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Asymptotic Error Expansions for Stiff Equations: an Analysis for the Implicit Midpoint and Trapezoidal Rules in the Strongly Stiff Case

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Summary. The structure of the global discretization error is studied for the implicit midpoint and trapezoidal rules applied to nonlinear *stiff* initial value problems. The point is that, in general, the global error contains nonsmooth (oscillating) terms at the dominant h^2-level. However, it is shown in the present paper that for special classes of stiff problems these nonsmooth terms contain an additional factor ε (where $-1/\varepsilon$ is the magnitude of the stiff eigenvalues). In these cases a "full" asymptotic error expansion exists in the *strongly stiff case* (ε sufficiently small compared to the stepsize h). The general case (where the oscillating error components are $O(h^2)$ and not $O(\varepsilon h^2)$) and applications of our results (extrapolation and defect correction algorithms) will be studied in separate papers.

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1 Introduction

During the recent years various convergence results have been derived for discretizations of nonlinear stiff initial value problems

$$\begin{aligned} &y'(t)=f(t, y(t)), \quad f\colon G\to \mathbb{R}^n, \quad G\subset\mathbb{R}\times\mathbb{R}^n \\ &y(0)=z_0 \\ &z(t)\ldots \textit{exact solution fixed by } z(0)=z_0. \end{aligned} \tag{1.1}$$

Most of these results are based on the concept of one-sided Lipschitz continuity and therefore cover a very general class of stiff problems. For many applications, however, simple convergence results (i.e., quantitative bounds for the global error) are too weak. If, for instance, error estimates (for local or global errors) are needed for the theoretical justification of stepsize control mechanisms or for the analysis of acceleration techniques, then assertions concerning the *structure* of the (global) discretization error should be available.

In the classical case of (nonstiff) problems with smooth data functions such results have been known for a long time: the existence of asymptotic expansions of the global error is well-known in a variety of situations (cf. for instance [11, 15]). For stiff problems, however, only few results of this type have been available so far (cf. [1, 2, 3, 8, 12, 16]). In particular, an analysis for the implicit Euler scheme can be found in [3] and in [12].

For the implicit midpoint rule and the implicit trapezoidal rule, B-convergence results (i.e., convergence results based on one-sided Lipschitz continuity) are well known (cf. [10, 13]). The main goal of our current research activity is the derivation of assertions concerning the structure of the global error for these methods. The relevant material will be partitioned into three papers:

(i) In the present paper the so-called strongly stiff case will be discussed for special classes of stiff problems and the existence of asymptotic expansions will be proved for the implicit midpoint rule and the trapezoidal rule.

(ii) In our second paper [5] we shall present a rigorous analysis of the error structure of the implicit midpoint rule for a rather general class of nonlinear stiff problems where (in contrast to the special class covered by Theorem 3.1 of Sect. 3 below) oscillations at the h^2-level turn out to be unavoidable – even in the strongly stiff case – and therefore asymptotic expansions do not exist. We shall describe the behavior of these oscillations in detail, so our results will be useful for practical applications. Whereas in the strongly stiff case these oscillations are very regular, the situation is different in the mildly stiff case where the oscillating terms are damped out as the integration proceeds, so an asymptotic expansion with a remainder term of full order ultimately reappears. The latter situation is similar to the implicit Euler scheme (cf. [3]).

(iii) Our third paper [6] will be devoted to applications of our theory. We shall present numerical experiments and an analysis for extrapolation and Iterated Defect Correction algorithms.

2 Preliminaries; Overview of Results

Note that in the *strongly stiff case* a full asymptotic expansion of the global error exists for the implicit Euler scheme (cf. [3, 12]). In the sequel we shall investigate the question to what extent the same is true for the implicit midpoint rule and the implicit trapezoidal rule. In particular, we shall characterize problem classes where this is indeed the case and we shall also present a counterexample where oscillating terms at the h^2-level occur, from which it is clear that asymptotic expansions cannot exist in general – not even in the strongly stiff case. (For the discussion of a general problem class where h^2-oscillations occur cf. our forthcoming paper [5].)

The particular problem class considered here is [1]

$$y'(t) = A(t)\, y(t) + \varphi(t, y(t)) \tag{2.1}$$

where

$$A(t) = T(t)\, \Lambda(t)\, T^{-1}(t), \qquad \Lambda(t) = \begin{pmatrix} c_1(t) & 0 \\ 0 & -\dfrac{c_2(t)}{\varepsilon} \end{pmatrix} \tag{2.2}$$

[1] This class of stiff problems is essentially equivalent to the class of problems considered in [3]

with smooth functions $T(t)$, $T^{-1}(t)$, $c_1(t)$ and $c_2(t)$. We assume

$$Re(c_2(t)) \geqq \kappa > 0 \tag{2.3}$$

where κ is significantly away from zero independently of ε. $\varepsilon>0$ is a small positive parameter characterizing the stiffness of the problem. We are considering the 2-dimensional case, i.e., $c_1(t)$ and $c_2(t)$ are scalar functions; but this is not a crucial restriction. All the material could easily be rewritten for problems which are more general in the sense that $c_1(t)$ and $c_2(t)$ are matrix functions of certain dimensions.[2]

If one would apply a multiparameter $(\varepsilon_1, \ldots, \varepsilon_k)$-theory the above assumption on the spectrum of $A(t)$ could probably be weakened; but we have not carried out an analysis for this more general case.

Most of our results refer to the case of a smooth function $\varphi(t, y)$, i.e., φ and those of its derivatives that appear in our analysis are assumed to be moderately sized. Sometimes, however, a slightly more general problem class with $\varphi = O(1/\varepsilon)$ is considered; but also in this case we assume that the appearing y-derivatives φ_y, φ_{yy} ... are $O(1)$ and not $O(1/\varepsilon)$. (Many stiff test problems with large inhomogeneities are of this type, e.g. the model problem of Prothero and Robinson.) Note that the t-derivatives φ_t, φ_{tt}, φ_{ty} ... never occur explicitly and so no assumptions about these derivatives are required.

We are of course assuming that the differential equation (2.1) admits smooth solutions; otherwise the problem would not be considered stiff. The existence of smooth solutions can be guaranteed by singular perturbation arguments under the assumption that $\varphi(t, y)$ and a certain number of its derivatives are of moderate size (cf. Lemma 3.1 below). For problems where φ is $O(1/\varepsilon)$, smooth solutions do usually not exist but only in special cases which can also be characterized by singular perturbation techniques. Such examples are also covered by our theory.

In general, the implicit midpoint and trapezoidal rules do not admit a full asymptotic expansion of the global error for problems of the type (2.1)–(2.3). We shall, however, characterize a number of subclasses where such an expansion exists in the strongly stiff case, i.e.,

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + \ldots + h^{2q} e_{2q}(t_\nu) + O(h^{2q+2}) \tag{2.4}$$

if $\varepsilon \ll h$. (Here ζ_ν denotes the numerical approximation for the exact solution value $z(t_\nu)$ at the gridpoint t_ν.)

Our argumentation is based on singular perturbation techniques. To this end we transform equation (2.1) according to

$$\bar{z}(t) := T^{-1}(t)\, z(t) \tag{2.5}$$

(with $T(t)$ from (2.2)):

$$\bar{z}'(t) = \Lambda(t)\, \bar{z}(t) + D(t)\, \bar{z}(t) + T^{-1}(t)\, \varphi(t, T(t)\, \bar{z}(t)) \tag{2.6}$$

[2] In this case one would say that – in view of assumption (2.2) – there are two 'clusters' of eigenvalues (namely the eigenvalues of $c_1(t)$ and $-c_2(t)/\varepsilon$) representing the non-stiff and the stiff part of the spectrum, respectively

where

$$D(t) := -T^{-1}(t)\,T'(t) = \begin{pmatrix} d_{11}(t) & d_{12}(t) \\ d_{21}(t) & d_{22}(t) \end{pmatrix}. \tag{2.7}$$

Since $A(t)$ depends on t it is not possible to decouple the 'stiff term' $A(t)\,z(t)$ by this transformation; the coupling is characterized by the matrix $D(t)$ (which is smooth due to our assumptions w.r.t. $T(t)$) whereas the degree of stiffness is characterized by the diagonal matrix $\Lambda(t)$ (with the stiff eigenvalue $-c_2(t)/\varepsilon$).

Our results below will show that the existence of an asymptotic error expansion depends on the type of coupling between the stiff and the non-stiff components (characterized by the matrix $D(t)$). We distinguish three cases:[3]

(i) full coupling, where all entries $d_{ij}(t)$ within $D(t)$ are $O(1)$,
(ii) weak coupling from the stiff to the non-stiff component, i.e., $d_{12}(t) = O(\varepsilon)$,
(iii) weak coupling from the non-stiff to the stiff component, i.e., $d_{21}(t) = O(\varepsilon)$.

A particular problem of the type (2.1) can be written in different ways. If, for instance, $\varphi(t, y) = B(t)y + \tilde{\varphi}(t, y)$ with a smooth matrix $B(t)$ then

$$y'(t) = A(t)\,y(t) + \varphi(t, y(t)) = (A(t) + B(t))\,y(t) + \tilde{\varphi}(t, y(t)) = \tilde{A}(t)\,y(t) + \tilde{\varphi}(t, y(t))$$

with another 'stiff matrix' $\tilde{A}(t)$. Condition (2.3) as well as the above coupling properties (i)–(iii) are only well-defined if they are invariant w.r.t. such a reformulation. It is shown in the Appendix that this is indeed the case.

A further question is whether the coupling properties (i)–(iii) are invariant w.r.t. a re-scaling $T \mapsto TS$ ($S = S(t)$ a smooth diagonal matrix such that TS, $(TS)^{-1}$ moderate). It is easy to see that this is also the case (cf. [17], Lemma 1.5).

W.r.t. the function $\varphi(t, y)$ we distinguish two cases:

a) The 'nonsmooth' case $\varphi(t, y) = O(1/\varepsilon)$: If the transformed function $\bar{\varphi}(t, \bar{y}) = T^{-1}(t)\,\varphi(t, T(t)\,\bar{y})$ (cf. (2.6)) satisfies a relation

$$\bar{\varphi}(t, \bar{y}) = \begin{pmatrix} 0 \\ \frac{1}{\varepsilon} j(t) \end{pmatrix} + \phi(t, \bar{y}) \tag{2.8}$$

with smooth functions $j(t)$ and $\phi(t, \bar{y})$, then the y-derivatives of $\bar{\varphi}$ and φ are moderate. Moreover, a singular perturbation argument in the spirit of [14] shows that (2.6) and consequently (2.1) admit smooth solutions. (With some additional technical effort it would also be possible to cover cases where the second component of $\bar{\varphi}(t, \bar{y})$ is of the form $\frac{1}{\varepsilon} \times$ some nonlinear smooth function.)

b) The 'smooth' case, where $\varphi(t, y)$ and some of its y-derivatives are $O(1)$.

As our discussion in Sects. 3 and 4 will show, the coupling properties (i)–(iii) introduced above are of essential importance for the existence of full asymptotic expansions. In Tables 1 and 2 we present a survey of our results. The cases a), b) above will be referred to as "φ nonsmooth" and "φ smooth", respectively.

[3] These special types of coupling were also considered by Van Veldhuizen in [17] where the stability properties of several methods, applied to linear problems $y'(t) = A(t)\,y(t)$, are discussed. In Van Veldhuizen's terminology the problem classes characterized by (ii), (iii) are denoted by $\mathscr{W}_{ts}$ and $\mathscr{W}_{st}$, respectively

Table 1. Existence of a full asymptotic expansion for the midpoint rule, q arbitrary, $\varepsilon \leqq Ch^{2q}$

Midpoint rule, $q \geqq 1$	Full coupling	$d_{12}(t) = O(\varepsilon)$	$d_{21}(t) = O(\varepsilon)$
φ nonsmooth	No	No	No
φ smooth	No	No	Yes

Table 2. Existence of a full asymptotic expansion for the trapezoidal rule, $q \geqq 2$, $\varepsilon \leqq Ch^{2q}$

Trapezoidal rule, $q \geqq 2$	Full coupling	$d_{12}(t) = O(\varepsilon)$	$d_{21}(t) = O(\varepsilon)$
φ nonsmooth	No	Yes	No
φ smooth	No	Yes	Yes

Table 1 displays the results for the implicit midpoint rule in the strongly stiff case $\varepsilon \leqq Ch^{2q}$. (For the meaning of q cf. (2.4).)

