Computing 43, 223–253 (1990)

Computing

Asymptotic Error Expansions for Stiff Equations: Applications

W. Auzinger, R. Frank and **G. Kirlinger,** Wien

Received April 18, 1989

Abstract — Zusammenfassung

Asymptotic Error Expansions for Stiff Equations: Applications. In a series of foregoing papers we have studied the structure of the global discretization error for the implicit Euler scheme and the implicit midpoint and trapezoidal rules applied to a general class of nonlinear stiff initial value problems. Full asymptotic error expansions (in the conventional sense) exist only in special situations; for the general case, asymptotic expansions in a weaker sense have been derived. In the present paper we demonstrate how these results can be used for an analysis of acceleration techniques applied to stiff problems. In particular, extrapolation and defect correction algorithms are considered. Various numerical results are presented and discussed.

AMS: 65B05, 65L05

Key words: stiff differential equations, asymptotic error expansions, extrapolation, defect correction

Asymptotische Fehlerentwicklungen für steife Differentialgleichungen: Anwendungen. In einer Reihe vorangegangener Arbeiten wurde die Struktur des globalen Diskretisierungsfehlers für das implizite Eulerverfahren sowie die implizite Mittelpunkts- und Trapezregel bei Anwendung auf eine allgemeine Klasse nichtlinearer steifer Anfangswertprobleme untersucht. Volle asymptotische Entwicklungen (im konventionellen Sinn) existieren nur in speziellen Situationen; für den allgemeinen Fall wurden asymptotische Fehlerentwicklungen in einem schwächeren Sinn hergeleitet. In der vorliegenden Arbeit wird gezeigt, wie beschleunigte Algorithmen, angewendet auf steife Probleme, mit Hilfe der erwähnten Resultate analysiert werden können. Im besonderen werden Extrapolation und die Methode der Defektkorrektur betrachtet. Verschiedenste numerische Resultate werden präsentiert und ausführlich diskutiert.

1. Introduction

The present paper is devoted to a study of acceleration techniques (extrapolation and defect correction) for the numerical solution of stiff initial value problems. The basic tool for an analysis of these methods are asymptotic expansions of the global error of the underlying discretization scheme. In the non-stiff case the existence of asymptotic error expansions has been well known for a long time; recently, similar results about global error structures have been derived for stiff problems. It turns out that in the stiff case asymptotic expansions exist only in a somewhat weaker sense. In [2], [3] and [4], in particular, we have investigated the structure of the global discretization error for the implicit Euler method and the implicit midpoint and trapezoidal rules applied to a class of nonlinear stiff initial value problems (concerning Euler's method cf. also [9]). In the present paper, these theoretical

Printed in Austria

results about global error structures are used for an analysis of acceleration techniques. Various numerical results are also presented.

The class of stiff problems considered in [2], [3] and [4] is the following:

$$y' = f(t,y) = A(t)y + \varphi(t,y),$$
$$y(0) = z_0 \tag{1.1}$$

where the stiffness is characterized by a small parameter ε ($0 < \varepsilon \ll 1$), i.e., the Jacobian along the true solution $z(t)$ of (1.1) has the structure

$$f_y(t,z(t)) = A(t) + \varphi_y(t,z(t)) = T(t)\Lambda(t)T^{-1}(t), \qquad \Lambda(t) = \begin{pmatrix} c_1(t) & 0 \\ 0 & -\dfrac{c_2(t)}{\varepsilon} \end{pmatrix} \tag{1.2}$$

with smooth functions $T(t)$, $T^{-1}(t)$, $c_1(t)$ and $c_2(t)$. It is assumed that

$$Re(c_2(t)) \geq \kappa > 0, \tag{1.3}$$

where $1/\kappa$ is of moderate size independently of ε. Furthermore we have assumed that $\varphi(t,y)$ is a sufficiently smooth function, with moderate derivatives up to a sufficiently high order.[1] $\varphi(t,y)$ itself can be admitted to be at $O(\varepsilon^{-1})$-level, as far as compatible with the existence of smooth solutions to (1.1).

For Euler's method the global error can be written as

$$\zeta_\nu - z(t_\nu) = he_1(t_\nu) + \cdots + h^q e_q(t_\nu) + R_\nu; \tag{1.4}$$

for the midpoint and trapezoidal rules,

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + \cdots + h^{2q} e_{2q}(t_\nu) + R_\nu. \tag{1.5}$$

Here, ζ_ν denotes the numerical approximation for the solution values $z(t_\nu) = z(\nu h)$ on a grid with stepsize h. The $e_i(t)$ are smooth solutions of certain linearized initial value problems—the so-called 'variational equations'. In contrast to the non-stiff case—for which these expansions are well-known to be asymptotically correct (i.e., $R_\nu = O(h^r)$ with a moderate O-constant, where $r = q + 1$ or $2q + 2$ in (1.4) or (1.5), resp.)—these expansions are only valid in a weaker sense:

(i) Asymptotic correctness does only hold in certain strongly stiff situations ('strongly stiff' means: ε sufficiently small compared to the stepsize h). More precisely:
- For Euler's method, expansion (1.4) is asymptotically correct if $\varepsilon \leq Ch^q$ (due to the occurrence of a factor ε within R_ν).
- For the implicit midpoint and trapezoidal rules, the same is true if $\varepsilon \leq Ch^{2q}$ and if certain *coupling properties* between the stiff and the non-stiff components are satisfied. The type of coupling, which plays an essential role here, depends on the size of the off-diagonal elements of the matrix[2]

$$-T^{-1}(t)T'(t) =: D(t) = \begin{pmatrix} d_{11}(t) & d_{12}(t) \\ d_{21}(t) & d_{22}(t) \end{pmatrix}. \tag{1.6}$$

If $d_{12}(t) = O(\varepsilon)$ (weak coupling from stiff to non-stiff component) or $d_{21}(t) = O(\varepsilon)$ (weak coupling from non-stiff to stiff component) then, in some cases, the factor ε does also appear within R_ν (see [3], Section 2, Tables 1 and 2), which entails the asymptotic correctness of (1.5) for sufficiently small $\varepsilon \ll h$.

In the other cases, the asymptotic correctness of the expansions (1.4), (1.5) is violated, i.e., the 'remainder term' R_ν is not at the desired $O(h^r)$-level. In [2] and [4] we have carried out a structural analysis of R_ν for these cases. R_ν often shows an exponentially damped behavior; in other cases it is systematically oscillating (cf. for instance (2.1)–(2.4) below).

(ii) In those cases where the expansion is not asymptotically correct, the coefficient functions $e_i(t)$ are usually not h-independent: They depend smoothly on a parameter $\chi = \chi(h,\varepsilon)$ (typically, $\chi = \varepsilon/h$ or ε/h^2).

(iii) The particular structure of R_ν (which must be studied in those cases where the expansion is not asymptotically correct) and the particular h-dependence of the $e_i(t)$ (cf. (ii)) depend on the 'degree of stiffness', i.e. on the ratio of h and ε. Therefore a representation for the global error which is uniformly valid for $h \to 0$ does not exist; different versions of these expansions hold for different subdomains of the 'ε-h-plane'.

The aim of the present paper is to demonstrate that error structures which suffer from the imperfections just mentioned are nevertheless useful for an analysis of acceleration techniques, namely *extrapolation* and *defect correction.*

Extrapolation. Here we are mainly interested in symmetric schemes; we consider polynomial h^2-extrapolation based on the implicit midpoint rule (IMR) or the implicit trapezoidal rule (ITR) with/without smoothing. In those strongly stiff cases where an asymptotically correct expansion exists, (cf. (i) above), the global error for fixed t is essentially a polynomial in h^2, and thus the optimal performance of extrapolation is obvious (this can be guaranteed by the same arguments as in the non-stiff case).

The analysis of Section 2 will show that in those strongly stiff cases where the 'remainder term' is systematically oscillating at a reduced h^p-level (cf. (i) above), extrapolation will also work satisfactorily. (It is by no means necessary that the global error is polynomial in h^2; any error behavior sufficiently smooth in h^2 will do as well.)

Only in 'mildly stiff' situations, i.e. if $\varepsilon \ll h^2$ is not satisfied, the smoothness of the global error w.r.t. h^2 deteriorates. We will see in Section 2 that extrapolation begins

[1] This smoothness assumption can be relaxed to some extent. For problems of singularly perturbed type, for instance, we have $f(t,y) = \begin{pmatrix} u(t,y) \\ \varepsilon^{-1}v(t,y) \end{pmatrix}$ where u, v and their derivatives are $O(1)$; thus the derivatives of the second component of f (resp. φ) are $O(\varepsilon^{-1})$.

[2] In [3], a slightly different notation was used, namely $A(t) = T(t)\Lambda(t)T^{-1}(t)$ (in contrast to (1.2)); thus also $D(t)$ has a slightly different meaning. This slight inconsistency is, however, of no relevance because, due to our smoothness assumptions w.r.t. φ, the 'type of coupling', defined by the size of the off-diagonal elements of $D(t)$, remains invariant w.r.t. such a reformulation (cf. the Lemma in the Appendix of [3]).

to 'stagnate' and does not show the full conventional order. The achievable level of accuracy is limited by $O(\varepsilon)$ in the worst case but is often much better, e.g. in the case of weak coupling (cf. (i) above) or if one applies smoothing, ... However, sufficiently far away from the start or from a stepsize change, the efficiency of extrapolation again improves due to the fact that in the mildly stiff case the asymptotic correctness of the expansion reappears (cf. Theorem 4.1 of [4]).

