{u}_N - P^+\mu_N = O(\epsilon h^{q+1}) \ .$$

Lemma 2 generalizes trivially to the situation where the nonlinearity ϕ depends on n, provided that the condition $\|\phi_n'(x)\| \le \ell$ with small ℓ for $\|x\| \le 2r$ holds uniformly in n, as is the case for the ϕ_n considered here. This extended version of Lemma 2 now implies

$$\widetilde{u}_n - \mu_n = O(\epsilon h^{q+1}) + O(h^p) \ , \quad 0 \le n \le N \ .$$

Together with (6.3) and (6.4) this gives

$$\widetilde{y}_n - \eta_n = O(\epsilon h^{q+1}) + O(h^p) \ , \quad 0 \le n \le N \ .$$

Using this improved estimate in (5.1) completes the proof of Theorem 1. □

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