For the trapezoidal rule it will turn out that an asymptotic expansion

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + O(h^4) \tag{2.9}$$

(i.e., $q = 1$) exists for any problem of the type (2.1)–(2.3) in the strongly stiff case $\varepsilon \leqq Ch^2$. For $q > 1$ this is not true in general; Table 2 displays the results for $q \geqq 2$ in the strongly stiff case $\varepsilon \leqq Ch^{2q}$.[4]

In those cases where a full asymptotic expansion cannot be guaranteed – and usually does not exist – (entries 'No') the remainder term shows a reduced order, namely h^2 for the midpoint rule (note that the midpoint rule is B-convergent of order 2) and h^4 (cf. (2.9)) for the trapezoidal rule (which is not trivial). In [5] we shall study these cases and describe quantitatively the *oscillating behavior* of the remainder term by discrete 'two-timing' singular perturbation techniques. In [5] we shall also consider situations where $\varepsilon \leqq Ch^{2q}$ is violated; it will turn out that in mildly stiff situations ($\varepsilon \approx h$ or even $h \ll \varepsilon$) the remainder term shows a rapidly decaying behavior (similarly as for the implicit Euler scheme).

In many existing papers on stiff problems, the considerations are restricted to semilinear equations

$$y'(t) = A\,y(t) + \varphi(t, y(t)) \tag{2.10}$$

with a constant matrix A. In our context this is a very special case: Since, for A constant, we have $D(t) \equiv D = 0$, both coupling conditions $d_{12}(t) = O(\varepsilon)$, $d_{21}(t) = O(\varepsilon)$ are trivially satisfied. So, by Table 2 (second column), a full asymptotic expansion exists for the trapezoidal rule. For the midpoint rule (Table 1,

[4] Actually, the result 'Yes' in the third column of Table 2 is even valid under the milder assumption $\varepsilon \leqq Ch^{2q-2}$ (cf. Theorem 4.2)

third column) this is only true if $\varphi(t, y)=O(1)$. (Examples 1 and 2 of Sect. 3 show that the requirement that $\varphi=O(1)$ is really essential here.)

Another important subclass of (2.1)–(2.3) consists of problems in singular perturbation form, where

$$A(t)=\begin{pmatrix} a_{11}(t) & a_{12}(t) \\ \frac{1}{\varepsilon}a_{21}(t) & \frac{1}{\varepsilon}a_{22}(t)\end{pmatrix} \tag{2.11}$$

with smooth functions $a_{ij}(t)$ and $a_{22}(t)\leqq -\kappa<0$. For problems of this type the coupling from the stiff to the non-stiff component is weak, i.e., $d_{12}(t)=O(\varepsilon)$ (cf. [9], Chapter 8).

3 The Implicit Midpoint Rule

Let us now consider the implicit midpoint discretization of (1.1):

$$\frac{1}{h}(\zeta_\nu-\zeta_{\nu-1})=f(\hat{t}_\nu, \tfrac{1}{2}(\zeta_{\nu-1}+\zeta_\nu)),$$
$$\zeta_0=z_0 \tag{3.1}$$

where $t_\nu=\nu h$ and $\hat{t}_\nu:=\frac{1}{2}(t_{\nu-1}+t_\nu)$. According to the ideas of Gragg [11] the global error of (3.1) can be written as

$$\zeta_\nu-z(t_\nu)=h^2e_2(t_\nu)+h^4e_4(t_\nu)+\ldots+h^{2q}e_{2q}(t_\nu)+R_\nu \tag{3.2}$$

where the functions $e_2(t)$, $e_4(t)$, ... are solutions of the variational equations

$$e_2'(t)=f_y(t,z(t))\,e_2(t)-\tfrac{1}{24}z'''(t)+\tfrac{1}{8}f_y(t,z(t))\,z''(t), \tag{3.3}$$

$$\begin{aligned} e_4'(t)=&f_y(t,z(t))\,e_4(t)-\tfrac{1}{1920}z^{V}(t)+\tfrac{1}{384}f_y(t,z(t))\,z^{IV}(t)\\ &-\tfrac{1}{24}e_2'''(t)+\tfrac{1}{8}f_y(t,z(t))\,e_2''(t)+\tfrac{1}{2}f_{yy}(t,z(t))[\tfrac{1}{8}z''(t)+e_2(t)]^2, \end{aligned} \tag{3.4}$$

$$\vdots$$

and where the remainder term R_ν satisfies the difference equation

$$\begin{aligned}\frac{1}{h}(R_\nu-R_{\nu-1})=&f_y(\hat{t}_\nu, z(\hat{t}_\nu))\frac{1}{2}(R_{\nu-1}+R_\nu)\\ &+G_\nu(\tfrac{1}{2}(R_{\nu-1}+R_\nu))+f_y(\hat{t}_\nu, z(\hat{t}_\nu))\,a_\nu+b_\nu-c_\nu.\end{aligned} \tag{3.5}$$

For each ν, G_ν denotes a certain smooth[5] function the concrete form of which is irrelevant for the present purpose. The inhomogeneous terms a_ν and c_ν are defined as

$$a_\nu:=\frac{1}{2}(I^-_{\nu,0}+I^+_{\nu,0})+\frac{h^2}{2}(I^-_{\nu,2}+I^+_{\nu,2})+\ldots+\frac{h^{2q}}{2}(I^-_{\nu,2q}+I^+_{\nu,2q}), \tag{3.6}$$

$$c_\nu:=\frac{1}{h}(I^+_{\nu,0}-I^-_{\nu,0})+h(I^+_{\nu,2}-I^-_{\nu,2})+\ldots+h^{2q-1}(I^+_{\nu,2q}-I^-_{\nu,2q}), \tag{3.7}$$

[5] Here the particular underlying assumption is that all higher derivatives f_{yy}, f_{yyy}, ... w.r.t. y are moderate; due to our smoothness assumptions w.r.t. φ this is of course the case for (2.1) where $f(t,y)=A(t)y+\varphi(t,y)$

where the $I^\pm_{\nu,k}$ are the remainder terms of the Taylor expansions

$$\begin{aligned} z\left(\hat{t}_\nu\pm\frac{h}{2}\right)=&z(\hat{t}_\nu)\pm\frac{h}{2}z'(\hat{t}_\nu)+\frac{h^2}{8}z''(\hat{t}_\nu)\pm\ldots\\ &\pm\frac{h^{2q+1}}{2^{2q+1}(2q+1)!}z^{(2q+1)}(\hat{t}_\nu)+I^\pm_{\nu,0}, \end{aligned} \tag{3.8}$$

$$\begin{aligned} e_2\left(\hat{t}_\nu\pm\frac{h}{2}\right)=&e_2(\hat{t}_\nu)\pm\frac{h}{2}e_2'(\hat{t}_\nu)+\frac{h^2}{8}e_2''(\hat{t}_\nu)\pm\ldots\\ &\pm\frac{h^{2q-1}}{2^{2q-1}(2q-1)!}e_2^{(2q-1)}(\hat{t}_\nu)+I^\pm_{\nu,2}, \end{aligned} \tag{3.9}$$

$$\vdots$$

Further, b_ν denotes the collection of all terms of the Taylor expansion of $f(\hat{t}_\nu, z(\hat{t}_\nu)+h^2e_2(\hat{t}_\nu)+\ldots+h^{2q}e_{2q}(\hat{t}_\nu))$ about $(\hat{t}_\nu, z(\hat{t}_\nu))$ which are at least $O(h^{2q+2})$. (b_ν is obviously not influenced by f_y and so it is indeed justified[5] to consider this $O(h^{2q+2})$.) All this can be shown by simple Taylor expansions (similarly as in [3] for the implicit Euler scheme). Note the occurrence of the Jacobian f_y within the inhomogeneities of (3.3, ...) and of (3.5).

The remainder equation (3.5) is of a similar type as the difference equation defining ζ_ν (cf. (3.1)). If it can be guaranteed that a_ν, b_ν and c_ν are at the $O(h^{2q+2})$-level then the usual B-convergence estimate (cf. for instance [13]) leads to $R_\nu=O(h^{2q+2})$ provided that $R_0=O(h^{2q+2})$. Now the point is that a_ν and c_ν (cf. (3.6–3.9)) depend on derivatives of the solutions $e_{2i}(t)$ of the variational equations (3.3, 3.4, ...) which are of course stiff. Therefore $a_\nu=O(h^{2q+2})$, $c_\nu=O(h^{2q+2})$ can only be guaranteed for *smooth* solutions $e_{2i}(t)$. This requires that special starting values must be chosen for the $e_{2i}(t)$ which do usually not vanish. But such a choice for the $e_{2i}(0)$ is usually not compatible with $R_0=O(h^{2q+2})$: Due to (3.2) for $\nu=0$ and due to the fact that $e_{2i}(0)\neq 0$ we have

$$R_0=\zeta_0-z(0)-h^2e_2(0)-\ldots-h^{2q}e_{2q}(0)=O(h^2) \tag{3.10}$$

and it must be expected that $R_\nu=O(h^2)$ and not $O(h^{2q+2})$.[6] This is indeed the case in Example 2 below where nonsmooth error terms occur at the $O(h^2)$-level.

However, for certain subclasses of (2.1) it will turn out that R_0 contains an additional factor ε, from which the desired estimate $R_\nu=O(h^{2q+2})$ can be concluded under the assumption $\varepsilon\leqq Ch^{2q}$ (strongly stiff case). These cases are studied in the present paper.

Before considering problem class (2.1) we shall first demonstrate some typical effects by means of simple scalar models.

[6] The idea to work with smooth solutions of the variational equation goes back to Dahlquist and Lindberg [8]; however, these authors proposed to choose ζ_0 as $\zeta_0=z(0)+h^2e_2(0)+\ldots+h^{2q}e_{2q}(0)$ such that $R_0=0$. This immediately leads to $R_\nu=O(h^{2q+2})$ but is difficult to realize in practice since the starting values $e_{2i}(0)$ defining smooth $e_{2i}(t)$ are usually not available

Example 1. Consider

$$y'(t) = -\frac{1}{\varepsilon} y(t) - e^{-t}, \quad 0 < \varepsilon \ll 1 \tag{3.11}$$

with the smooth solution

$$z(t) = -\frac{\varepsilon}{1-\varepsilon} e^{-t} \tag{3.12}$$

(fixed by the initial condition $z(0) = -\varepsilon/(1-\varepsilon)$). For $q=1$, (3.2) reads

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + R_\nu, \tag{3.13}$$

and for (3.11) the first variational equation (3.3) is

$$e_2'(t) = -\frac{1}{\varepsilon} e_2(t) - \frac{\varepsilon}{24(1-\varepsilon)} e^{-t} + \frac{1}{8(1-\varepsilon)} e^{-t}. \tag{3.14}$$

This has the smooth solution

$$e_2(t) = \left(\frac{\varepsilon}{8(1-\varepsilon)^2} - \frac{\varepsilon^2}{24(1-\varepsilon)^2}\right) e^{-t} = O(\varepsilon) \tag{3.15}$$

The remainder term R_ν satisfies (cf. (3.5))

$$\frac{1}{h}(R_\nu - R_{\nu-1}) = -\frac{1}{\varepsilon}\frac{1}{2}(R_{\nu-1} + R_\nu) - \frac{1}{\varepsilon} a_\nu - c_\nu \tag{3.16}$$

where, according to (3.6)–(3.9),

$$-\frac{1}{\varepsilon} a_\nu = O(h^4), \quad c_\nu = O(h^4) \tag{3.17}$$

for the smooth solution $e_2(t)$ (cf. (3.15)). (That even $a_\nu = O(\varepsilon h^4)$ – and not only $a_\nu = O(h^4)$ – follows from the definition of a_ν and the fact that $z^{(k)}(t) = O(\varepsilon)$ and $e_2^{(k)}(t) = O(\varepsilon)$.)

R_0 is now fixed by the requirement that (3.13) is satisfied for $\nu = 0$ with $\zeta_0 = z(0)$:

$$R_0 = \zeta_0 - z(0) - h^2 e_2(0) = -h^2 e_2(0), \tag{3.18}$$

so, $R_0 = O(\varepsilon h^2)$ due to (3.15). In the strongly stiff case $\varepsilon \leqq C h^2$ we therefore have $R_0 = O(h^4)$. Now from (3.16) and (3.17),

$$R_\nu = \left(\frac{1 - \frac{h}{2\varepsilon}}{1 + \frac{h}{2\varepsilon}}\right) R_{\nu-1} - \frac{h}{1 + \frac{h}{2\varepsilon}} \underbrace{\left(\frac{1}{\varepsilon} a_\nu + c_\nu\right)}_{O(h^4)}, \tag{3.19}$$

hence $R_\nu = O(h^4)$. So for (3.11) the existence of an asymptotic expansion is trivial. This is not only true for $q=1$ but also for $q>1$ if 'strongly stiff' is understood by $\varepsilon \leqq C h^{2q}$.