Defect correction. In contrast to extrapolation, defect correction is an acceleration technique that works on fixed grids; cf. the begin of Section 3 for a description of the algorithm. Here the key point in the analysis is the smoothness of the global error with respect to t (and not w.r.t. h or h^2). Such an analysis, again based on our results from [4], is presented in Section 3.

2. Extrapolation

2.1. *Theoretical Considerations*

We will now discuss extrapolation based on the IMR applied to a stiff problem of the type (1.1)–(1.3) with full coupling between the stiff and the non-stiff components. Here—in contrast to the special cases mentioned above—an asymptotically correct expansion does *not* exist (not even in the strongly stiff case). Thus for the analysis of extrapolation the conventional argument is of no use. It can, however, be studied on the basis of Theorem 3.1 or Theorem 4.1 of [4].

First we consider situations where Theorem 3.1 of [4] can be applied. To this end we assume that $\varepsilon \le Ch_i^2$ holds (with some moderate constant C) for all stepsizes h_i used for extrapolation. A simplified version of Theorem 3.1 of [4] (which gives sufficient information for the analysis of one extrapolation step) reads as follows:[3]

Assume $\varepsilon \le Ch^2$ (C moderate) and denote

$$\chi := \frac{\varepsilon}{h^2}. \tag{2.1}$$

Then the global error of the IMR can be written as

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + R_\nu, \qquad \nu = 0, 1, \ldots, N \tag{2.2}$$

where the h-independent function $e_2(t)$ is a smooth solution of the first variational equation (see [4], (2.5)) and where

[3] It should be emphasized that our results from [2], [3] and [4] are not only valid for equidistant grids: Our various theorems are formulated for a subinterval (with constant stepsize h) of the whole integration interval and can be applied inductively to describe the error structure for arbitrary, *non-equidistant* grids. (This requires inductive assumptions about the starting values for $e_2(t)$ and $\beta_2(t;\chi)$ which have been suppressed in (2.2)–(2.4).) For the present purpose, however, we omit the merely technical details of such a discussion; we consider only one extrapolation interval and we assume that the integration starts on a smooth solution $z(t)$ of (1.1).

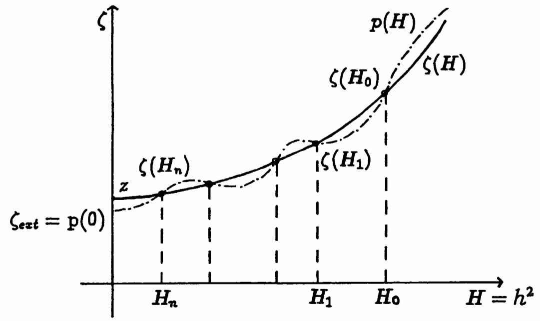

Figure 1

$$R_\nu = T(t_\nu)\begin{pmatrix} 0 \\ h^2\beta_2(t_\nu;\chi) \end{pmatrix}(-1)^\nu + O(h^4). \tag{2.3}$$

Here, $\beta_2(t;\chi)$ is a smooth function in t which depends smoothly on the parameter χ and which is a solution of[4]

$$\beta_2'(t;\chi) = \left(d_{22}(t) - \frac{4\chi}{c_2(t)}\right)\beta_2(t;\chi). \tag{2.4}$$

In Figure 1, $\zeta_N = \zeta(H) = \zeta(h^2)$ denotes the numerical approximation at the endpoint $t_N = t_{ext}$ of the extrapolation interval, generated by the IMR on a grid with stepsize h. $z(t_{ext}) = \zeta(0)$ is the true solution at this point. h^2-extrapolation with a polynomial $p(H)$ of degree n is based on the values $\zeta(H_0), \ldots, \zeta(H_n)$ (where $H_0 > H_1 > \cdots > H_n$). The extrapolated approximation is $\zeta_{ext} = p(0)$; the extrapolation error can be written as[5]

$$\begin{aligned}\zeta_{ext} - \zeta(0) &= -\zeta[0, H_0, \ldots, H_n](0 - H_0)(0 - H_1)\cdots(0 - H_n) \\ &= \zeta[0, H_0, \ldots, H_n](-1)^n H_0 H_1 \cdots H_n.\end{aligned} \tag{2.5}$$

In those special situations where an expansion in the conventional sense exists, the $(n+1)$-th divided difference in (2.5) is of course $O(1)$ (since, then, $\zeta(H) = polynomial(H) + O(H^{n+1})$). Thus the factor[6] $H_0 H_1 \cdots H_n = h_0^2 h_1^2 \cdots h_n^2 = O(h_n^{2n+2})$ determines the order of extrapolation for these regular situations. In the stiff situation considered here the point is that $\zeta[0, H_0, \ldots, H_n] = O(1)$ is not true in

[4] For the meaning of $c_2(t)$ and $d_{22}(t)$ cf. (1.2) and (1.6), respectively.

[5] The identity

$$p(0) - \zeta(0) = -\frac{1}{(n+1)!}\frac{d^{n+1}\zeta(\vartheta)}{dH^{n+1}}(-1)^{n+1}H_0 H_1 \cdots H_n \qquad \text{for some } \vartheta \in [0, H_0]$$

cannot be applied directly: The representation for $\zeta(H)$ given in Theorem 3.1 of [4] (or (2.2)–(2.4) above)—which allows us to study the behavior of the $(n+1)$-th derivative of $\zeta(H)$—is only valid for $\varepsilon \le CH$; but it cannot be guaranteed that $\vartheta \in [0, H_0]$ also satisfies $\varepsilon \le C\vartheta$.

[6] For extrapolation algorithms there is always a fixed relation between the h_i. So it is justified to write $O(h_0^2 \cdots h_n^2) = O(h_n^{2n+2})$.

general; to understand to what extent extrapolation will work successfully, the magnitude of $\zeta[0,H_0,\dots,H_n]$ has to be studied.

Defining

$$\eta(H) := \zeta(H) - \zeta(0) \tag{2.6}$$

we may rewrite the $(n+1)$-th divided difference in (2.5) as

$$\zeta[0,H_0,\dots,H_n] = \eta[0,H_0,\dots,H_n]. \tag{2.7}$$

$\eta(H_i) = \eta(h_i^2)$ is the global error of the IMR with stepsize h_i at $t = t_{ext}$; furthermore, $\eta(0) = 0$. The $\eta(H_i)$ can be written as

$$\eta(H_i) = H_i g(H_i) \tag{2.8}$$

with certain $g(H_i)$ which can be expressed in terms of $e_2(t_{ext})$ and $\beta_2(t_{ext};\chi)$ from (2.2)–(2.4) above. Now we use the following Lemma (which can be proved by induction).

Lemma 2.1. (*Product formula for divided differences.*)

$$(uv)[x_0,\dots,x_k] = \sum_{\ell=0}^{k} u[x_0,\dots,x_\ell]v[x_\ell,\dots,x_k]. \tag{2.9}$$

Straightforward application of (2.9) to η (cf. (2.8)) leads us to

$$\eta[0,H_0,\dots,H_n] = g[H_0,\dots,H_n]. \tag{2.10}$$

(Here, $x_0 = 0$, $x_1 = H_0$, $x_2 = H_1,\dots$, and the first factor $u[x_0]$ has been identified with the linear factor H in (2.8); thus the sum in (2.9) reduces to one non-vanishing term.)

Due to (2.7) and (2.10), the extrapolation error (2.5) (involving a $(n+1)$-th divided difference of ζ) can be expressed as

$$\zeta_{ext} - \zeta(0) = g[H_0,\dots,H_n](-1)^n H_0 H_1 \cdots H_n \tag{2.11}$$

involving the n-th divided difference of g at the nodes $H_i = h_i^2$. The extrapolation error will show the full conventional order $O(h_0^2 \cdots h_n^2)$ provided that $g[H_0,\dots,H_n] = O(1)$. So, due to

$$g[H_0,\dots,H_n] = \frac{1}{n!}\frac{d^n g(H)}{dH^n} \quad \text{for some} \quad H \in [H_n, H_0], \tag{2.12}$$

the degree of smoothness of the function $g(H)$, $H_n \le H \le H_0$, is essential.

Let us at first consider one extrapolation step ($n = 1$). Due to the representation (2.2)–(2.4) for the global error we have $g(H) = \bar{g}(H) + O(H)$ where[7]

$$\bar{g}(H) = e_2(t_{ext}) + T(t_{ext}) \begin{pmatrix} 0 \\ \beta_2\left(t_{ext};\dfrac{\varepsilon}{H}\right) \end{pmatrix} \tag{2.13}$$

[7] We assume that the extrapolation point t_{ext} is always an even grid point.

and where $\beta_2(t_{ext};\chi)$ is smooth w.r.t. $\chi = \varepsilon/H$. Due to

$$g[H_0,H_1] = \bar{g}'(H) + O(1) \quad \text{for some} \quad H \in [H_1,H_0], \tag{2.14}$$

$\bar{g}'(H)$ is the crucial quantity. The only critical term in $\bar{g}'(H)$ originates from $\beta_2\left(t_{ext};\dfrac{\varepsilon}{H}\right)$ which is smooth w.r.t. $\chi = \dfrac{\varepsilon}{H}$ (but not w.r.t. H):

$$\frac{d}{dH}\beta_2\left(t_{ext};\frac{\varepsilon}{H}\right) = \frac{d}{dx}\beta_2(t_{ext};\chi)\cdot\frac{d\chi}{dH} = O\left(\frac{\varepsilon}{H^2}\right), \tag{2.15}$$

and so, due to (2.11), the extrapolation error can finally be estimated by

$$\zeta_{ext} - \zeta(0) = -g[H_0,H_1]H_0H_1 = \left(O\left(\frac{\varepsilon}{H_1^2}\right) + O(1)\right)H_0H_1 = O(\varepsilon) + O(h_1^4). \tag{2.16}$$

For one extrapolation step we conclude:

Proposition 2.1. *If the stepsize h_1 satisfies $\varepsilon \le Ch_1^4$ with some moderate constant C, then one step of h^2-extrapolation based on the IMR delivers the full conventional order $O(h_1^4)$. For stepsizes h_1 only satisfying $\varepsilon \le Ch_1^2$ but not $\varepsilon \le Ch_1^4$ the order of extrapolation reduces; the achievable level of accuracy is limited by $O(\varepsilon)$.*

The case of $n \ge 2$ extrapolation steps can be treated analogously. Instead of (2.2)–(2.4), more information about the error structure, namely an expansion up to the $O(h^{2n+2})$-level, is required. For an $O(h^6)$-expansion see Theorem 3.1 of [4]; longer expansions are also discussed in [4]. The essence of these results is that for $\varepsilon \le CH$ the global error of the IMR at $t = t_{ext}$ can be written as $Hg(H)$ with

$$g(H) = \bar{g}(H) + O(H^n) \tag{2.17}$$

where $\bar{g}$ depends smoothly on $\chi = \dfrac{\varepsilon}{H}$. Due to

$$g[H_0,\dots,H_n] = \frac{1}{n!}\bar{g}^{(n)}(H) + O(1) \quad \text{for some} \quad H \in [H_n,H_0], \tag{2.18}$$

$\bar{g}^{(n)}(H)$ is the crucial quantity. Among several $\dfrac{\varepsilon}{H}$-dependent terms which now appear in $\bar{g}(H)$ the term $\beta_2\left(t_{ext};\dfrac{\varepsilon}{H}\right)$ is again the most critical one. Since

$$\frac{d^n}{dH^n}\beta_2\left(t_{ext};\frac{\varepsilon}{H}\right) = O\left(\frac{\varepsilon}{H^{n+1}}\right), \tag{2.19}$$

the error after n extrapolation steps can be estimated by

$$\begin{aligned}\zeta_{ext} - \zeta(0) &= g[H_0,\dots,H_n](-1)^n H_0 \cdots H_n = \left(O\left(\frac{\varepsilon}{H_n^{n+1}}\right) + O(1)\right)H_0 \cdots H_n \\ &= O(\varepsilon) + O(h_n^{2n+2}).\end{aligned} \tag{2.20}$$

For n extrapolation steps we conclude:

Proposition 2.2. *If the finest stepsize h_n satisfies $\varepsilon \le Ch_n^{2n+2}$ with some moderate constant C, then all steps of h^2-extrapolation based on the IMR deliver the full conventional order. The order of extrapolation begins to reduce as soon as the relation $\varepsilon \le Ch_i^{2i+2}$ is violated. The accuracy of extrapolation begins to stagnate and the achievable level of accuracy is limited by $O(\varepsilon)$.*

Mildly stiff case. Propositions 2.1 and 2.2 refer to the case where all stepsize satisfy $\varepsilon \le Ch_i^2$; for a numerical verification see Subsection 2.2. A different behavior is observed if $\varepsilon \le Ch^2$ is violated. Theorem 4.1 of [4] refers to such a situation: It describes the error structure of the IMR for $\varepsilon \le Ch$. In this case the amplitude of the oscillation occurring in R_ν (cf. (2.3)) is not a smooth function but is strongly decaying. This means that a full asymptotic expansion 'reappears' as the integration proceeds. So—while it cannot be expected in this case that extrapolation works successfully at grid points t_{ext} immediately after the start (or after a change of stepsize)—the damping properties of R_ν can be exploited algorithmically: Extrapolation will work successfully at points t_{ext} sufficiently far away from the starting point if it is based on the so-called 'global' connection strategy. For an experimental illustration of this point we refer to Subsection 2.2.

2.2. *Numerical Examples, Discussion*

Now we present and discuss a number of numerical results for extrapolation based on the IMR and ITR; these methods are also compared with extrapolation based on the semi-implicit midpoint rule. Further topics addressed include smoothing, global vs. local extrapolation and the effect of roundoff errors.

Most of the computations were performed in high accuracy; our intention was to demonstrate the correctness of our theoretical results in a way unaffected by roundoff errors. We used double precision arithmetic on a CDC-Cyber 180 (96 bit mantissa $\approx$ 29 decimal digits). However, for practical purposes the influence of roundoff errors cannot be neglected. We have therefore also done some experiments in single and double precision IEEE arithmetic (24 resp. 53 bit mantissa) to study roundoff error sensitivity.

These computations were based on an experimental program which was not intended to be a 'production code' (no control of stepsize or order, ...).

Our test problems were taken from the class (1.1)–(1.3); the data were chosen as follows.

Different choices for $A(t)$:

- t-dependent stiff matrix

$$A(t) = \begin{pmatrix} 1+e^{-t} & \alpha\cos t \\ \beta\cos t & 1+e^{-t} \end{pmatrix} \cdot \begin{pmatrix} \cos t & 0 \\ 0 & -\dfrac{1+e^{-t}}{\varepsilon} \end{pmatrix} \cdot \begin{pmatrix} 1+e^{-t} & \alpha\cos t \\ \beta\cos t & 1+e^{-t} \end{pmatrix}^{-1}, \tag{2.21}$$

where α and β are chosen as 1 or ε. These parameters characterize the type of coupling:

- $\alpha = \beta = 1$: full coupling between stiff and non-stiff components
- $\alpha = \varepsilon$: weak coupling from stiff to non-stiff component
- $\beta = \varepsilon$: weak coupling from non-stiff to stiff component

- Constant stiff matrix $A(t) \equiv A$:

$$A = \begin{pmatrix} 2+\dfrac{1}{\varepsilon} & -2-\dfrac{2}{\varepsilon} \\ 1+\dfrac{1}{\varepsilon} & -1-\dfrac{2}{\varepsilon} \end{pmatrix} \tag{2.22}$$

Different choices for $\varphi(t, y)$:

- $\varphi(t, y) = O(1/\varepsilon)$:

$$\varphi(t, y) = \frac{1}{\varepsilon}\begin{pmatrix} \dfrac{\alpha\cos^2 t}{1+e^{-t}} \\ \cos t \end{pmatrix} + \begin{pmatrix} \sin(t+y_2) \\ \cos(t+y_1) \end{pmatrix} \tag{2.23}$$

where $\alpha = 1$ or $\alpha = \varepsilon$ is chosen according to α in (2.21).

- $\varphi(t, y) = O(1)$:

$$\varphi(t, y) = \begin{pmatrix} \sin(t+y_2) \\ \cos(t+y_1) \end{pmatrix} \tag{2.24}$$

- $\varphi(t, y) = \varphi(y) = O(1)$ (autonomous):

$$\varphi(y) = \begin{pmatrix} \sin(y_1+y_2) \\ \cos(y_1-y_2) \end{pmatrix} \tag{2.25}$$

These data can be combined in various ways yielding stiff problems (1.1) of different 'degree of difficulty'. Note that $\varphi = O(1/\varepsilon)$ is usually not compatible with the existence of a smooth solution; however, $\varphi(t, y)$ in (2.23) is constructed in such a way that, if combined with $A(t)$ from (2.21) (with equal choice of α in (2.21) and (2.23)), a smooth solution does exist.

Implicit Midpoint Rule.

At first we verify our assertions from Subsection 2.1 about the behavior of the extrapolated IMR. To this end we consider test problem (1.1) with $A(t)$ from (2.21), full coupling between stiff and nonstiff components ($\alpha = \beta = 1$) and $\varphi(t, y)$ from (2.23). For this example a conventional asymptotic error expansion does not exist; the error structure is described by Theorem 3.1 of [4] (see also (2.2)–(2.4) above).

For $\varepsilon = 10^{-10}$ a smooth solution is fixed by the initial value

$$y(t_0) = y(1) = \begin{pmatrix} 5.1493496017702\ldots D+00 \\ 2.3673213796469\ldots D+00 \end{pmatrix}. \tag{2.26}$$

Table 2.1 shows the L_2-norm of the global error after integration over the interval $[1, 2]$ and extrapolation at $t_{ext} = 2$.