Example 2. The situation is quite different for the model problem of Prothero and Robinson,

$$y'(t) = -\frac{1}{\varepsilon}(y(t) - e^{-t}) - e^{-t},$$
$$y(0) = 1 \tag{3.20}$$

with the (smooth) solution

$$z(t) = e^{-t}. \tag{3.21}$$

The first variation equation,

$$e_2'(t) = -\frac{1}{\varepsilon} e_2(t) + \frac{1}{24} e^{-t} - \frac{1}{8\varepsilon} e^{-t} \tag{3.22}$$

has the smooth solution

$$e_2(t) = \left(\frac{\varepsilon}{24(1-\varepsilon)} - \frac{1}{8(1-\varepsilon)}\right) e^{-t} \tag{3.23}$$

with

$$e_2(0) = \left(\frac{\varepsilon}{24(1-\varepsilon)} - \frac{1}{8(1-\varepsilon)}\right) \to -\frac{1}{8} = O(1) \quad \text{for } \varepsilon \to 0. \tag{3.24}$$

Therefore,

$$R_0 = -h^2 e_2(0) \to \frac{h^2}{8} \quad \text{for } \varepsilon \to 0 \tag{3.25}$$

so we only have $R_\nu = O(h^2)$. The dominant term within R_ν is oscillating at the h^2-level:

$$R_\nu \approx \left(\frac{1 - \frac{h}{2\varepsilon}}{1 + \frac{h}{2\varepsilon}}\right)^\nu R_0 \approx \frac{h^2}{8}(-1)^\nu \quad \text{for } 0 < \varepsilon \ll 1. \tag{3.26}$$

An asymptotic expansion does not exist. However, the oscillation shows a very regular behavior for $\varepsilon \ll 1$.

The crucial difference between Examples 1 and 2 is the behavior of the respective inhomogeneities $\varphi_1(t) = -e^{-t}$ (Example 1) and $\varphi_2(t) = \left(\frac{1}{\varepsilon} - 1\right) e^{-t}$ (Example 2). φ_1 and its derivatives are $O(1)$, whereas φ_2 and its derivatives are $O(1/\varepsilon)$, which causes the breakdown of the asymptotic expansion. (This situation is analogous to that one illustrated in the third column of Table 1 above.)

The solutions of (3.11) and (3.20) are identical except the additional factor $-\varepsilon/(1-\varepsilon)$ in (3.12). The same is true for the smooth solutions $e_2(t)$ of (3.14), (3.22) and for the respective global errors. So the difference between these models seems to be of a trivial nature. For vector problems, however, where smooth and stiff components are usually coupled, it is essential whether the effects of the stiff components are $O(\varepsilon h^2)$ or $O(h^2)$.

We shall now discuss the existence of an asymptotic error expansion for problem class (2.1). As a first step we briefly describe the structure of smooth solutions of (2.1) by singular perturbation techniques. The following lemma is a standard in singular perturbation theory.

Lemma 3.1. *Consider a problem of the type* (2.1) *and assume that* $\varphi(t, y)$ *and a sufficient number of its derivatives are* $O(1)$. *Then any smooth solution possesses an* ε*-expansion of the form*

$$z(t)=T(t)\,\bar{z}(t) \quad \textit{with} \quad \bar{z}(t)=\begin{pmatrix} X_0(t)+\varepsilon X_1(t)+\dots \\ \varepsilon Y_1(t)+\dots \end{pmatrix}. \tag{3.27}$$

Proof. Consider (2.1) in its transformed form (2.6). Denoting

$$\bar{z}(t)=\begin{pmatrix} x(t) \\ y(t) \end{pmatrix}, \qquad T^{-1}(t)\,\varphi(t, T(t)\,\bar{z}(t))=\begin{pmatrix} \bar{\varphi}_1(t, x(t), y(t)) \\ \bar{\varphi}_2(t, x(t), y(t)) \end{pmatrix} \tag{3.28}$$

and multiplying the second component of (2.6) by ε we obtain

$$x'(t)=c_1(t)\,x(t)+d_{11}(t)\,x(t)+d_{12}(t)\,y(t)+\bar{\varphi}_1(t, x(t), y(t)), \tag{3.29}$$

$$\varepsilon y'(t)=-c_2(t)\,y(t)+\varepsilon d_{21}(t)\,x(t)+\varepsilon d_{22}(t)\,y(t)+\varepsilon\bar{\varphi}_2(t, x(t), y(t)). \tag{3.30}$$

The ansatz

$$x(t)=X_0(t)+\varepsilon X_1(t)+\dots \tag{3.31}$$

$$y(t)=Y_0(t)+\varepsilon Y_1(t)+\dots \tag{3.32}$$

is inserted into (3.29, 3.30). Expanding

$$\begin{aligned}\bar{\varphi}_i(t, x(t), y(t))=&\,\bar{\varphi}_i(t, X_0(t), Y_0(t))+\varepsilon\bar{\varphi}_{ix}(t, X_0(t), Y_0(t))\,X_1(t)\\ &+\varepsilon\bar{\varphi}_{iy}(t, X_0(t), Y_0(t))\,Y_1(t)+\dots\end{aligned} \tag{3.33}$$

and equating coefficients of powers of ε we obtain

Coefficients of ε^1:

$$X_0'(t)=c_1(t)\,X_0(t)+d_{11}(t)\,X_0(t)+d_{12}(t)\,Y_0(t)+\bar{\varphi}_1(t, X_0(t), Y_0(t)), \tag{3.34}$$

$$0=-c_2(t)\,Y_0(t) \tag{3.35}$$

Coefficients of ε^1:

$$\begin{aligned}X_1'(t)=&\,c_1(t)\,X_1(t)+d_{11}(t)\,X_1(t)+d_{12}(t)\,Y_1(t)\\ &+\bar{\varphi}_{1x}(t, X_0(t), X_0(t))\,X_1(t)+\bar{\varphi}_{1y}(t, X_0(t), Y_0(t))\,Y_1(t),\end{aligned} \tag{3.36}$$

$$0=-c_2(t)\,Y_1(t)+d_{21}(t)\,X_0(t)+d_{22}(t)\,Y_0(t)+\bar{\varphi}_2(t, X_0(t), Y_0(t))-Y_0'(t) \tag{3.37}$$

$$\vdots$$

From (3.35), $Y_0(t)\equiv 0$. The $X_i(t)$, $i\geq 0$, are solutions of the smooth differential equations (3.34), (3.36), ... whereas the $Y_i(t)$, $i\geq 1$, are defined by algebraic equations (3.37), ... □

In the proof of Lemma 3.1 we did not check the asymptotic correctness of (3.27), i.e. whether a remainder term in the ansatz (3.31), (3.32) is indeed at a certain ε^p-level. The reader interested in this point is referred to [3] (proof of Lemma 3.1).

Remark 3.1. In the general case of a 'nonsmooth' $\bar{\varphi}$ (cf. (2.8)), (3.35) obviously has to be replaced by

$$0=-c_2(t)\,Y_0(t)+j(t). \tag{3.38}$$

So, in general, $Y_0(t)\not\equiv 0$. (For details cf. for instance [14], Chap. 4.)

Remark 3.2. In general, a solution of (2.1) does not only contain smooth terms but also 'transient' terms which are rapidly decaying away from $t=0$. The detailed structure (after transformation (2.5), (2.6)), which can be described by singular perturbation techniques (cf. [14]) is

$$\bar{z}(t)=\underbrace{\begin{pmatrix} X_0(t)+\varepsilon X_1(t)+\dots \\ \varepsilon Y_1(t)+\dots \end{pmatrix}}_{\tilde{Z}(t,\varepsilon)}+\underbrace{\begin{pmatrix} \varepsilon m_0(t/\varepsilon)+\dots \\ n_0(t/\varepsilon)+\varepsilon n_1(t/\varepsilon)+\dots \end{pmatrix}}_{\bar{M}(t/\varepsilon)} \tag{3.39}$$

with a certain transient term $\bar{M}(t/\varepsilon)$ which is smooth with respect to t/ε but not with respect to t. A solution $\bar{z}(t)$ will be called "arbitrarily smooth" if *all* transient terms identically vanish. For the present purpose a certain *degree of smoothness* is required, i.e., the leading transient terms up to a certain ε^k-level must vanish. If $\bar{M}(t/\varepsilon)=O(\varepsilon^k)$ then

$$\frac{d^l}{dt^l}\,\bar{M}(t/\varepsilon)=O(\varepsilon^{k-l}) \tag{3.40}$$

so up to $l=k$ all derivatives $\dfrac{d^l}{dt^l}\,\bar{z}(t)$ remain bounded.

In the following we assume that the given solution $z(t)=T(t)\,\bar{z}(t)$ is sufficiently smooth (in the above sense) such that the terms $\frac{1}{2}\cdot(I^-_{\nu,0}+I^+_{\nu,0})$, ... and $\dfrac{1}{h}(I^+_{\nu,0}-I^-_{\nu,0})$, ... which appear within a_ν and c_ν (cf. (3.6), (3.7)) are $O(h^{2q+2})$. This assumption means that our results about the structure of the global error (Theorems 3.1, 4.1, 4.2 and 4.4) are only valid after a transient phase. We do not describe the error structure in the transients. (After the proofs of these theorems we shall, however, shortly discuss the influence of a transient phase. We shall show that, immediately after a transient phase, the global error satisfies the assumptions of our theorems.)

The proof of Theorem 3.1 below is based on the idea to *construct special smooth solutions of the variational Eq.* (3.3, ...). Again a certain degree of smoothness is required to ensure that the terms $\frac{h^2}{2}(I^-_{\nu,2}+I^+_{\nu,2}), \ldots$ and $h(I^+_{\nu,2}-I^-_{\nu,2}), \ldots$ which appear within a_ν and c_ν are $O(h^{2q+2})$. The technical details of such a construction are essentially the same as for the implicit Euler scheme (cf. [3], Lemma 3.1 and Proposition 3.2). The interested reader is referred to [3].

Given a sufficiently smooth $z(t)$, and having constructed sufficiently smooth solutions $e_{2i}(t)$ of the variational equations we have

$$a_\nu=O(h^{2q+2}), \quad b_\nu=O(h^{2q+2}), \quad c_\nu=O(h^{2q+2}). \tag{3.41}$$

Theorem 3.1. *Consider a problem of the type* (2.1); *assume that* $\varphi(t,y)=O(1)$ *is sufficiently smooth and that*

$$d_{21}(t)=O(\varepsilon) \tag{3.42}$$

(weak coupling from the non-stiff to the stiff component). Assume $\varepsilon \leqq C h^{2q}$ *(strongly stiff case). Let* $[0, t_E]$ *be a subinterval of the whole integration interval with constant stepsize h and asssume inductively*[7] *that – after transformation by* $T^{-1}(t)$ *(cf.* (2.2), (2.5)) *– the accumulated global error* $T^{-1}(0)(\zeta_0-z(0))$ *at* $t=0$ *satisfies*

$$T^{-1}(0)(\zeta_0-z(0))=h^2\begin{pmatrix}x_2+O(\varepsilon)\\ O(\varepsilon)\end{pmatrix}+\ldots+h^{2q}\begin{pmatrix}x_{2q}+O(\varepsilon)\\ O(\varepsilon)\end{pmatrix}+O(h^{2q+2}) \tag{3.43}$$

with certain x_{2i} *which are independent of h and* ε. *Then the global error of the implicit midpoint rule on* $[0, t_E]$ *admits an asymptotic expansion*

$$\zeta_\nu-z(t_\nu)=h^2 e_2(t_\nu)+h^4 e_4(t_\nu)+\ldots+h^{2q}e_{2q}(t_\nu)+R_\nu \tag{3.44}$$

with smooth, h-independent functions $e_{2i}(t)$ *which are solutions of the variational Eq.* (3.3, …); *further,*

$$R_\nu=O(h^{2q+2}) \tag{3.45}$$

at all grid points $t_\nu=\nu h$, $\nu=0, 1, \ldots, t_E/h$.

Proof. Transformation of the first variational equation according to

$$\bar{e}_2(t):=T^{-1}(t)\,e_2(t) \tag{3.46}$$

yields

$$\begin{aligned}\bar{e}_2'(t)&=\Lambda(t)\,\bar{e}_2(t)+D(t)\,\bar{e}_2(t)+T^{-1}(t)\,\varphi_y(t,z(t))\,T(t)\,\bar{e}_2(t)\\ &\quad-\tfrac{1}{24}T^{-1}(t)z'''(t)+\tfrac{1}{8}\Lambda(t)\,T^{-1}(t)(T(t)\,\bar{z}(t))''+\tfrac{1}{8}T^{-1}(t)\varphi_y(t,z(t))\,z''(t).\end{aligned} \tag{3.47}$$

This is a linear equation of a similar type as (2.6); instead of the smooth nonlinear term $T^{-1}(t)\,\varphi(t, T(t)\,\bar{z}(t))$ now the smooth linear term $T^{-1}(t)\,\varphi_y(t,z(t))\,T(t)\,\bar{e}_2(t)$ plus an additional inhomogeneity appears. The crucial point is the occurrence of $\Lambda(t)=O(1/\varepsilon)$ within this inhomogeneity which is therefore $O(1/\varepsilon)$ in general. But under the special assumption (3.42) it is $O(1)$ which can be seen as follows:

[7] "Inductively" refers to an induction w.r.t. several subintervals with constant stepsize h. This induction will be discussed in more detail immediately after the proof of the Theorem

Expressing $T^{-1}(t)\,T''(t)$ by[8]

$$T^{-1}(t)\,T''(t)=D^2(t)-D'(t), \tag{3.48}$$

rewriting the 'critical term' involving $\Lambda(t)$ as

$$\tfrac{1}{8}\Lambda(t)\,T^{-1}(t)(T(t)\,\bar{z}(t))''=\tfrac{1}{8}\Lambda(t)\,\bar{z}''(t)-\tfrac{1}{4}\Lambda(t)\,D(t)\,\bar{z}'(t)+\tfrac{1}{8}\Lambda(t)[D^2(t)-D'(t)]\,\bar{z}(t), \tag{3.49}$$

and taking account of

$$\bar{z}(t)=\begin{pmatrix}O(1)\\ O(\varepsilon)\end{pmatrix} \tag{3.50}$$

(cf. (3.27)) we see that (3.49) is indeed $O(1)$ if (3.42) holds.[9]

So, Eq. (3.47) satisfies the assumptions of Lemma 3.1 and therefore its smooth solutions $\bar{e}_2(t)$ can be characterized by

$$\bar{e}_2(t)=\begin{pmatrix}X_{0,2}(t)+\varepsilon X_{1,2}(t)+\ldots\\ \varepsilon Y_{1,2}(t)+\ldots\end{pmatrix} \tag{3.51}$$

(cf. (3.27)) where the functions $X_{0,2}(t)$, $X_{1,2}(t)$, … are solutions of smooth linear differential equations analogous to (3.34), (3.36), …; the starting values $X_{0,2}(0)$, $X_{1,2}(0)$, … can be chosen arbitrarily. The starting values $Y_{1,2}(0)$, … are then fixed by algebraic equations analogous to (3.37), ….