Table 2.1

GLOBAL ERROR	EPSILON = 1E−10					
h	IMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	1.129D−01					
1/8	2.749D−02	9.862D−04				
1/16	6.840D−03	4.477D−05	1.800D−05			
1/32	1.708D−03	2.669D−06	1.382D−07	1.455D−07		
1/64	4.269D−04	1.654D−07	1.511D−09	6.597D−10	9.238D−11	
1/128	1.067D−04	1.058D−08	2.591D−10	2.872D−10	2.857D−10	2.859D−10
OBSERVED ORDER						
	2.04					
	2.01	4.46				
	2.00	4.07	7.03			
	2.00	4.01	6.52	7.79		
	2.00	3.97	2.54	1.20	−1.63	

For $\varepsilon = 10^{-5}$ a smooth solution is fixed by

$$y(t_0) = y(1) = \begin{pmatrix} 5.1493565980022\ldots\mathrm{D}+00 \\ 2.3673531720112\ldots\mathrm{D}+00 \end{pmatrix}. \tag{2.27}$$

Table 2.2 shows the L_2-norm of the global error after integration over the interval $[1, 2]$ and extrapolation at $t_{ext} = 2$.

Table 2.2

GLOBAL ERROR	EPSILON = 1E−5					
h	IMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	1.128D−01					
1/8	2.746D−02	1.014D−03				
1/16	6.812D−03	7.321D−05	1.047D−05			
1/32	1.680D−03	3.069D−05	2.785D−05	2.813D−05		
1/64	4.006D−04	2.650D−05	2.622D−05	2.619D−05	2.618D−05	
1/128	8.500D−05	2.065D−05	2.026D−05	2.016D−05	2.014D−05	2.013D−05
OBSERVED ORDER						
	2.04					
	2.01	3.79				
	2.02	1.25	−1.41			
	2.07	0.21	0.09	0.10		
	2.24	0.36	0.37	0.38	0.38	

These results are in full accordance with our analysis of Subsection 2.1: The first extrapolation step shows the full order $O(h^4)$ as long as $Ch^4 \geq \varepsilon$, two extrapolation steps show the order $O(h^6)$ as long as $Ch^6 \geq \varepsilon, \ldots$. In other words:

Extrapolation yields an improvement in accuracy as long as the error is significantly larger than ε but "stagnates" at the $O(\varepsilon)$-level.

For problems (1.1) with a smooth function $\varphi(t, y) = O(\varepsilon^0)$ and for which the coupling from the non-stiff to the stiff component is weak, the extrapolated IMR performs significantly better. For this case it has been shown in [3] (Theorem (3.1) that an asymptotically correct expansion (with a remainder term $R_\nu = O(h^{2q+2})$) exists in the strongly stiff case $\varepsilon \leq Ch^{2q}$. This is due to the fact that—compared with the general case where $R_\nu = O(h^2)$ (cf. (2.2)–(2.4))—the 'critical' terms in R_ν have an additional factor ε, such that

$$R_\nu = O(\varepsilon h^2) + O(h^{2q+2}). \tag{2.28}$$

For this case a structural analysis of R_ν can be carried out in a completely analogous way as in Theorem 3.1 of [4] for the general case. Based on this analysis, extrapolation can be studied in the same way as in Subsection 2.1 above. It turns out that, due to the additional factor ε in (2.28), extrapolation yields an improvement in accuracy down to the $O(\varepsilon^2)$-level; n extrapolation steps show the full order $O(h^{2n+2})$ as long as $Ch^{2n+2} \geq \varepsilon^2$. For a numerical verification we consider test problem (1.1) with $A(t)$ from (2.21), weak coupling non-stiff → stiff ($\alpha = 1, \beta = \varepsilon$) and $\varphi(t, y)$ from (2.24).

For $\varepsilon = 10^{-5}$ a smooth solution is fixed by the initial value

$$y(t_0) = y(1) = \begin{pmatrix} 5.5215049678384\ldots\mathrm{D}+00 \\ 2.8913720760101\ldots\mathrm{D}-05 \end{pmatrix}. \tag{2.29}$$

Table 2.3 shows the L_2-norm of the global error after integration over the interval $[1, 2]$ and extrapolation at $t_{ext} = 2$. In contrast to Table 2.2, the error level $\varepsilon^2 = 10^{-10}$ is indeed achieved.

Table 2.3

GLOBAL ERROR	EPSILON = 1E−5					
h	IMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	1.273D−02					
1/8	3.106D−03	1.027D−04				
1/16	7.720D−04	6.124D−06	3.125D−07			
1/32	1.927D−04	3.789D−07	4.174D−09	1.236D−09		
1/64	4.816D−05	2.392D−08	8.643D−10	8.848D−10	8.837D−10	
1/128	1.204D−05	1.835D−09	6.836D−10	6.808D−10	6.800D−10	6.798D−10
OBSERVED ORDER						
	2.04					
	2.01	4.07				
	2.00	4.01	6.22			
	2.00	3.99	2.27	0.48		
	2.00	3.70	0.34	0.38	0.38	

Smoothing. Due to the occurring oscillations it appears reasonable to apply smoothing: Replacing ζ_ν by

$$\tfrac{1}{4}(\zeta_{\nu-1} + 2\zeta_\nu + \zeta_{\nu+1}) \tag{2.30}$$

entails a cancellation of oscillating terms. In particular, the oscillating component $\beta_2(t_\nu;\chi)(-1)^\nu$ occurring in (2.3) at the h^2-level is smoothed out to the h^4-level. This is useful due to the following reasons:

(a) For extrapolation the term $\beta_2(t;\chi)$ is 'critical' (not because of the factor $(-1)^\nu$ but) due to its h-dependence via $\chi = \varepsilon/h^2$ (cf. (2.15), (2.19)). Thus the fact that this term is 'damped out' by smoothing should be advantageous. Indeed, an analysis in the spirit of Subsection 2.1 shows that extrapolation will work significantly better if preceded by a smoothing step (cf. Tables 2.4 and 2.5).

(b) It may happen that $\beta_2(t;\chi)$, which is a solution of (2.4), is exponentially increasing even if the original problem (and also the first variational equation defining $e_2(t)$) does not admit exponentially increasing solutions. In such a case the IMR behaves badly; but this bad behavior can be improved to some extent by means of smoothing. (Cf. Tables 2.5 and 2.6 for a numerical illustration.)

Table 2.4 illustrates the effect of smoothing on extrapolation. It refers to the same example as Table 2.2; but now we have used one smoothing step (2.30) at $t_\nu = t_{ext} = 2$ prior to extrapolation.

Table 2.4

GLOBAL ERROR		EPSILON = 1E−5		** SMOOTHING **		
h	IMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	4.383D−02					
1/8	1.152D−02	8.004D−04				
1/16	2.917D−03	5.017D−05	3.078D−06			
1/32	7.315D−04	3.128D−06	5.287D−08	1.369D−08		
1/64	1.830D−04	1.960D−07	1.019D−09	7.363D−10	7.899D−10	
1/128	4.576D−05	1.279D−08	5.692D−10	5.693D−16	5.687D−10	5.685D−10
OBSERVED ORDER						
	1.93					
	1.98	4.00				
	2.00	4.00	5.86			
	2.00	4.00	5.70	4.22		
	2.00	3.94	0.84	0.37	0.47	

Compared to Table 2.2, a significant improvement is observed.

Ascher's example. An interesting example demonstrating the somewhat limited applicability of symmetric schemes has been given by Ascher in [1]. It is a linear example of the type (1.1) with

$$A(t) = \begin{pmatrix} -1 + \dfrac{\gamma t}{\varepsilon} & 1 + t - \dfrac{t}{\varepsilon}(1+\gamma t) \\ \dfrac{\gamma}{\varepsilon} & -\dfrac{1}{\varepsilon}(1+\gamma t) \end{pmatrix} \tag{2.31}$$

and

$$\varphi(t,y) \equiv \varphi(t) = \begin{pmatrix} \dfrac{t}{\varepsilon}\sin t \\ \dfrac{1}{\varepsilon}\sin t \end{pmatrix} \tag{2.32}$$

A simple calculation shows that the lower right element $d_{22}(t)$ of the 'coupling matrix' $D(t) = -T^{-1}(t)T'(t)$ (cf. (1.6)) is

$$d_{22}(t) = \gamma + O(\varepsilon). \tag{2.33}$$

Thus for the IMR the 'amplitude function' $\beta_2(t;\chi)$ is strongly increasing in t if $\gamma \gg 1$—in contrast to the stability of Ascher's problem: A singular perturbation analysis shows that strongly increasing solutions never occur, not even for strongly positive γ. This is exactly the situation addressed in (b) above. The IMR performs indeed very badly for $\gamma \gg 1$. Table 2.5 shows the L_2-norm of the global error after integration over the interval $[0,1]$ (and using global extrapolation) for $\varepsilon = 10^{-10}$ and $\gamma = 100$, starting from the initial value

$$y(0) = \begin{pmatrix} 1 \\ 1 + \varepsilon(\gamma - 1) + O(\varepsilon^2) \end{pmatrix} = \begin{pmatrix} 1.0 \\ 1.0000000099000\ldots \end{pmatrix} \tag{2.34}$$

defining a smooth solution.