Similar considerations can be carried out recursively for the other transformed variational equations the inhomogeneities of which involve 'critical terms' similar to (3.49). So any smooth solution of any of the variational equations is of the form

$$\bar{e}_{2i}(t)=\begin{pmatrix}X_{0,2i}(t)+\varepsilon X_{1,2i}(t)+\ldots\\ \varepsilon Y_{1,2i}(t)+\ldots\end{pmatrix} \tag{3.52}$$

where the starting values $X_{k,2i}(0)$ can be chosen arbitrarily. Now we make use of the degree of freedom for the starting values $X_{0,2i}(0)$ at the ε^0-level, choosing

$$X_{0,2i}(0):=x_{2i}, \quad i=1,2,\ldots,q \tag{3.53}$$

with x_{2i} from the inductive assumption (3.43). Further we define R_0 such that

$$\zeta_0-z(0)=h^2 e_2(0)+\ldots+h^{2q}e_{2q}(0)+R_0 \tag{3.54}$$

is satisfied with $\zeta_0-z(0)$ satisfying (3.43). Premultiplying (3.54) by $T^{-1}(0)$ we obtain due to (3.43), (3.46), (3.53):

$$\begin{aligned}T^{-1}(0)\,R_0&=T^{-1}(0)(\zeta_0-z(0))-h^2\bar{e}_2(0)-\ldots-h^{2q}\bar{e}_{2q}(0)\\ &=O(h^2\varepsilon)+\ldots+O(h^{2q}\varepsilon)+O(h^{2q+2})=O(h^{2q+2}) \quad \text{for } \varepsilon\leqq Ch^{2q},\end{aligned} \tag{3.55}$$

[8] (3.48) can be shown by differentiating $T^{-1}(t)\,T'(t)$ and using $(T^{-1}(t))'\,T(t)=-T^{-1}(t)\,T'(t)=D(t)$

[9] Here the silent assumption is made that not only $d_{21}(t)$ but also its derivatives $d_{21}^{(k)}(t)$ are $O(\varepsilon)$

so

$$R_0 = O(h^{2q+2}). \tag{3.56}$$

Now – with a starting value at the $O(h^{2q+2})$-level – the desired estimate $R_\nu = O(h^{2q+2})$ (cf. (3.45)) can be estimated by B-convergence techniques. This estimate is completely analogous to the B-convergence estimate for the global error of the midpoint rule presented by Kraaijevanger in [13]. The critical point within such an estimate is the occurrence of the term $f_y(\hat{t}_\nu, z(\hat{t}_\nu))\, a_\nu = [A(\hat{t}_\nu) + \varphi_y(\hat{t}_\nu, z(\hat{t}_\nu))]\, a_\nu$ within the inhomogeneity of (3.5). Despite (3.41) it cannot be concluded that this is always $O(h^{2q+2})$ because $A(t) = O(1/\varepsilon)$. A more refined argumentation is necessary: Following the idea of Kraaijevanger [13] we introduce the auxiliary quantities

$$R_\nu^+ := R_\nu + I_\nu^+, \qquad R_\nu^- := R_{\nu-1} + I_\nu^- \tag{3.57}$$

where

$$I_\nu^\pm := I_{\nu,0}^\pm + h^2 I_{\nu,2}^\pm + \ldots + h^{2q} I_{\nu,2q}^\pm = O(h^{2q+2}) \tag{3.58}$$

(for the definition of the $I_{\nu,2i}^\pm$ cf. (3.8), (3.9)). Due to

$$a_\nu = \frac{1}{2}(I_\nu^- + I_\nu^+), \qquad c_\nu = \frac{1}{h}(I_\nu^+ - I_\nu^-) \tag{3.59}$$

(cf. (3.6), (3.7)) one obtains after some simple manipulations

$$\frac{1}{h}(R_\nu^+ - R_\nu^-) = f_y(\hat{t}_\nu, z(\hat{t}_\nu))\, \frac{1}{2}(R_\nu^- + R_\nu^+)$$

$$+ G_\nu(-a_\nu) + \Phi_\nu\left(\frac{1}{2}(R_\nu^- + R_\nu^+)\right) + b_\nu \tag{3.60}$$

where $\Phi_\nu(\cdot)$ is defined as

$$\Phi_\nu(R) := G_\nu(R - a_\nu) - G_\nu(-a_\nu) \tag{3.61}$$

satisfying $\Phi_\nu(0) = 0$, $\|\Phi_\nu(R)\| \leq L_\Phi \|R\|$ (L_Φ of moderate size). Due to (3.41) and due to $R_\nu^- - R_{\nu-1}^+ = I_\nu^- - I_{\nu-1}^+ = O(h^{2q+3})$ the usual B-convergence techniques lead to the recursion

$$\|R_\nu^+\| \leq \frac{1 + \dfrac{h(m + L_\Phi)}{2}}{1 - \dfrac{h(m + L_\Phi)}{2}} \|R_{\nu-1}^+\| + O(h^{2q+3}) \tag{3.62}$$

(here $\|\cdot\|$ denotes the Euclidean norm and m is the corresponding one-sided Lipschitz bound for f). From this the desired result

$$R_\nu = O(h^{2q+2}) \tag{3.63}$$

follows by a simple argumentation. □

Theorem 3.1 can be applied inductively to describe the error structure for *nonequidistant* grids: From (3.52) we conclude that at the endpoint $t = t_E$ of the current subinterval the (transformed) global error can be written as

$$\tilde{h}^2 \left(\frac{h}{\tilde{h}}\right)^2 \begin{pmatrix} X_{0,2}(t_E) + O(\varepsilon) \\ O(\varepsilon) \end{pmatrix} + \ldots + \tilde{h}^{2q} \left(\frac{h}{\tilde{h}}\right)^{2q} \begin{pmatrix} X_{0,2q}(t_E) + O(\varepsilon) \\ O(\varepsilon) \end{pmatrix} + O(\tilde{h}^{2q+2}), \tag{3.64}$$

where $\tilde{h}$ denotes the stepsize in the subinterval following $[0, t_E]$. So the global error at $t = t_E$ has the same structure as assumed in (3.43), and the induction proceeds to the next subinterval.

The begin of this induction is trivial if, in the very first subinterval, the integration starts on a smooth solution of the original problem. If there is a transient phase, however, the above argumentation does not work (because smooth solutions of the variational equations do not exist in the transients). However, (3.43) can also be assumed immediately after the transient phase: Since the B-convergence theory shows that the global error of the midpoint rule is (essentially) proportional to the length of the integration interval (if the integration starts on the true solution) and since the length of the transient phase is always $O(\varepsilon)$, the error bound immediately after the transients contains a factor ε. If one assumes further that the stepsizes in the transients are adjusted to the gradually improving smoothness of the solution such that local errors are approximately equidistributed, then the error after the transients is $O(\varepsilon h^2)$ (where h denotes the stepsize *after* the transient phase). So – immediately after the transients – (3.43) is valid with $x_2 = x_4 = \ldots = x_{2q} = 0$.

4 The Implicit Trapezoidal Rule

Recall that for the implicit midpoint rule the critical point is the occurrence of the Jacobian $f_y(t, z(t))$ within the inhomogeneities of the variational equations (3.3, ...) and of the remainder equation (3.5). Because of these critical terms our results for the midpoint rule are restricted to problems with smooth $\varphi(t, y)$ and a special type of coupling (cf. Theorem 3.1). For the implicit trapezoidal rule it will turn out that f_y does not appear within any inhomogeneous term. Therefore the structure of the variational equations is very similar to that for the implicit Euler scheme (cf. [3]). But now the crucial point is that the trapezoidal rule is not B-stable and not even D-stable in the sense of Van Veldhuizen [17]. Due to this *lack of stability* it is not obvious how to estimate the remainder term R_ν in the B-sense.

Let us therefore at first discuss the stability properties of the trapezoidal rule in some detail. The trapezoidal rule

$$\frac{1}{h}(\zeta_\nu - \zeta_{\nu-1}) = \frac{1}{2}(f(t_{\nu-1}, \zeta_{\nu-1}) + f(t_\nu, \zeta_\nu)),$$

$$\zeta_0 = z_0 \tag{4.1}$$

Table 3

Trapez. rule	$\zeta_0=h^2\begin{pmatrix}1\\0\end{pmatrix}$	$\zeta_0=h^2\begin{pmatrix}1\\1\end{pmatrix}$
$\omega=1$ $(d_{12}(t)=O(1))$	2.71 E−02	4.27 E+05
$\omega=\varepsilon$ $(d_{12}(t)=O(\varepsilon))$	5.03 E−02	4.23 E−02

contains the "explicit term" $f(t_{\nu-1}, \zeta_{\nu-1})$ which impairs stability: If the integration does not start on a smooth solution then $f(t_0, \zeta_0)$ is large (typically $O(1/\varepsilon)$); this may result in a catastrophic error propagation. This observation does not contradict the B-convergence estimate for the trapezoidal rule given by Kraaijevanger in ([13], Theorem 3.1): If in the transients a very small stepsize is used to ensure small local errors, then the ratio between the stepsizes in and after the transients is large; in this case Kraaijevanger's convergence bound blows up.

However, under the special coupling condition $d_{12}(t)=O(\varepsilon)$ (weak coupling from the stiff to the non-stiff component) the trapezoidal rule can be shown to be fully stable; this will be proved in Theorem 4.3 below.

Let us illustrate the situation by a numerical example:

Example 3. Consider

$$y'(t)=T(t)\,\Lambda T^{-1}(t)\,y(t),\qquad y(0)=0 \tag{4.2}$$

with

$$T(t)=\begin{pmatrix}\cos t & \omega\sin t\\ -\sin t & \cos t\end{pmatrix},\qquad \Lambda=\begin{pmatrix}1 & 0\\ 0 & -\dfrac{1}{\varepsilon}\end{pmatrix}. \tag{4.3}$$

For $\omega=1$ the stiff and the non-stiff components are fully coupled whereas for $\omega=\varepsilon$ the coupling from the stiff to the non-stiff component is weak. $z(t)\equiv 0$ is the (smooth) solution of (4.2). Instead of $\zeta_0=z(0)=0$ we consider perturbed starting values at the h^2-level:

$$\zeta_0=h^2\begin{pmatrix}1\\0\end{pmatrix} \tag{4.4}$$

defines another smooth solution (close to $z(t)\equiv 0$) whereas

$$\zeta_0=h^2\begin{pmatrix}1\\1\end{pmatrix} \tag{4.5}$$

is also close to $z(0)=0$ but does not define a smooth solution. Table 3 shows the respective numerical approximations at $t=1$, obtained by the trapezoidal rule with $h=0.1$, for $\varepsilon=10^{-10}$: In the case of a general coupling and a starting value on a non-smooth solution the trapezoidal rule shows indeed a strongly unstable behavior, whereas in the other cases full stability is observed.