Table 2.5

GLOBAL ERROR		EPSILON = 1E−10		GAMMA = 100
h	IMR	1st EX	2nd EX	
1/600	3.273D+41			
1/1200	6.907D+40	1.702D+40		
1/2400	1.653D+40	9.880D+38	8.054D+37	
OBSERVED ORDER				
	2.24			
	2.06	4.11		

Smoothing prior to extrapolation (at each of the 300 extrapolation points) has the effect shown in Table 2.6.

Local vs. global extrapolation. Mildly stiff case. In extrapolation algorithms one usually applies a so-called local connection strategy ('local extrapolation'), where after each extrapolation point the integration is continued from the most accurate

Table 2.6

GLOBAL ERROR		EPSILON = 1E−10		GAMMA = 100	** SMOOTHING **
h	IMR	1st EX	2nd EX		
1/600	2.127D+00				
1/1200	5.325D−01	7.990D−04			
1/2400	1.331D−01	4.421D−05	6.114D−06		
OBSERVED ORDER					
	2.00				
	2.00	4.18			

extrapolated value. In mildly stiff cases, however (i.e., if ε is not significantly smaller than h), local extrapolation seems not be very favourable: Recall that for $\varepsilon \not\leq Ch^2$ the 'remainder term' R_ν of the asymptotic expansion of the IMR is dominant at the first grid points but strongly decaying with increasing t_ν (cf. Theorem 4.1 of [4]). Using local extrapolation means that a new starting value is chosen after performing extrapolation—and therefore the remainder term reappears after each extrapolation interval. Thus, local extrapolation makes no use of the damping properties of R_ν. It seems to be advisable to use 'global extrapolation', i.e., to continue the different approximations on the different grids on their own. (Only after a change of stepsize, where the reappearance of irregular error terms is unavoidable, local extrapolation should be used.)

We have performed a number of experiments with local and global extrapolation. To our experience, the local and global versions often behave similarly, especially in strongly stiff situations; but in the mildly stiff case global extrapolation yields much better results. Tables 2.7 and 2.8 illustrate such a situation. The results refer to the same example as Table 2.2 above, but the stepsize is now significantly smaller (mildly stiff case).

Table 2.7

GLOBAL ERROR		EPSILON = 1E−5		** LOCAL EXTRAPOLATION **
h	IMR	1st EX	2nd EX	
1/600	1.479D−07			
1/1200	1.221D−07	1.136D−07		
1/2400	8.338D−08	7.047D−08	6.760D−08	
OBSERVED ORDER				
	0.28			
	0.55	0.69		

In view of these results the question arises whether, for a practical implementation, it is advisable to avoid stepsize changes to a certain extent with the aim of applying

Table 2.8

GLOBAL ERROR		EPSILON = 1E−5		** GLOBAL EXTRAPOLATION **
h	IMR	1st EX	2nd EX	
1/600	2.493D−06			
1/1200	6.233D−07	8.106D−12		
1/2400	1.558D−07	9.466D−08	4.423D−13	
OBSERVED ORDER				
	2.00			
	2.00	6.42		

global extrapolation as often as possible. This may be reasonable under severe accuracy requirements (stepsize used so small that the situation is mildly stiff).

Implicit Trapezoidal Rule.

Asymptotic error expansions for the ITR have been studied in [3]. In most cases the error structure of the ITR is 'more perfect' than for the IMR. In particular, an asymptotically correct expansion exists in certain situations where this is not the case for the IMR (see [3], Section 2, Tables 1 & 2). Moreover, the h^4-expansion

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + O(h^4) \qquad \text{for } \varepsilon \leq Ch^2 \tag{2.35}$$

holds for any problem of the type (1.1)–(1.3) (cf. Theorem 4.1 of [3])—in contrast to the IMR where oscillations occur at the h^2-level (cf. (2.3)). It is therefore obvious that for $\varepsilon \leq Ch^2$ one step of h^2-extrapolation will perform successfully. (For the IMR this can only be guaranteed under the more stringent assumption $\varepsilon \leq Ch^4$—cf. Proposition 2.1 above).

Theorem 4.1 of [3] does not describe the *structure* of the $O(h^4)$-remainder term in (2.35). However, such a structural analysis can be done in a completely analogous way as in [4] for the IMR (cf. Theorem 3.1 of [4], see also (2.2)–(2.4) above). The major difference is that for the ITR the typical h-dependent, oscillating terms occur only at the $O(h^4)$-level. On the basis of such a structural analysis, extrapolation can be studied analogously as for the IMR in Subsection 2.1 (Propositions 2.1 and 2.2), and the following conclusion can be drawn:

Proposition 2.3. *If the finest stepsize h_n satisfies $\varepsilon \leq Ch_n^{2n}$ with some moderate constant C, then all steps of h^2-extrapolation based on the ITR deliver the full conventional order. The order of extrapolation begins to reduce as soon as the relation $\varepsilon \leq Ch_i^{2i}$ is violated. The accuracy of extrapolation begins to stagnate and the achievable level of accuracy is limited by $O(\varepsilon h^2)$.*

Note that, compared to Proposition 2.2 (IMR), the achievable accuracy is $O(\varepsilon h^2)$ (vs. $O(\varepsilon)$) and the stepsize restrictions are milder. This is due the fact that for the ITR the 'critical' error terms are $O(h^4)$ (vs. $O(h^2)$).

Table 2.9 shows a result for extrapolated ITR which illustrates this behavior; it refers to the same test problem as Table 2.2 above.

Table 2.9

GLOBAL ERROR EPSILON = 1E−5

h	ITR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	5.391D−03					
1/8	1.408D−03	8.085D−05				
1/16	3.534D−04	1.755D−06	3.518D−06			
1/32	8.842D−05	9.481D−08	1.588D−08	3.971D−08		
1/64	2.211D−05	5.719D−09	2.217D−10	3.442D−11	1.295D−10	
1/128	5.528D−06	3.764D−10	2.535D−11	2.840D−11	2.838D−11	2.850D−11
OBSERVED ORDER						
	1.94					
	1.99	5.53				
	2.00	4.21	7.79			
	2.00	4.05	6.16	10.17		
	2.00	3.93	3.13	0.28	2.19	

In a number of special cases the irregular error terms have an additional factor ε (cf. Table 2 of [3]), and therefore the 'level of stagnation' of the extrapolated ITR is then even $O(\varepsilon^2 h^2)$. This can also be verified by numerical experiments. We have also applied smoothing to the ITR; generally speaking, the improvement of accuracy effected by smoothing is less significant than for the IMR.

Recall that all the above numerical results were obtained in very high accuracy (CDC-Cyber double precision); the effect of roundoff errors is not visible. However, it is a well-known fact that the trapezoidal rule is not B-stable, except in special cases (weak coupling stiff → non-stiff; cf. Theorem 4.3 of [3]). A high sensitivity with respect to roundoff errors must therefore be expected—but does actually not occur. This point will further be discussed at the end of the present subsection, where numerical results for different machine precisions are compared.

Semi-implicit Midpoint Rule.

Recently, extrapolation based on semi-implicit methods has been proposed by several authors (cf. [5], [9]). In particular, a semi-implicit (two-step) midpoint rule (SIMR) has been proposed by Bader and Deuflhard (cf. [5]) and has also been implemented in a code called METAN1. For this method a rigorous analysis of the error structure has not been done so far but could be carried out by similar techniques as in [3], [4] for the IMR and ITR.

By construction, the SIMR is very suitable for the integration of semilinear autonomous problems of the type $y' = Ay + \varphi(y)$ with a constant stiff matrix A. We applied the ITR and the SIMR to such a problem, with A from (2.22), $\varepsilon = 10^{-10}$ and $\varphi(y)$ from (2.25). A smooth solution is fixed by the initial value

$$y(t_0) = y(1) = \begin{pmatrix} 2.8169452699600\ldots\mathrm{D}{+}00 \\ 1.4084726350403\ldots\mathrm{D}{+}00 \end{pmatrix}. \tag{2.36}$$

Table 2.10 (ITR) and Table 2.11 (SIMR) show the L_2-norm of the global error after integration over the interval $[1, 2]$ and extrapolation at $t_{ext} = 2$.

Table 2.10

GLOBAL ERROR EPSILON = 1E−10

h	ITR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	3.638D−01					
1/8	9.483D−02	5.182D−03				
1/16	2.426D−02	7.319D−04	4.352D−04			
1/32	6.104D−03	5.325D−05	8.007D−06	1.226D−06		
1/64	1.528D−03	3.411D−06	8.804D−08	3.765D−08	4.261D−08	
1/128	3.823D−04	2.144D−07	1.319D−09	5.760D−11	8.983D−11	1.316D−10
OBSERVED ORDER						
	1.94					
	1.97	2.82				
	1.99	3.78	5.76			
	2.00	3.96	6.51	5.03		
	2.00	3.99	6.06	9.35	8.89	

Table 2.11

GLOBAL ERROR EPSILON = 1E−10

h	SIMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	5.515D−01					
1/8	2.950D−02	2.232D−01				
1/16	2.696D−02	2.611D−02	1.297D−02			
1/32	6.151D−03	7.848D−04	2.578D−03	2.825D−03		
1/64	1.516D−03	2.845D−05	2.198D−05	6.324D−05	7.457D−05	
1/128	3.780D−04	1.539D−06	2.543D−07	9.047D−08	3.388D−07	4.121D−07
OBSERVED ORDER						
	4.22					
	0.13	3.10				
	2.13	5.06	2.33			
	2.02	4.79	6.87	5.48		
	2.00	4.21	6.43	9.45	7.78	

The major motivation for the use of semi-implicit schemes is of course their low computational cost (no Newton iteration; a fixed Jacobian is used in each extrapolation interval.). Thus, the fact that the extrapolated ITR yields a better accuracy for the above example (Tables 2.10 vs. 2.11) should not suggest that the ITR is more efficient in this case.

The practical applicability of semi-implicit methods is, however, restricted. Since the Jacobian matrix is 'frozen' at the begin of each extrapolation interval, one may run into troubles in the case of a t-dependent stiff matrix $A(t)$. The following example illustrates this situation: Consider the simple linear equation

$$y' = A(t)y \tag{2.37}$$

with $A(t)$ from (2.21) (full coupling, i.e., $\alpha = \beta = 1$). For $\varepsilon = 10^{-10}$ a smooth solution is fixed by the initial value

$$y(t_0) = y(1) = \begin{pmatrix} 4.3736149438019\ldots\mathrm{D}+00 \\ 1.7275456946077\ldots\mathrm{D}+00 \end{pmatrix}. \tag{2.38}$$

We solved this problem in 'autonomized' form (in [5] the SIMR is only formulated for autonomous problems). Table 2.12 (ITR) and Table 2.13 (SIMR) show the L_2-norm of the global error after integration over the interval [1, 2] and extrapolation at $t_{ext} = 2$.

Table 2.12

GLOBAL ERROR EPSILON = 1E−10

h	ITR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	1.666D−02					
1/8	4.186D−03	2.909D−05				
1/16	1.048D−03	1.656D−06	1.728D−07			
1/32	2.620D−04	1.014D−07	2.217D−09	4.909D−10		
1/64	6.550D−05	6.309D−09	3.202D−11	2.655D−12	7.408D−13	
1/128	1.638D−05	3.938D−10	4.897D−13	1.074D−14	3.705D−16	3.533D−16

OBSERVED ORDER

	1.99					
	2.00	4.13				
	2.00	4.03	6.28			
	2.00	4.01	6.11	7.53		
	2.00	4.00	6.03	7.95	10.97	

Table 2.13

GLOBAL ERROR EPSILON = 1E−10

h	SIMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	1.304D+36					
1/8	2.223D+68	2.965D+68				
1/16	2.292D+130	3.056D+130	3.260D+130			
1/32	3.541D+249	4.722D+249	5.036D+249	5.116D+249		
1/64	1.920D+478	2.560D+478	2.731D+478	2.774D+478	2.785D+478	

*** EXPONENT OVERFLOW ***

We also applied the extrapolated semi-implicit Euler method proposed by Hairer and Lubich (cf. [9]) to this problem. The same catastrophic behavior was observed.

We have modified the SIMR by updating the Jacobian not only at the starting point but at each grid point t_ν ('semi-implicit updated midpoint rule,' SIUMR). Table 2.14 shows the results for the same test problem as in Tables 2.12 and 2.13. The computational effort of this modified scheme is nearly the same as for a fully implicit method—but also the results are of the same quality (compare Table 2.14 with Table 2.12).

Table 2.14

GLOBAL ERROR EPSILON = 1E−10

h	SIUMR	1st EX	2nd EX	3rd EX	4th EX	5th EX
1/4	1.366D−02					
1/8	4.091D−03	9.017D−04				
1/16	1.057D−03	4.572D−05	1.134D−05			
1/32	2.663D−04	2.657D−06	2.135D−07	3.686D−08		
1/64	6.669D−05	1.634D−07	2.878D−09	4.656D−10	6.120D−10	
1/128	1.668D−05	1.017D−08	4.244D−11	2.575D−12	7.593D−13	1.619D−13

OBSERVED ORDER

	1.74					
	1.95	4.30				
	1.99	4.10	5.73			
	2.00	4.02	6.21	6.31		
	2.00	4.01	6.08	7.50	9.65	

From these numerical experiences the following conclusion may be drawn: Semi-implicit methods are often very efficient, but their domain of applicability is restricted. For a practical implementation an 'embedded' scheme is desirable where a suitable control mechanism decides whether the semi-implicit version (fixed Jacobian) or a 'fully-implicit' version (including updates of the Jacobian) has to be used. Unfortunately, such an option is not included in present codes.

Roundoff error sensitivity.

All the above experiments were carried out in high precision arithmetic. In practical computations, however, one will use conventional (e.g., single or double IEEE) arithmetic, where for the above examples the effect of roundoff errors cannot be neglected. In particular, the trapezoidal rule is not B-stable for a general problem of the type (1.1) (unless the coupling stiff → non-stiff is weak—cf. Theorem 4.3 of [3]); thus it cannot be expected that every numerical perturbation will be propagated in a stable way.

We have done a lot of experiments in single and double precision IEEE arithmetic (24 resp. 53 bit mantissa). In many cases it turned out that the resulting extrapolation tableaus differed considerably from the high precision results. However, this was not only observed for the ITR but for any other integration scheme used. This can be explained as follows: Consider a stiff problem of the type (1.1) with full coupling. All entries $a_{ij}(t)$ in the matrix $A(t)$ are $O(1/\varepsilon)$, and rounding into a floating point system causes a relative error of the magnitude[8] *eps* which corresponds to an absolute error of the magnitude eps/ε. Thus, after rounding, the right hand side of the given problem is only specified to an absolute accuracy eps/ε. The effect of such a data inaccuracy on the solution is also $O(eps/\varepsilon)$ (due to the well-conditioned behavior of the problem class considered); thus the effects of the inevitably occurring data errors are significant if ε is very small. For $\varepsilon = 10^{-10}$, for instance, the reasonable error level is limited by 10^{-6} in the case of $eps \approx 10^{-16}$ (IEEE double precision) resp. 10^{+3} for $eps \approx 10^{-7}$ (IEEE single precision). (For double precision arithmetic on a CDC Cyber we have $eps \approx 10^{-29}$; therefore the data error is not visible in the above tables.)

Our numerical experience shows that the effects of these data errors are so dominant that a significant roundoff error sensitivity is not observable, not even for the ITR. This is not surprising since, even if one takes into account that roundoff error propagation may be influenced by the conventional Lipschitz constant $L \sim 1/\varepsilon$, the resulting roundoff error level should not be worse than $O(eps/\varepsilon)$.

Another point is that condition estimates based on one-sided Lipschitz continuity (condition numbers like e^{mt}) are not always sharp. Consider for instance example (1.1) with $\varphi(t, y) = O(1)$ (cf. (2.24)) and weak coupling (stiff $\rightarrow$ non-stiff or vice versa[9]), i.e., $\alpha = \varepsilon$ or $\beta = \varepsilon$. In this case, sharper condition estimates can be derived by means of singular perturbation techniques and it turns out that the effect of data errors is not $O(eps/\varepsilon)$ but only $O(eps)$. Therefore from the point of view of roundoff error sensitivity the case $\alpha = 1$, $\beta = \varepsilon$, for which the ITR is not B-stable, is of particular interest. But not even in this case an increased roundoff error sensitivity could be observed. To illustrate this point, we have integrated this example using the ITR and IMR and IEEE single precision arithmetic. Table 2.15 and 2.16 display

Table 2.15

GLOBAL ERROR	EPSILON = 1E−10				
h	ITR	1st EX	2nd EX	3rd EX	4th EX
1/4	2.306E−02				
1/8	5.688E−03	1.020E−04			
1/16	1.417E−03	6.199E−06	1.110E−16		
1/32	3.533E−04	1.431E−06	9.537E−07	9.537E−07	
1/64	8.774E−05	9.537E−07	9.537E−07	9.537E−07	9.537E−07
OBSERVED ORDER					
	2.02				
	2.00	4.04			
	2.00	2.12	−33.00		
	2.01	2.58	0.00	0.00	

[8] By *eps* we denote the relative accuracy of the underlying floating point system.

[9] In these cases the stiff matrix $A(t)$ is of the form $A(t) = \begin{pmatrix} O(1) & O(1) \\ O(\varepsilon^{-1}) & O(\varepsilon^{-1}) \end{pmatrix}$ resp. $A(t) = \begin{pmatrix} O(1) & O(\varepsilon^{-1}) \\ O(1) & O(\varepsilon^{-1}) \end{pmatrix}$.

the resp. results for $\varepsilon = 10^{-10}$; the integration was started from

$$y(t_0) = y(1) = \begin{pmatrix} 5.5214845585481\ldots D+00 \\ 2.8913452182389\ldots D-10 \end{pmatrix} \tag{2.39}$$

defining a smooth solution.