The variational equations and the remainder equation for the trapezoidal rule can again be derived following the ideas of Gragg ([11]). Since each trapezoidal step involves the evaluation of $f(t, y)$ at two different grid points $t_{\nu-1}$ and t_ν, one might expect that the variational equations are influenced by the t-derivatives $f_t, f_{tt}, f_{ty}, \ldots$ which are of course large for problems of the type (2.1) (unless $A(t)\equiv A\equiv const.$ and φ is smooth). However, within the derivation of these variational equations it turns out that these derivatives do actually not occur:

$$\zeta_\nu - z(t_\nu)=h^2 e_2(t_\nu)+h^4 e_4(t_\nu)+\ldots+h^{2q}e_{2q}(t_\nu)+R_\nu \tag{4.6}$$

where

$$e_2'(t)=f_y(t, z(t))\,e_2(t)+\tfrac{1}{12}z'''(t), \tag{4.7}$$

$$e_4'(t)=f_y(t, z(t))\,e_4(t)-\tfrac{1}{120}z^{V}(t)+\tfrac{1}{12}e_2'''(t)+\tfrac{1}{2}f_{yy}(t, z(t))\,e_2^2(t), \tag{4.8}$$

$$\vdots$$

The remainder equation reads

$$\frac{1}{h}(R_\nu-R_{\nu-1})=\frac{1}{2}\big(f_y(t_{\nu-1}, z(t_{\nu-1}))\,R_{\nu-1}+f_y(t_\nu, z(t_\nu))\,R_\nu\big) + \frac{1}{2}\big(G_{\nu-1}(R_{\nu-1})+G_\nu(R_\nu)\big)+b_\nu-c_\nu+d_\nu. \tag{4.9}$$

Here, c_ν is defined exactly in the same way as for the midpoint rule (cf. (3.7)); b_ν and d_ν are defined as the collection of those terms arising from the various Taylor expansions which contain at least a factor h^{2q+2}. (For the precise description of these quantities cf. [4].)

Our analysis is again based on smooth solutions $e_{2i}(t)$ of the variational equations (4.7, ...). For smooth $e_{2i}(t)$ it is again easy to verify that

$$b_\nu=O(h^{2q+2}),\qquad c_\nu=O(h^{2q+2}),\qquad d_\nu=O(h^{2q+2}). \tag{4.10}$$

Our first result is valid for any problem of the type (2.1) without additional assumptions (cf. (2.9)):

Theorem 4.1. *Consider a problem of the type* (2.1) *and assume* $\varepsilon\le Ch^2$. *Let* $[0, t_E]$ *be a subinterval of the whole integration interval with constant stepsize h and assume inductively that – after transformation by* $T^{-1}(t)$ *(cf.* (2.2), (2.5)) *–, the accumulated global error* $T^{-1}(0)(\zeta_0-z(0))$ *at* $t=0$ *satisfies*

$$T^{-1}(0)(\zeta_0-z(0))=h^2\begin{pmatrix}x_2+O(\varepsilon)\\ O(\varepsilon)\end{pmatrix}+\begin{pmatrix}O(h^4)\\ O(\varepsilon h^2)\end{pmatrix} \tag{4.11}$$

where x_2 *is independent of h and* ε. *Then the global error of the implicit trapezoidal rule on* $[0, t_E]$ *admits an asymptotic expansion*

$$\zeta_\nu-z(t_\nu)=h^2 e_2(t_\nu)+R_\nu \tag{4.12}$$

with a smooth, h-independent function $e_2(t)$ which is a solution of the variational Eq. (4.7); *further,*

$$R_\nu = T(t_\nu)\begin{pmatrix} O(h^4) \\ O(\varepsilon h^2) \end{pmatrix} = O(h^4) \tag{4.13}$$

at all grid points $t_\nu = \nu h$, $\nu = 0, 1, \ldots, t_E/h$.

Proof. Transformation of the variational Eq. (4.7) according to $\bar{e}_2(t) := T^{-1}(t)\, e_2(t)$ yields

$$\dot{\bar{e}}_2(t) = \Lambda(t)\, \bar{e}_2(t) + D(t)\, \bar{e}_2(t) + T^{-1}(t)\, \varphi_y(t, z(t))\, T(t)\, \bar{e}_2(t) + \tfrac{1}{12} T^{-1}(t)\, z'''(t). \tag{4.14}$$

This is a linear equation of a similar type as (2.6); in contrast to (3.47) the inhomogeneity of (4.14) is always $O(1)$.[10] Therefore (4.14) satisfies the assumptions of Lemma 3.1; so its smooth solutions $\bar{e}_2(t)$ are of the form

$$\bar{e}_2(t) = \begin{pmatrix} X_{0,2}(t) + \varepsilon X_{1,2}(t) + \ldots \\ \varepsilon Y_{1,2}(t) + \ldots \end{pmatrix} \tag{4.15}$$

where the starting values within the first component can be chosen arbitrarily. Now we make use of the degree of freedom for the starting value $X_{0,2}(0)$ at the ε^0-level, choosing

$$X_{0,2}(0) := x_2 \tag{4.16}$$

with x_2 from the inductive assumption (4.11). Further we define R_0 such that

$$\zeta_0 - z(0) = h^2 e_2(0) + R_0 \tag{4.17}$$

is satisfied with $\zeta_0 - z(0)$ satisfying (4.11). Premultiplying (4.17) by $T^{-1}(0)$ we obtain due to (4.11), (4.16):

$$\begin{aligned} T^{-1}(0)\, R_0 &= T^{-1}(0)(\zeta_0 - z(0)) - h^2\, \bar{e}_2(0) \\ &= h^2 \begin{pmatrix} O(\varepsilon) \\ O(\varepsilon) \end{pmatrix} + \begin{pmatrix} O(h^4) \\ O(\varepsilon h^2) \end{pmatrix} = \begin{pmatrix} O(h^4) \\ O(\varepsilon h^2) \end{pmatrix} \quad \text{for } \varepsilon \leqq C h^2. \end{aligned} \tag{4.18}$$

Now we consider the remainder Eq. (4.9) for problem (2.1):

$$\frac{1}{h}(R_\nu - R_{\nu-1}) = \frac{1}{2}(A(t_{\nu-1})\, R_{\nu-1} + A(t_\nu)\, R_\nu) + \frac{1}{2}(H_{\nu-1}(R_{\nu-1}) + H_\nu(R_\nu)) + i_\nu \tag{4.19}$$

where, for each ν, $H_\nu(R) := \varphi_y(t_\nu, z(t_\nu))\, R + G_\nu(R)$ is a smooth function satisfying

$$H_\nu(0) = 0, \tag{4.20}$$

and

$$i_\nu := b_\nu - c_\nu + d_\nu = O(h^4) \tag{4.21}$$

by construction (cf. (4.10)).

[10] This is true independently of the type of coupling between the stiff and the non-stiff component and for any smooth solution $z(t)$ (not only for $z(t)$ satisfying (3.27))

After multiplication of (4.19) by $T_{\nu-\frac{1}{2}}^{-1} := T^{-1}(t_{\nu-\frac{1}{2}})$ and after some simple manipulations we obtain the transformed remainder equation

$$\begin{aligned} \frac{1}{h}(\rho_\nu - \rho_{\nu-1}) = {} & \frac{1}{2}\left(I + \frac{h}{2}\Theta_{\nu-1}^{+}\right)(\Lambda_{\nu-1}\, \rho_{\nu-1} + \bar{H}_{\nu-1}(\rho_{\nu-1})) + \frac{1}{2}\Theta_{\nu-1}^{+}\, \rho_{\nu-1} \\ & + \frac{1}{2}\left(I - \frac{h}{2}\Theta_\nu^{-}\right)(\Lambda_\nu\, \rho_\nu + \bar{H}_\nu(\rho_\nu)) + \frac{1}{2}\Theta_\nu^{-}\, \rho_\nu + \bar{\imath}_\nu \end{aligned} \tag{4.22}$$

where $T_\nu := T(t_\nu)$, $\Lambda_\nu := \Lambda(t_\nu)$ and

$$\begin{aligned} \rho_\nu &:= T_\nu^{-1} R_\nu, \qquad \bar{\imath}_\nu := T_{\nu-\frac{1}{2}}^{-1}\, i_\nu = O(h^4), \\ \Theta_{\nu-1}^{+} &:= -T_{\nu-\frac{1}{2}}^{-1} \frac{2}{h}(T_{\nu-\frac{1}{2}} - T_{\nu-1}), \\ \Theta_\nu^{-} &:= -T_{\nu-\frac{1}{2}}^{-1} \frac{2}{h}(T_\nu - T_{\nu-\frac{1}{2}}), \end{aligned} \tag{4.23}$$

and with the smooth functions

$$\bar{H}_\nu(\rho) := T_\nu^{-1} H_\nu(T_\nu \rho) \tag{4.24}$$

satisfying

$$\bar{H}_\nu(0) = 0 \tag{4.25}$$

(cf. (4.20)).

Because of the lack of stability of the trapezoidal rule of the recursion $\rho_0 \mapsto \rho_1 \mapsto \ldots \mapsto \rho_\nu \mapsto \ldots$ has now to be studied very carefully. In particular we shall discuss two steps $\rho_{\nu-1} \mapsto \rho_\nu$ and $\rho_\nu \mapsto \rho_{\nu+1}$ in detail to describe a certain oscillating effect. Inductively assuming

$$\rho_{\nu-1} = \begin{pmatrix} h^4 x_{\nu-1} \\ \varepsilon h^2 y_{\nu-1} \end{pmatrix} \tag{4.26}$$

with certain moderate quantities $x_{\nu-1}$, $y_{\nu-1}$ (for the begin of this induction cf. (4.18)) we shall express x_ν, y_ν and $x_{\nu+1}$, $y_{\nu+1}$ in

$$\rho_\nu = \begin{pmatrix} h^4 x_\nu \\ \varepsilon h^2 y_\nu \end{pmatrix}, \qquad \rho_{\nu+1} = \begin{pmatrix} h^4 x_{\nu+1} \\ \varepsilon h^2 y_{\nu+1} \end{pmatrix} \tag{4.27}$$

in terms of $x_{\nu-1}$ and $y_{\nu-1}$. We shall show

$$h^4 x_{\nu+1} = h^4(1 + O(h))\, x_{\nu-1} + O(h^5)\, y_{\nu-1} + O(h^5), \tag{4.28}$$

$$\varepsilon h^2 y_{\nu+1} = \varepsilon h^2(1 + O(h))\, y_{\nu-1} + O(\varepsilon h^4)\, x_{\nu-1} + O(\varepsilon h^4) \tag{4.29}$$

(cf. (4.44) below). From this recursion the desired structure $\begin{pmatrix} O(h^4) \\ O(\varepsilon h^2) \end{pmatrix}$ of the transformed remainder term can be concluded for arbitrary grid points by standard arguments.

First we rewrite (4.22) as

$$\left(I-\frac{h}{2}\Theta_\nu^-\right)\left[\left(I-\frac{h}{2}\Lambda_\nu\right)\rho_\nu-\frac{h}{2}\bar{H}_\nu(\rho_\nu)\right]$$
$$=\left(I+\frac{h}{2}\Theta_{\nu-1}^+\right)\left[\left(I+\frac{h}{2}\Lambda_{\nu-1}\right)\rho_{\nu-1}+\frac{h}{2}\bar{H}_{\nu-1}(\rho_{\nu-1})\right]+h\bar{\iota}_\nu. \tag{4.30}$$

For each ν we define the auxiliary quantity

$$\tilde{\rho}_\nu:=\underbrace{\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}\left(I-\frac{h}{2}\Theta_\nu^-\right)^{-1}\left(I+\frac{h}{2}\Theta_{\nu-1}^+\right)\left(I+\frac{h}{2}\Lambda_{\nu-1}\right)}_{=:\Gamma_\nu}\rho_{\nu-1} \tag{4.31}$$

(the result of one step of the "principal" homogeneous part of (4.30) starting from $\rho_{\nu-1}$). It is easy to verify that the 'growth-matrix' Γ_ν is of the form

$$\Gamma_\nu=\begin{pmatrix} 1+O(h) & O(h)\left(1-\dfrac{c_2(t_{\nu-1})h}{2\varepsilon}\right) \\ \dfrac{O(h)}{1+\dfrac{c_2(t_\nu)h}{2\varepsilon}} & (1+O(h))\dfrac{1-\dfrac{c_2(t_{\nu-1})h}{2\varepsilon}}{1+\dfrac{c_2(t_\nu)h}{2\varepsilon}}\end{pmatrix}. \tag{4.32}$$

For $\varepsilon \leqq C h^2$ this can be written as

$$\Gamma_\nu=\begin{pmatrix} 1+O(h) & \dfrac{h^2}{\varepsilon}\gamma(t_{\nu-1})+O\left(\dfrac{h^3}{\varepsilon}\right) \\ O(\varepsilon) & -1+O(h)\end{pmatrix} \tag{4.33}$$

with a certain smooth function $\gamma(t)$ which is defined in terms of data functions. (To derive (4.33) from (4.32) condition (2.3) and the smoothness of the data functions, in particular that of $c_2(t)$, are essential.)