Table 2.16

GLOBAL ERROR	EPSILON = 1E−10				
h	IMR	1st EX	2nd EX	3rd EX	4th EX
1/4	1.273E−02				
1/8	3.107E−03	1.020E−04			
1/16	7.725E−04	5.722E−06	4.768E−07		
1/32	1.936E−04	4.768E−07	9.537E−07	9.537E−07	
1/64	4.721E−05	1.431E−06	1.431E−06	1.431E−06	1.431E−06
OBSERVED ORDER					
	2.04	4.30			
	2.01	4.16	5.70		
	2.00	3.58	−1.00	−24.04	
	2.04	−1.58	−0.58	−0.58	−0.58

The achievable accuracy is of course limited by $eps \approx 10^{-7}$; but there is no significant difference between the results in Tables 2.15 and 2.16. The ITR does not suffer from an increased roundoff error sensitivity.

The only possibility to visualize the instability of the ITR is to apply starting perturbations which do not define smooth solutions. Tables 2.17 and 2.18 display the results for the same situation as in Tables 2.15 and 2.16 above but with a

Table 2.17

GLOBAL ERROR	EPSILON = 1E−10				
h	ITR	1st EX	2nd EX	3rd EX	4th EX
1/4	6.177E+00				
1/8	1.649E+00	1.402E−01			
1/16	4.381E−01	3.435E−02	2.729E−02		
1/32	9.712E−02	1.655E−02	1.995E−02	2.070E−02	
1/64	2.328E−02	1.333E−03	3.185E−04	7.154E−06	7.391E−05
OBSERVED ORDER					
	1.90				
	1.91	2.03			
	2.17	1.05	0.45		
	2.06	3.63	5.97	11.50	

perturbed initial value

$$\tilde{y}(t_0) = y(t_0) + \begin{pmatrix} 10^{-7} \\ 10^{-7} \end{pmatrix} \tag{2.40}$$

with $y(t_0)$ from (2.39).

Table 2.18

GLOBAL ERROR		EPSILON = 1E−10			
h	IMR	1st EX	2nd EX	3rd EX	4th EX
1/4	1.273E−02				
1/8	3.106E−03	1.030E−04			
1/16	7.725E−04	5.246E−06	1.434E−06		
1/32	1.926E−04	4.872E−07	1.000E−07	1.000E−07	
1/64	4.721E−05	1.434E−06	1.434E−06	1.434E−06	1.434E−06
OBSERVED ORDER					
	2.04				
	2.01	4.30			
	2.00	3.43	3.84		
	2.03	−1.56	−3.84	−3.84	

Here the instability of the ITR is clearly visible, especially on the coarser grids.

Summarizing, we may say that the lack of stability of the ITR seems to be of minor practical relevance. To our experience, instability effects only occur if 'artifical' perturbations are imposed. We never observed unstable propagation of roundoff errors. Note, however, that in a transient phase the lack of stability of the ITR cannot be neglected; the stepsize has to be controlled carefully to avoid instability.

3. Defect Correction

3.1. *Theoretical Considerations*

Iterated defect correction (IDeC) is an acceleration technique which can be used successfully for the integration of stiff problems—provided that a suitable basic method is used. A B-convergence analysis of defect correction (based on the backward Euler scheme and the implicit midpoint rule) was given in [6], [7]. These results are somewhat restricted (only semi-linear problems are covered) and the proofs are extremely technical because they do not rely upon the existence of asymptotic error expansions.

To show how an analysis of defect correction can be based on our results about global error structures, we shall now sketch a convergence proof of IDeC based on the IMR.

Description of the algorithm (see [6], [7] for more details):

Assume that a 'basic approximation' ζ_ν is computed by the IMR on a grid with stepsize h. The ζ_ν are interpolated by a piecewise polynomial function $P^{[0]}(t)$ of a sufficiently high degree. For the IMR (where the global error contains oscillating terms) it is usually recommendable to interpolate at *even* grid points only, i.e.,

$$P^{[0]}(t_\nu) = \zeta_\nu, \qquad \nu = 0, 2, \ldots \tag{3.1}$$

Introducing the *defect*[10]

$$d^{[0]}(t) := \frac{d}{dt} P^{[0]}(t) - f(t, P^{[0]}(t)) \tag{3.2}$$

we form the so-called *neighbouring problem*

$$y' = f(t, y) + d^{[0]}(t),$$
$$y(0) = y_0 \tag{3.3}$$

with the exact solution $P^{[0]}(t)$. Now the neighbouring problem is solved by the IMR, yielding an approximation $\pi_\nu^{[0]}$ for $P^{[0]}(t_\nu)$. The quantity $\pi_\nu^{[0]} - P^{[0]}(t_\nu)$ (global error of the IMR for the neighbouring problem) is an estimate for the 'original' global error $\zeta_\nu - z(t_\nu)$, leading to an improved approximation

$$\zeta_\nu^{[1]} := \zeta_\nu - (\pi_\nu^{[0]} - P^{[0]}(t_\nu)) \tag{3.4}$$

for $z(t_\nu)$. This process can be continued iteratively. For a discussion of further algorithmic details (local/global connection strategy, nonequidistant grids, ...) we refer to [6].

Sketch of IDeC analysis for $\varepsilon \leq Ch^2$.

For what follows we assume that the reader is familiar with the concepts used in [4]. Once more we recall the error structure of the IMR (cf. Theorem 3.1 of [4]) applied to an original problem of the type (1.1)–(1.3) for the case $\varepsilon \leq Ch^2$ ($\chi := \varepsilon/h^2$ of moderate size):

$$\zeta_\nu - z(t_\nu) = h^2 e_2(t_\nu) + h^4 e_4(t_\nu; \chi) + R_\nu \tag{3.5}$$

where $e_2(t)$ and $e_4(t; \chi)$ are smooth solutions of the variational equations (cf. [4], (2.5)) and

$$R_\nu = T(t_\nu) \begin{pmatrix} h^4 \alpha_4(t_\nu; \chi)(-1)^\nu \\ h^2 \beta_2(t_\nu; \chi)(-1)^\nu + h^4 \beta_4(t_\nu; \chi)(-1)^\nu \end{pmatrix} + O(h^6). \tag{3.6}$$

Here $\beta_2(t; \chi)$ is a solution of

$$\beta_2'(t; \chi) = \left(d_{22}(t) - \frac{4\chi}{c_2(t)} \right) \beta_2(t; \chi), \tag{3.7}$$

and $\alpha_4(t; \chi)$ and $\beta_4(t; \chi)$ are smooth functions (defined in [4], (3.45), (3.47)).

[10] At those gridpoints where two adjacent polynomials meet the corresponding one-sided derivative is used.

The global error of the IMR applied to the neighbouring problem (3.3) can be written analogously:

$$\pi_\nu^{[0]} - P^{[0]}(t_\nu) = h^2 e_2^{[0]}(t_\nu) + h^4 e_4^{[0]}(t_\nu; \chi) + R_\nu^{[0]} \tag{3.8}$$

where, for instance, $e_2^{[0]}(t)$ is a smooth solution of

$$\frac{d}{dt} e_2^{[0]}(t) = f_y(t, P^{[0]}(t)) e_2^{[0]}(t) - \frac{1}{24} \frac{d^3}{dt^3} P^{[0]}(t) + \frac{1}{8} f_y(t, P^{[0]}(t)) \frac{d^2}{dt^2} P^{[0]}(t) \tag{3.9}$$

and

$$R_\nu^{[0]} = T^{[0]}(t_\nu) \begin{pmatrix} h^4 \alpha_4^{[0]}(t_\nu; \chi)(-1)^\nu \\ h^2 \beta_2^{[0]}(t_\nu; \chi)(-1)^\nu + h^4 \beta_4^{[0]}(t_\nu; \chi)(-1)^\nu \end{pmatrix} + O(h^6). \tag{3.10}$$

Here $\beta_2^{[0]}(t; \chi)$, for instance, is a solution of

$$\frac{d}{dt} \beta_2^{[0]}(t; \chi) = \left(d_{22}^{[0]}(t) - \frac{4\chi}{c_2^{[0]}(t)} \right) \beta_2^{[0]}(t; \chi). \tag{3.11}$$

The data functions $c_i^{[0]}(t)$, $d_{ij}^{[0]}(t), \dots$ originate from the Jacobian f_y taken along the true solution $P^{[0]}(t)$ of the neighbouring problem:

$$f_y(t, P^{[0]}(t)) = T^{[0]}(t) \Lambda^{[0]}(t) T^{[0]-1}(t), \qquad \Lambda^{[0]}(t) = \begin{pmatrix} c_1^{[0]}(t) & 0 \\ 0 & -\dfrac{c_2^{[0]}(t)}{\varepsilon} \end{pmatrix} \tag{3.12}$$

and $D^{[0]}(t) = (d_{ij}^{[0]}(t)) := -T^{[0]-1}(t) \dfrac{d}{dt} T^{[0]}(t)$.