From (4.31) and (4.33),

$$\tilde{\rho}_\nu=\Gamma_\nu\rho_{\nu-1}=\begin{pmatrix} h^4(1+O(h))\,x_{\nu-1}+h^4(1+O(h))\,\gamma(t_{\nu-1})\,y_{\nu-1} \\ O(\varepsilon)\,h^4 x_{\nu-1}-\varepsilon h^2(1+O(h))\,y_{\nu-1}\end{pmatrix}=:\begin{pmatrix} h^4\tilde{x}_\nu \\ \varepsilon h^2\tilde{y}_\nu\end{pmatrix}. \tag{4.34}$$

The difference $\rho_\nu-\tilde{\rho}_\nu$ satisfies (cf. (4.30), (4.31)):

$$\left(I-\frac{h}{2}\Theta_\nu^-\right)\left(I-\frac{h}{2}\Lambda_\nu\right)(\rho_\nu-\tilde{\rho}_\nu)$$
$$=\frac{h}{2}\left(I-\frac{h}{2}\Theta_\nu^-\right)\bar{H}_\nu(\rho_\nu)+\frac{h}{2}\left(I+\frac{h}{2}\Theta_{\nu-1}^+\right)\bar{H}_{\nu-1}(\rho_{\nu-1})+h\bar{\iota}_\nu \tag{4.35}$$

or equivalently,

$$\rho_\nu-\tilde{\rho}_\nu=\frac{h}{2}\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}(\bar{H}_\nu(\rho_\nu)-\bar{H}_\nu(\tilde{\rho}_\nu))$$
$$+\frac{h}{2}\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}\left[\bar{H}_\nu(\tilde{\rho}_\nu)+\left(I-\frac{h}{2}\Theta_\nu^-\right)^{-1}\left(I+\frac{h}{2}\Theta_{\nu-1}^+\right)\bar{H}_{\nu-1}(\rho_{\nu-1})\right]$$
$$+h\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}\left(I-\frac{h}{2}\Theta_\nu^-\right)^{-1}\bar{\iota}_\nu. \tag{4.36}$$

Hence, due to (4.25), since $\left\|\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}\right\|$ is moderate (due to assumption (2.3)) and since $\left(I-\frac{h}{2}\Theta_\nu^-\right)^{-1}=I+O(h)$[11], $\left(I+\frac{h}{2}\Theta_{\nu-1}^+\right)=I+O(h)$:

$$\|\rho_\nu-\tilde{\rho}_\nu\|\leqq Bh\|\rho_\nu-\tilde{\rho}_\nu\|+Bh[\|\tilde{\rho}_\nu\|+\|\rho_{\nu-1}\|+h^4], \tag{4.37}$$

where B denotes some generic, moderate bound depending on the Lipschitz bounds of the smooth functions $\bar{H}_{\nu-1}(\rho)$, $\bar{H}_\nu(\rho)$ and on the O-constant occurring in (4.21). From (4.37),

$$\|\rho_\nu-\tilde{\rho}_\nu\|\leqq Bh[\|\tilde{\rho}_\nu\|+\|\rho_{\nu-1}\|+h^4] \tag{4.38}$$

with some other moderate bound B.[11]

Observing that $\frac{h}{2}\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}$ is a diagonal matrix of the form

$$\frac{h}{2}\left(I-\frac{h}{2}\Lambda_\nu\right)^{-1}=\begin{pmatrix} \dfrac{h}{2}\dfrac{1}{1-\dfrac{h}{2}c_1(t_\nu)} & 0 \\ 0 & \dfrac{h}{2}\dfrac{1}{1+\dfrac{c_2(t_\nu)h}{2\varepsilon}}\end{pmatrix}=\begin{pmatrix} O(h) & 0 \\ 0 & O(\varepsilon)\end{pmatrix} \tag{4.39}$$

and using once more (4.36) and (4.38) we can estimate the components of $\rho_\nu-\tilde{\rho}_\nu$ by

$$h^4|x_\nu-\tilde{x}_\nu|\leqq Bh\|\rho_\nu-\tilde{\rho}_\nu\|+Bh[\|\tilde{\rho}_\nu\|+\|\rho_{\nu-1}\|+h^4]\leqq Bh[\|\tilde{\rho}_\nu\|+\|\rho_{\nu-1}\|+h^4],$$
$$\varepsilon h^2|y_\nu-\tilde{y}_\nu|\leqq B\varepsilon\|\rho_\nu-\tilde{\rho}_\nu\|+B\varepsilon[\|\tilde{\rho}_\nu\|+\|\rho_{\nu-1}\|+h^4]\leqq B\varepsilon[\|\tilde{\rho}_\nu\|+\|\rho_{\nu-1}\|+h^4]. \tag{4.40}$$

Hence

$$h^4|x_\nu-\tilde{x}_\nu|\leqq Bh[h^4L_{11}|x_{\nu-1}|+(h^4+\varepsilon h^2)L_{12}|y_{\nu-1}|+h^4],$$
$$\varepsilon h^2|y_\nu-\tilde{y}_\nu|\leqq B\varepsilon[h^4L_{21}|x_{\nu-1}|+(h^4+\varepsilon h^2)L_{22}|y_{\nu-1}|+h^4] \tag{4.41}$$

[11] Valid under some mild stepsize restriction (if necessary)

with certain a-priori bounds $L_{ij}=O(1)$ (note that $h^4+\varepsilon h^2=O(h^4)$ by assumption $\varepsilon\leqq Ch^2$). So

$$\rho_\nu=\begin{pmatrix} h^4(\tilde{x}_\nu+(x_\nu-\tilde{x}_\nu)) \\ \varepsilon h^2(\tilde{y}_\nu+(y_\nu-\tilde{y}_\nu)) \end{pmatrix}$$

$$=\begin{pmatrix} h^4(1+O(h))\,x_{\nu-1}+h^4((1+O(h))\,\gamma(t_{\nu-1})+O(h))\,y_{\nu-1}+O(h^5) \\ O(\varepsilon)\,h^4 x_{\nu-1}-\varepsilon h^2(1+O(h))\,y_{\nu-1}+O(\varepsilon h^4) \end{pmatrix}. \tag{4.42}$$

Now we apply the same argumentation to the next step $\rho_\nu\mapsto\rho_{\nu+1}$, obtaining

$$\rho_{\nu+1}=\begin{pmatrix} h^4(1+O(h))\,x_\nu+h^4((1+O(h))\,\gamma(t_\nu)+O(h))\,y_\nu+O(h^5) \\ O(\varepsilon)\,h^4\,x_\nu-\varepsilon h^2(1+O(h))\,y_\nu+O(\varepsilon h^4) \end{pmatrix}$$

$$=\begin{pmatrix} h^4(1+O(h))\,x_{\nu-1}+h^4((1+O(h))\underbrace{(\gamma(t_{\nu-1})-\gamma(t_\nu))}_{O(h)}+O(h))\,y_{\nu-1}+O(h^5) \\ O(\varepsilon)\,h^4 x_{\nu-1}+\varepsilon h^2(1+O(h))\,y_{\nu-1}+O(\varepsilon h^4) \end{pmatrix}. \tag{4.43}$$

Hence

$$\rho_{\nu+1}=\rho_{\nu-1}+\begin{pmatrix} O(h^5)\,x_{\nu-1}+O(h^5)\,y_{\nu-1}+O(h^5) \\ O(\varepsilon h^4)\,x_{\nu-1}+O(\varepsilon h^3)\,y_{\nu-1}+O(\varepsilon h^4) \end{pmatrix}. \tag{4.44}$$

The crucial point is that – due to an *oscillating effect* caused by the entry $-1+O(h)$ within Γ_ν (cf. (4.33)) – no accumulation of h^4 terms occurs!

Now the desired estimate (4.13) follows from (4.44) by a standard argument. □

Similarly as Theorem 3.1 above, Theorem 4.1 can be applied inductively to describe the effects of nonequidistant grids. It is essential here (cf. (4.13)) that the second component of the transformed remainder term is $O(\varepsilon h^2)$ at *all* grid points (and therefore also at the endpoint t_E of the current subinterval). Together with (4.15) this shows that a relation analogous to (4.11) holds for $t=t_E$, and so the induction continues.

Again the begin of this induction is trivial if, in the very first subinterval, the integration starts on a smooth solution of the original problem. In the presence of a transient phase we can use the same argumentation as for the midpoint rule: From the *B*-convergence bound for the trapezoidal rule (cf. [13]) and from the fact that the length of the transient phase is $O(\varepsilon)$ it can be concluded that (for a sufficiently small stepsize ensuring small local errors) the global error is $O(\varepsilon h^2)$ immediately after a transient phase (where h denotes the stepsize *after* the transients); so our inductive assumption (4.11) is satisfied with $x_2=0$.

Concerning the grids within the transient phase there is, however, a fundamental difference to the midpoint rule: The convergence bound in [13] for the trapezoidal rule depends in a sensitive way on the ratio between the different stepsizes, and therefore the error bound $O(\varepsilon h^2)$ can only be guaranteed if a fixed (or at least slightly varying) stepsize is used in the transients. It is therefore

not obvious (in contrast to the midpoint rule[12]) whether the desired error level $O(\varepsilon h^2)$ can be ensured in the case of strongly varying stepsizes within the transient phase (adjusted to the strongly varying smoothness of the solution). A singular perturbation analysis for the trapezoidal rule following a transient solution would have to be carried out to gain further insight to this point; however, this is outside the scope of the present paper.

Remark 4.1. Note that Theorem 4.1 can be used to derive convergence bounds for the trapezoidal rule which are in a certain sense sharper than that one given in [13]. Assume, for instance, that only two different stepsizes are used, namely a very small stepsize h_1 within the transients and a large stepsize h_2 afterwards. The bound given in [13] becomes very large for this special non-equidistant grid because the ratio h_2/h_1 is very large. But if we apply the bound from [13] only to cover the first subinterval (to ensure the error level $O(\varepsilon h_2^2)$ at the end of the transient phase) and estimate the error in the second subinterval on the basis of Theorem 4.1 we end up with a global error bound of a strongly improved quality.

The question arises whether Theorem 4.1 can be extended to the general case $q>1$. A closer look at the above proof shows that this cannot be expected – not even for $\varepsilon\leqq Ch^{2q}$ – because of the occurrence of the entry $\frac{h^2}{\varepsilon}\gamma(t_{\nu-1})$ within Γ_ν (cf. (4.33)).[13] The following example shows that Theorem 4.1 is indeed sharp.

Example 4. Consider

$$y'(t)=A(t)(y(t)-g(t))+g'(t),$$
$$y(0)=g(0) \tag{4.45}$$

where $A(t)=T(t)\Lambda(t)\,T^{-1}(t)$ with

$$T(t)=\begin{pmatrix} e^{t/10} & \sin t \\ \sin t & e^{t/10} \end{pmatrix},\quad \Lambda(t)=\begin{pmatrix} e^{-t/10} & 0 \\ 0 & -\frac{e^{-t/5}}{\varepsilon} \end{pmatrix} \tag{4.46}$$

and with the smooth solution

$$z(t)=g(t)=\begin{pmatrix} e^{-t} \\ e^{-t} \end{pmatrix}. \tag{4.47}$$

The inhomogeneity of (4.45) is $\varphi(t)(\equiv\varphi(t,y))=g'(t)-A(t)\,g(t)=O(1/\varepsilon)$, i.e., φ is of the 'nonsmooth type'. This example shows a full coupling between the stiff and the non-stiff component (all entries $d_{ij}(t)$ within $D(t)=-T^{-1}(t)\,T'(t)$

[12] The midpoint rule is *B*-stable and therefore not only the effect of local error accumulation but also that of starting perturbations can be estimated by *B*-convergence bounds. So the inductive application of *B*-convergence estimates *within* the transients yields – even for strongly varying stepsizes – the desired error level $O(\varepsilon h^2)$ at the end of the transient phase

[13] Terms at the εh^2-level in the second component multiplied by $\frac{h^2}{\varepsilon}\gamma(t_{\nu-1})$ result in h^4-terms in the first component – even under the more stringent assumption $\varepsilon\leqq Ch^{2q}$

Table 4a

Difference quotients	Global error	1st DQ	2nd DQ	3rd DQ	4th DQ
$h=1/8$	2.10E−03	4.00E−03	8.15E−03	4.21E−02	5.13E−01
$h=1/16$	5.23E−04	1.03E−03	2.16E−03	2.00E−02	5.74E−01
$h=1/32$	1.31E−04	2.62E−04	5.48E−04	9.81E−03	6.09E−01
$h=1/64$	3.27E−05	6.59E−05	1.38E−04	4.91E−03	6.24E−01
$h=1/128$	8.17E−06	1.65E−05	3.44E−05	2.46E−03	6.30E−01

Table 4b

Observed order	Global error	1st DQ	2nd DQ	3rd DQ	4th DQ
$h=1/8$					
	2.00	1.95	1.92	1.08	−0.16
$h=1/16$					
	2.00	1.98	1.98	1.02	−0.09
$h=1/32$					
	2.00	1.99	2.00	1.00	−0.04
$h=1/64$					
	2.00	1.99	2.00	0.99	−0.01
$h=1/128$					

are $O(1)$). We integrated (4.45) for $\varepsilon=10^{-10}$ using the trapezoidal rule. The above tables display the L_2-norm of the *difference quotients* (taken with respect to adjacent grid points t and $t-h$) of the global error at $t=1$ together with the observed orders.[14] Tables 4a and 4b show that Theorem 4.1 is indeed sharp: The nonsmooth (oscillating) part of the global error is $O(h^4)$, its 1st difference quotient is $O(h^3)$, ..., its k-th difference quotient is $O(h^{4-k})$ and is dominant for $k\geqq 3$.

The existence of a full asymptotic expansion of an arbitrary order ($q>1$) in the strongly stiff case can only be guaranteed under additional assumptions (cf. Table 2 above); these special cases are discussed in the following.

For the proof of our next theorem a slight reformulation of the given problem is required:

$$y'(t)=\tilde{A}(t)\,y(t)+\tilde{\varphi}(t,y(t)) \tag{4.48}$$

with

$$\tilde{A}(t):=A(t)+\varphi_y(t,z(t))=\tilde{T}(t)\,\tilde{\Lambda}(t)\,\tilde{T}^{-1}(t), \tag{4.49}$$

$$\tilde{\varphi}(t,y):=\varphi(t,y)-\varphi_y(t,z(t))\,y \tag{4.50}$$

so $\tilde{\varphi}_y(t,z(t))\equiv 0$. Due to the Lemma of the Appendix, the type of coupling expressed by the off-diagonal elements of $\tilde{D}(t)=-\tilde{T}^{-1}(t)\,\tilde{T}'(t)$ is the same as for $D(t)=-T^{-1}(t)\,T'(t)$ (with $T(t)$ from (2.2)).

[14] The computations were performed on a CDC Cyber 180 in double precision (mantissa length ≈ 29 decimal digits)

Theorem 4.2. *Consider a problem of the type* (2.1); *assume that* $\varphi(t,y)=O(1)$ *is sufficiently smooth and that*

$$d_{21}(t)=O(\varepsilon) \tag{4.51}$$

(weak coupling from the non-stiff to the stiff component). Assume $q\geqq 2$, $\varepsilon\leqq C h^{2q-2}$ *(strongly stiff case). Let* $[0,t_E]$ *be a subinterval of the whole integration interval with constant stepsize* h *and assume inductively that – after transformation by* $\tilde{T}^{-1}(t)$ *(cf.* (4.49)) *– the accumulated global error* $\tilde{T}^{-1}(0)(\zeta_0-z(0))$ *at* $t=0$ *satisfies*

$$\begin{aligned}\tilde{T}^{-1}(0)(\zeta_0-z(0)) &= h^2\begin{pmatrix} x_{0,2}+\varepsilon x_{1,2}+O(\varepsilon^2)\\ O(\varepsilon^2)\end{pmatrix}+\dots+h^{2q}\begin{pmatrix} x_{0,2q}+\varepsilon x_{1,2q}+O(\varepsilon^2)\\ O(\varepsilon^2)\end{pmatrix}\\ &\quad+\begin{pmatrix} O(h^{2q+2})\\ O(\varepsilon h^{2q})\end{pmatrix}\end{aligned} \tag{4.52}$$

with certain $x_{k,2i}$ *which are independent of* h *and* ε. *Then the global error of the implicit trapezoidal rule on* $[0,t_E]$ *admits an asymptotic expansion*

$$\zeta_\nu-z(t_\nu)=h^2 e_2(t_\nu)+h^4 e_4(t_\nu)+\dots+h^{2q}e_{2q}(t_\nu)+R_\nu \tag{4.53}$$

with smooth, h-independent functions $e_{2i}(t)$ *which are solutions of the variational Eqs.* (4.7, ...); *further,*

$$R_\nu=\tilde{T}(t_\nu)\begin{pmatrix} O(h^{2q+2})\\ O(\varepsilon h^{2q})\end{pmatrix}=O(h^{2q+2}) \tag{4.54}$$

at all grid points $t_\nu=\nu h$, $\nu=0,1,\dots,t_E/h$.

Proof. By assumption on $\varphi(t,y)$ and by Lemma 3.1 the transformed smooth solution $\tilde{z}(t):=\tilde{T}^{-1}(t)\,z(t)$ of the original problem has the form

$$\tilde{z}(t)=\begin{pmatrix} O(1)\\ O(\varepsilon)\end{pmatrix}. \tag{4.55}$$

Let $\tilde{e}_2(t):=\tilde{T}^{-1}(t)\,e_2(t)$. Due to $\tilde{\varphi}_y(t,z(t))\equiv 0$ the first transformed variational equation reads

$$\tilde{e}_2'(t)=\tilde{\Lambda}(t)\,\tilde{e}_2(t)+\tilde{D}(t)\,\tilde{e}_2(t)+\tfrac{1}{12}\tilde{T}^{-1}(t)\,z'''(t) \tag{4.56}$$

with the inhomogeneity

$$\begin{aligned}\tfrac{1}{12}\tilde{T}^{-1}(t)\,z'''(t) &= \tfrac{1}{12}\tilde{T}^{-1}(t)(\tilde{T}(t)\,\tilde{z}(t))'''\\ &= \tfrac{1}{12}\tilde{z}'''(t)-\tfrac{1}{4}\tilde{D}(t)\,\tilde{z}''(t)+\tfrac{1}{4}\tilde{T}^{-1}(t)\,\tilde{T}''(t)\,\tilde{z}'(t)\\ &\quad+\tfrac{1}{12}\tilde{T}^{-1}(t)\,\tilde{T}'''(t)\,\tilde{z}(t).\end{aligned} \tag{4.57}$$

Expressing $\tilde{T}^{-1}(t)\,\tilde{T}''(t)$ and $\tilde{T}^{-1}(t)\,\tilde{T}'''(t)$ by means of $\tilde{D}(t)$ (cf. (3.48)), taking account of (4.55) and using assumption (4.51) we conclude

$$\tfrac{1}{12}\,\tilde{T}^{-1}(t)\,z'''(t)=\begin{pmatrix}O(1)\\O(\varepsilon)\end{pmatrix}. \tag{4.58}$$

Denoting

$$\tilde{e}_2(t)=\begin{pmatrix}\tilde{x}_2(t)\\\tilde{y}_2(t)\end{pmatrix},\quad \tfrac{1}{12}\,\tilde{T}^{-1}(t)\,z'''(t)=\begin{pmatrix}\tilde{\imath}_2(t)\\\varepsilon\tilde{\jmath}_2(t)\end{pmatrix} \tag{4.59}$$

and multiplying the second component of (4.56) by ε we end up with

$$\tilde{x}_2'(t)=\tilde{c}_1(t)\,\tilde{x}_2(t)+\tilde{d}_{11}(t)\,\tilde{x}_2(t)+\tilde{d}_{12}(t)\,\tilde{y}_2(t)+\tilde{\imath}_2(t) \tag{4.60}$$

$$\varepsilon\,\tilde{y}_2'(t)=-\tilde{c}_2(t)\,\tilde{y}_2(t)+\underbrace{\varepsilon\tilde{d}_{21}(t)\,\tilde{x}_2(t)}_{O(\varepsilon^2)}+\varepsilon\tilde{d}_{22}(t)\,\tilde{y}_2(t)+\varepsilon^2\tilde{\jmath}_2(t) \tag{4.61}$$

where $\tilde{d}_{21}(t)=O(\varepsilon)$ by assumption (4.51) and due the Lemma of the Appendix. Using the ansatz

$$\tilde{x}_2(t)=\tilde{X}_{0,2}(t)+\varepsilon\tilde{X}_{1,2}(t)+\varepsilon^2\tilde{X}_{2,2}(t)+\ldots \tag{4.62}$$

$$\tilde{y}_2(t)=\tilde{Y}_{0,2}(t)+\varepsilon\,\tilde{Y}_{1,2}(t)+\varepsilon^2\,\tilde{Y}_{2,2}(t)+\ldots \tag{4.63}$$

and proceeding analogously as in the proof of Lemma 3.1 we conclude that, for any smooth solution of (4.60), (4.61) (with arbitrarily chosen starting values $\tilde{X}_{2,i}(0)$) not only $\tilde{Y}_{0,2}(t)\equiv 0$ but even $\tilde{Y}_{1,2}(t)\equiv 0$ holds. This argumentation can be continued recursively to the other variational equations. So any smooth solution $\tilde{e}_{2i}(t)=\tilde{T}^{-1}(t)\,e_{2i}(t)$ is of the form

$$\tilde{e}_{2i}(t)=\begin{pmatrix}\tilde{X}_{0,2i}(t)+\varepsilon\tilde{X}_{1,2i}(t)+\varepsilon^2\tilde{X}_{2,2i}(t)+\ldots\\ \varepsilon^2\,\tilde{Y}_{2,2i}(t)+\ldots\end{pmatrix}. \tag{4.64}$$

In the same way as in the proof of Theorem 3.1 (cf. (3.53)–(3.55)) we now choose

$$\tilde{X}_{0,2i}(0):=x_{0,2i}, \tag{4.65}$$

$$\tilde{X}_{1,2i}(0):=x_{1,2i} \tag{4.66}$$

with $x_{0,2i}$, $x_{1,2i}$ from (4.52). Further we define R_0 such that

$$\zeta_0-z(0)=h^2\,e_2(0)+\ldots+h^{2q}\,e_{2q}(0)+R_0 \tag{4.67}$$

is satisfied with $\zeta_0-z(0)$ satisfying (4.52). Premultiplying (4.67) by $\tilde{T}^{-1}(0)$ we obtain due to (4.52) and (4.65), (4.66):

$$\tilde{\rho}_0:=\tilde{T}^{-1}(0)\,R_0=\tilde{T}^{-1}(0)(\zeta_0-z(0))-h^2\,\tilde{e}_2(0)-\ldots-h^{2q}\tilde{e}_{2q}(0)$$

$$=h^2\begin{pmatrix}O(\varepsilon^2)\\O(\varepsilon^2)\end{pmatrix}+\ldots+h^{2q}\begin{pmatrix}O(\varepsilon^2)\\O(\varepsilon^2)\end{pmatrix}+\begin{pmatrix}O(h^{2q+2})\\O(\varepsilon h^{2q})\end{pmatrix}=\begin{pmatrix}O(h^{2q+2})\\O(\varepsilon h^{2q})\end{pmatrix}. \tag{4.68}$$

The rest of the argumentation (stability analysis for the remainder term) is completely analogous as in the proof of Theorem 4.1 (with an additional factor h^{2q-2}). So, for all ν,

$$\tilde{\rho}_\nu=\tilde{T}^{-1}(t_\nu)\,R_\nu=\begin{pmatrix}O(h^{2q+2})\\O(\varepsilon h^{2q})\end{pmatrix}=O(h^{2q+2}), \tag{4.69}$$

which completes the proof. □

The inductive applicability of Theorem 4.2 is again obvious if the integration starts on a smooth solution. But after a transient phase only a global error level $O(\varepsilon h^2)$ can be guaranteed (on the basis of B-convergence bounds) which too weak to start the induction. For an extension of our result for such situations a more sophisticated analysis would be required for the transient phase; but this is out of the scope of the present paper.

At the begin of the present subsection we have illustrated the lack of stability of the trapezoidal rule by a numerical example. Recall (cf. Table 3) that in the case $d_{12}(t)=O(\varepsilon)$ full stability was observed. Indeed, the trapezoidal rule is stable for problems with this type of coupling:

Theorem 4.3. *Consider two steps $(t_{\nu-1},\xi_{\nu-1})\mapsto(t_\nu,\xi_\nu)$ and $(t_{\nu-1},\eta_{\nu-1})\mapsto(t_\nu,\eta_\nu)$ of the trapezoidal rule applied to a problem of the type (2.1)–(2.3), where $A(t)$ satisfies the coupling condition $d_{12}(t)=O(\varepsilon)$ and where $\varphi(t,y)$ is allowed to be of the 'nonsmooth type' $\varphi=O(1/\varepsilon)$. Then the stability estimate*

$$\|\xi_\nu-\eta_\nu\|\leqq(1+O(h))\,\|\xi_{\nu-1}-\eta_{\nu-1}\| \tag{4.70}$$

holds.

Proof. The difference $\delta_\nu:=\xi_\nu-\eta_\nu$ satisfies

$$\frac{1}{h}(\delta_\nu-\delta_{\nu-1})=\frac{1}{2}(A(t_{\nu-1})\,\delta_{\nu-1}+A(t_\nu)\,\delta_\nu)$$

$$+\frac{1}{2}((\varphi(t_{\nu-1},\eta_{\nu-1}+\delta_{\nu-1})-\varphi(t_{\nu-1},\eta_{\nu-1}))+(\varphi(t_\nu,\eta_\nu+\delta_\nu)-\varphi(t_\nu,\eta_\nu))). \tag{4.71}$$

Ignoring the smooth, nonlinear terms for the moment, we consider the auxiliary quantity

$$\tilde{\delta}_\nu:=\Big(I-\frac{h}{2}A(t_\nu)\Big)^{-1}\Big(I+\frac{h}{2}A(t_{\nu-1})\Big)\,\delta_{\nu-1}, \tag{4.72}$$

or equivalently

$$\tilde{\delta}_\nu=T_\nu\,\Gamma_\nu\,T_{\nu-1}^{-1}\,\delta_{\nu-1} \tag{4.73}$$

(for the definition of Γ_ν cf. (4.31)). Due to the smoothness of the data functions, due to condition (2.3) and due to the coupling condition $d_{12}(t)=O(\varepsilon)$ – which carries over to the discrete analoga Θ_ν and $\Theta^+_{\nu-1}$ of $D(t)$ – it follows by some simple manipulations that

$$\Gamma_\nu=\left(I-\frac{h}{2}A(\hat{t}_\nu)\right)^{-1}\left(I+\frac{h}{2}A(\hat{t}_\nu)\right)+O(h) \tag{4.74}$$

Note that relation (4.74) is not only valid for $\varepsilon \ll h$ but for arbitrary constellations of ε and h (only some mild stepsize restriction $h\leqq h_0$ might be necessary). Note further that assumption $d_{12}(t)=O(\varepsilon)$ is essential; otherwise the $O(h)$-term in (4.74) would be affected by ε^{-1} (cf. (4.32)).

From (4.74) and due to $T_\nu=T_{\nu-\frac{1}{2}}(I+O(h))$, $T_{\nu-1}^{-1}=T_{\nu-\frac{1}{2}}^{-1}(I+O(h))$:

$$\begin{aligned}\tilde{\delta}_\nu&=\left[T_{\nu-\frac{1}{2}}\left(I-\frac{h}{2}A(\hat{t}_\nu)\right)^{-1}\left(I+\frac{h}{2}A(\hat{t}_\nu)\right)T_{\nu-\frac{1}{2}}^{-1}+O(h)\right]\delta_{\nu-1}\\&=\left[\left(I-\frac{h}{2}A(\hat{t}_\nu)\right)^{-1}\left(I+\frac{h}{2}A(\hat{t}_\nu)\right)+O(h)\right]\delta_{\nu-1}\end{aligned} \tag{4.75}$$

and therefore

$$\|\tilde{\delta}_\nu\|\leqq(1+O(h))\,\|\delta_{\nu-1}\| \tag{4.76}$$

because $\left\|\left(I-\frac{h}{2}A(\hat{t}_\nu)\right)^{-1}\left(I+\frac{h}{2}A(\hat{t}_\nu)\right)\right\|\leqq\left(1+\frac{h\mu}{2}\right)\Big/\left(1-\frac{h\mu}{2}\right)$ where $\mu:=\max_t$ log-norm $A(t)$.

Now the effects of the nonlinear terms can be estimated by a standard argumentation based on the moderate Lipschitz continuity of $\varphi(\cdot, y)$ (similarly as in the proof of Theorem 4.1). This results in

$$\|\delta_\nu-\tilde{\delta}_\nu\|\leqq Ch[\|\tilde{\delta}_\nu\|+\|\delta_{\nu-1}\|]\leqq C'h\|\delta_{\nu-1}\| \tag{4.77}$$

with certain moderate constants C, C'. The desired estimate (4.70) follows directly from (4.76) and (4.77). □

This stability property is the basis for

Theorem 4.4. *Consider a problem of the type* (2.1) *where $\varphi(t, y)$ is allowed to be of the 'nonsmooth type' $\varphi=O(1/\varepsilon)$ and assume*

$$d_{12}(t)=O(\varepsilon) \tag{4.78}$$

(weak coupling from the stiff to the non-stiff component). Assume $\varepsilon\leqq Ch^{2q}$ (strongly stiff case). Let $[0, t_E]$ be a subinterval of the whole integration interval with constant stepsize h and assume inductively that – after transformation by $T^{-1}(t)$ (cf. (2.2), (2.5)) *– the accumulated global error $T^{-1}(0)(\zeta_0-z(0))$ at $t=0$ satisfies*

$$T^{-1}(0)(\zeta_0-z(0))=h^2\begin{pmatrix}x_2+O(\varepsilon)\\O(\varepsilon)\end{pmatrix}+\ldots+h^{2q}\begin{pmatrix}x_{2q}+O(\varepsilon)\\O(\varepsilon)\end{pmatrix}+O(h^{2q+2}) \tag{4.79}$$

with certain x_{2i} which are independent of h and ε. Then the global error of the implicit trapezoidal rule on $[0, t_E]$ admits an asymptotic expansion

$$\zeta_\nu-z(t_\nu)=h^2e_2(t_\nu)+h^4e_4(t_\nu)+\ldots+h^{2q}e_{2q}(t_\nu)+R_\nu \tag{4.80}$$

with smooth, h-independent functions $e_{2i}(t)$ which are solutions of the variational Eq. (4.7, …); *further,*

$$R_\nu=O(h^{2q+2}) \tag{4.81}$$

at all grid points $t_\nu=\nu h$, $\nu=0, 1, \ldots, t_E/h$.

Proof (sketch). Recall that smooth solutions of the variational equations (4.7, …) for the trapezoidal rule are always of the form

$$e_{2i}(t)=T(t)\begin{pmatrix}X_{0,2i}(t)+\varepsilon X_{1,2i}(t)+\ldots\\Y_{1,2i}(t)+\ldots\end{pmatrix}. \tag{4.82}$$

Now one can proceed in the usual way (cf. (3.52)–(3.56) in the proof of Theorem 3.1), ending up with

$$R_0=O(h^{2q+2}). \tag{4.83}$$

From this and from (4.10) the desired estimate (4.81) can immediately be concluded because the trapezoidal rule is fully stable under assumption (4.78) (cf. Theorem 4.3). □

Concerning the induction w.r.t. several subintervals with constant stepsize the same arguments apply as given for the midpoint rule after the proof of Theorem 3.1: For nonequidistant, strongly varying grids within a transient phase – adjusted the the gradually improving smoothness of the solution – the global error level $O(\varepsilon h^2)$ after the transients can now be guaranteed by convergence bounds based on Theorem 4.3.

Appendix

Lemma. *Let $A(t)=T(t)\Lambda(t)T^{-1}(t)$ satisfying* (2.2), (2.3) *be given and let $B(t)$ denote some smooth, moderate matrix. Then*

$$\tilde{A}(t):=A(t)+B(t)=\tilde{T}(t)\tilde{\Lambda}(t)\tilde{T}^{-1}(t) \tag{A.1}$$

where

$$\tilde{\Lambda}(t)=\begin{pmatrix}\tilde{c}_1(t) & 0\\0 & -\dfrac{\tilde{c}_2(t)}{\varepsilon}\end{pmatrix} \tag{A.2}$$

with smooth functions $\tilde{T}(t)$, $\tilde{T}^{-1}(t)$, $\tilde{c}_1(t)$, $\tilde{c}_2(t)$. Further

$$Re(\tilde{c}_2(t))\geqq\tilde{\kappa}>0,\quad \tilde{\kappa}=\kappa+O(\varepsilon) \tag{A.3}$$

and $\tilde{D}(t) := -\tilde{T}^{-1}(t)\,\tilde{T}'(t)$ *has the same coupling properties as* $D(t) = -T^{-1}(t)\,T'(t)$.

Proof. In the following we omit the argument t. From

$$A + B = T(\Lambda + T^{-1}BT)\,T^{-1} \tag{A.4}$$

and from $T^{-1}BT = O(1)$ we conclude

$$\tilde{c}_1 = c_1 + O(1), \qquad \tilde{c}_2 = c_2 + O(\varepsilon) \tag{A.5}$$

by Gerschgorin's Theorem. From this (A.3) follows immediately (due to (2.3)). Let

$$E \equiv \begin{pmatrix} e_{11} & e_{12} \\ e_{21} & e_{22} \end{pmatrix} := \tilde{T}^{-1}T. \tag{A.6}$$

Now we make use of the freedom of scaling the matrix $\tilde{T}$. We assume that $\tilde{T}$ is scaled such that

$$e_{11} \geqq 0, \quad e_{22} \geqq 0, \quad |e_{11}| + |e_{12}| = 1, \quad |e_{21}| + |e_{22}| = 1. \tag{A.7}$$

By (A.6) and (A.7), $\tilde{T}^{-1}$ has a moderate norm. Therefore

$$\tilde{T}^{-1}BT = \tilde{\Lambda}E - E\Lambda \tag{A.8}$$

is also moderate. But this is only possible if e_{12} and e_{21} are $O(\varepsilon)$. From this and from (A.7) we conclude

$$E = I + O(\varepsilon). \tag{A.9}$$

Hence, $E^{-1} = T^{-1}\tilde{T}$ is a moderate matrix and therefore not only $\tilde{T}^{-1}$ is moderate but also $\tilde{T}$. The smoothness of E, E^{-1} $\tilde{T}$, $\tilde{T}^{-1}$, $\tilde{c}_1$ and $\tilde{c}_2$ is an immediate consequence of the smoothness of the given data functions.

Now we discuss the coupling properties of $\tilde{D}$. First we express $\tilde{D}$ by D in the following way:

$$\tilde{D} = -\tilde{T}^{-1}\tilde{T}' = -\tilde{T}^{-1}TT^{-1}\tilde{T}' = -ET^{-1}\tilde{T}'; \tag{A.10}$$

due to $(T^{-1}\tilde{T})' = T^{-1}\tilde{T}' + (T^{-1})'\tilde{T}$ this results in

$$\tilde{D} = -E(E^{-1})' + E(T^{-1})'\tilde{T} \tag{A.11}$$

where $E(E^{-1})' = O(\varepsilon)$ due to (A.9). Using $0 = (TT^{-1})' = T(T^{-1})' + T'T^{-1}$ we rewrite the second term in (A.11) as

$$E(T^{-1})'\tilde{T} = \tilde{T}^{-1}T(T^{-1})'\tilde{T} = -\tilde{T}^{-1}T'T^{-1}\tilde{T} = EDE^{-1}. \tag{A.12}$$

From (A.11) and (A.12),

$$\tilde{D} = EDE^{-1} - E\,(E^{-1})' = EDE^{-1} + O(\varepsilon) \tag{A.13}$$

from which the invariance of the coupling properties follows as a consequence of (A.9). □

References

1. Auzinger, W., Frank, R., Macsek, F.: Asymptotic error expansions for stiff equations. Part 1: The strongly stiff case. Report Nr. 67/68, Institut fuer Angewandte und Numerische Mathematik, TU Wien 1986
2. Auzinger, W., Frank, R., Macsek, F.: Asymptotic error expansions for stiff equations. Part 2: The mildly stiff case. Report Nr. 68/86, Institut fuer Angewandte und Numerische Mathematik, TU Wien 1986
3. Auzinger, W., Frank, R., Macsek, F.: Asymptotic error expansions for stiff equations: The implicit Euler scheme. Report Nr. 72/87, Institut fuer Angewandte und Numerische Mathematik, TU Wien 1987. SIAM J. Numer. Anal. (to appear)
4. Auzinger, W., Frank, R.: Asymptotic error expansions for stiff equations: An analysis for the implicit midpoint and trapezoidal rules in the strongly stiff case. Report Nr. 73/88, Institut fuer Angewandte und Numerische Mathematik, TU Wien 1988. (Extended version of the present paper)
5. Auzinger, W., Frank, R.: Asymptotic error expansions for stiff equations: The implicit midpoint rule, Report Nr. 77/88, Institut fuer Angewandte und Numerische Mathematik, TU Wien 1988
6. Auzinger, W., Frank, R., Kirlinger, G.: Asymptotic error expansions for stiff equations: Applications. Report Nr. 78/89, Institut fuer Angewandte und Numerische Mathematik, TU Wien 1989
7. Bader, G., Deuflhard, P.: A semi-implicit midpoint rule for stiff systems of ordinary differential equations. Numer. Math. **41**, 373–398 (1983)
8. Dahlquist, G., Lindberg, B.: On some implicit one-step methods for stiff differential equations. Dept. of Computer Sciences, Royal Institute of Technology, Report TRITA-NA-7302, 1973
9. Dekker, K., Verwer, J.G.: Stability of Runge-Kutta methods for stiff nonlinear differential equations. CWI Monograph 2, North-Holland 1984
10. Frank, R., Schneid, J., Ueberhuber, C.W.: The concept of *B*-convergence. SIAM J. Numer. Anal. **18**, 753–780 (1981)
11. Gragg, W.B.: Repeated extrapolation to the limit in the numerical solution of ordinary differential equations. Thesis, UCLA 1963
12. Hairer, E., Lubich, C.: Extrapolation at stiff differential equations. Numer. Math. **52**, 377–400 (1988)
13. Kraaijevanger, J.F.B.M.: *B*-Convergence of the implicit midpoint rule and the trapezoidal rule. BIT 25, 652–666 (1985)
14. O'Malley Jr., R.E.: Introduction to singular perturbations. Academic Press, New York 1974
15. Stetter, H.J.: Asymptotic expansions for the error of discretization algorithms for nonlinear functional equations. Numer. Math. **7**, 18–31 (1965)
16. Van Veldhuizen, M.: Asymptotic expansions of the global error for the implicit midpoint rule (stiff case). Computing **33**, 185–192 (1984)
17. Van Veldhuizen, M.: *D*-Stability. SIAM J. Numer. Anal. **18**, 45–64 (1981)

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