Let m denote the degree of the interpolating polynomial. We split $P^{[0]}(t)$ into

$$P^{[0]}(t) = P^*(t) + P^{**}(t) \tag{3.13}$$

where $P^*(t)$ interpolates the function[11]

$$\psi(t) := z(t) + h^2 e_2(t) + h^4 e_4(t; \chi) + T(t) \begin{pmatrix} h^4 \alpha_4(t; \chi) \\ h^2 \beta_2(t; \chi) + h^4 \beta_4(t; \chi) \end{pmatrix} \tag{3.14}$$

and $P^{**}(t)$ interpolates the remaining $O(h^6)$-terms in (3.6). By assumption $\varepsilon \le Ch^2$, the parameter χ is of moderate size, and since e_4 and the α's and β's depend smoothly on χ the function $\psi(t)$ is smooth. So, from well-known approximation properties of polynomial interpolation,

$$\frac{d^i}{dt^i} \left(P^*(t) - \psi(t) \right) = O(h^{m+1-i}). \tag{3.15}$$

From (3.14) and due to the smoothness of ψ,

$$\frac{d^i}{dt^i} (\psi(t) - z(t)) = O(h^2) \tag{3.16}$$

[11] Since $P^{[0]}(t)$ interpolates at even grid points only, the factor $(-1)^\nu$ does not appear in (3.14).

(recall that $z(t)$ is assumed to be a smooth solution of the original problem). Furthermore

$$\frac{d^i}{dt^i} P^{**}(t) = O(h^{6-i}). \tag{3.17}$$

From (3.15), (3.16) and (3.17) we conclude for $m \ge 4$

$$\frac{d^i}{dt^i} (P^{[0]}(t) - z(t)) = \frac{d^i}{dt^i} (P^*(t) - \psi(t)) + \frac{d^i}{dt^i} (\psi(t) - z(t)) + \frac{d^i}{dt^i} P^{**}(t) = O(h^2),$$
$$i = 0, 1, 2, 3. \tag{3.18}$$

From (3.18) and due our smoothness assumptions w.r.t. the higher derivatives of f (cf. Section 1),

$$f_y(t, P^{[0]}(t)) = f_y(t, z(t)) + f_{yy}(t, z(t)) \underbrace{(P^{[0]}(t) - z(t))}_{O(h^2)} + \cdots = f_y(t, z(t)) + O(h^2). \tag{3.19}$$

Equations (3.18) and (3.19) imply that *the difference between the data functions entering the variational equations for* $e_2(t)$ (cf. [4], (2.5)) *and* $e_2^{[0]}(t)$ (cf. (3.9)) *is* $O(h^2)$.

Next we show that also the starting values $e_2(0)$, $e_2^{[0]}(0)$ differ only by $O(h^2)$. To this end we recall that the representation (3.5)–(3.7) for the global error w.r.t. the original problem is based on a *special choice for the starting values* $e_2(0)$, $e_4(0; \chi)$ (cf. [4], Section 2 and the proof of Theorem 3.1). These special starting values can be explicitly expressed in terms of the data functions $c_i(t), d_{ij}(t), \dots$. For the neighbouring problem we use an analogous construction; this means that the starting values $e_2^{[0]}(0)$, $e_4^{[0]}(0; \chi)$ are determined by analogous expressions in terms of the $c_i^{[0]}(t)$, $d_{ij}^{[0]}(t), \dots$. Thus, once it has been shown that[12]

$$c_i^{[0]}(t) = c_i(t) + O(h^2), \qquad d_{ij}^{[0]}(t) = d_{ij}(t) + O(h^2), \dots \tag{3.20}$$

then indeed

$$e_2^{[0]}(0) = e_2(0) + O(h^2). \tag{3.21}$$

From the fact that the data functions as well as the starting values defining $e_2(t)$, $e_2^{[0]}(t)$ differ by $O(h^2)$ we obtain the 'similarity relation'

$$e_2^{[0]}(t) = e_2(t) + O(h^2). \tag{3.22}$$

(3.20) further implies

$$\beta_2^{[0]}(t; \chi) = \beta_2(t; \chi) + O(h^2). \tag{3.23}$$

From (3.22) and (3.23) the desired IDeC error estimate

$$\zeta_\nu^{[1]} - z(t_\nu) = O(h^4) \tag{3.24}$$

follows immediately.

[12] For the proof of (3.20) cf. the paragraph following (3.24).

It remains to be shown that (3.20) indeed holds. Due to (3.19) we have

$$T^{[0]}(t)\Lambda^{[0]}(t)T^{[0]-1}(t) = T(t)\Lambda(t)T^{-1}(t) + O(h^2); \tag{3.25}$$

from this the desired estimate (3.20) can be concluded by the same arguments as used for the proof of the Lemma in the Appendix of [3].

The argumentation can be generalized to the case of more than one IDeC step (we omit the technical details). Summarizing, we have:

Proposition 3.1. *If the stepsize h satisfies $\varepsilon \leq Ch^2$ with some moderate constant C, then k IDeC steps based on the IMR and interpolation at even grid points with piecewise polynomials of degree (at least) 2k + 2 deliver the full conventional order $O(h^{2k+2})$.*

Notice the rather mild assumption $\varepsilon \leq Ch^2$ (for an arbitrary number of IDeC steps) in contrast to the restrictive assumption $\varepsilon \leq Ch^{2k+2}$ in the case of k extrapolation steps (cf. Proposition 2.2).

The case $\varepsilon \leq Ch$.

If $\varepsilon \leq Ch^2$ is not satisfied (mildly stiff case), the amplitude of the oscillating global error terms is no longer smooth but strongly decaying (cf. Theorem 4.1 of [4]): Instead of $(-1)^\nu$ the factors

$$\Pi_\nu := \prod_{\mu=1}^{\nu} \left(\frac{1 - \dfrac{c_2(t_\mu - \frac{h}{2})h}{2\varepsilon}}{1 + \dfrac{c_2(t_\mu - \frac{h}{2})h}{2\varepsilon}} \right) \tag{3.26}$$

appear. Therefore the derivatives of a polynomial $P^{[0]}(t)$ interpolating the ζ_ν (ν even) are not of moderate size. Consequently, the necessary similarity relations (3.18) do not hold. To analyze defect correction in this more difficult case we use a slightly modified representation for the global error of the neighbouring problem: Split $P^{[0]}(t)$ into

$$P^{[0]}(t) = P^*(t) + P^{**}(t) \tag{3.27}$$

where $P^*(t)$ interpolates the smooth part of ζ_ν, i.e.,

$$P^*(t_\nu) = z(t_\nu) + h^2 e_2(t_\nu) \tag{3.28}$$

and P^{**} interpolates the non-smooth remainder term R_ν (which behaves like (3.26)). A modified variational equation can be derived for the neighbouring problem (3.3) where the smooth function $P^*(t)$ plays the role of $P^{[0]}(t)$:

$$\frac{d}{dt}e_2^{[0]}(t) = f_y(t, P^*(t))e_2^{[0]}(t) - \frac{1}{24}\frac{d^3}{dt^3}P^*(t) + \frac{1}{8}f_y(t, P^*(t))\frac{d^2}{dt^2}P^*(t). \tag{3.29}$$

For a suitable choice of the starting value $e_2^{[0]}(0)$ it can be shown that the global error $\pi_\nu^{[0]} - P^{[0]}(t_\nu)$ can be written as

$$\pi_\nu^{[0]} - P^{[0]}(t_\nu) = h^2 e_2^{[0]}(t_\nu) + R_\nu^{[0]} \tag{3.30}$$

where $R_\nu^{[0]}$ is the solution of a nonlinear difference equation of a similar type as the equation defining R_ν (cf. [4], (2.6)) but with the additional inhomogeneous term

$$\frac{d}{dt}P^{**}(t_\nu - \tfrac{h}{2}) - \frac{1}{h}(P^{**}(t_\nu) - P^{**}(t_{\nu-1})) + f_y(t_\nu - \tfrac{h}{2}, P^*(t_\nu - \tfrac{h}{2}))(\tfrac{1}{2}(P^{**}(t_{\nu-1}) + P^{**}(t_\nu)) - P^{**}(t_\nu - \tfrac{h}{2})). \tag{3.31}$$

Since P^{**} interpolates the remainder term R_ν of the original problem which decays like Π_ν (cf. (3.26)), it can be shown that the critical inhomogeneous term (3.31) also exhibits a damping behavior. Now a discrete singular perturbation analysis (in the spirit of [4]) can be performed for the remainder equation defining $R_\nu^{[0]}$ and it can be shown that also $R_\nu^{[0]}$ essentially decays like Π_ν. It can further be shown that the starting value $e_2^{[0]}(0)$ can be fixed such that $e_2^{[0]}(0) - e_2(0) = O(h^2)$, from which $e_2^{[0]}(t) - e_2(t) = O(h^2)$ follows by the same arguments as in the case $\varepsilon \leq Ch^2$.

We omit the technical details of this argumentations, which are somewhat lengthy.

The essence of these results is:

- R_ν and $R_\nu^{[0]}$ are $O(h^2)$ at the first grid points, and a 'similarity relation' $R_\nu^{[0]} - R_\nu = O(h^4)$ does not hold (due to the occurrence of the inhomogeneous term (3.31) for which there is no *pendant* within the equation defining R_ν). However, R_ν as well as $R_\nu^{[0]}$ exhibit a decaying behavior with increasing ν.
- Therefore—since the similarity relation $h^2 e_2^{[0]}(t) - h^2 e_2(t) = O(h^4)$ is satisfied—the desired error estimate $\zeta_\nu^{[1]} - z(t_\nu) = O(h^4)$ does not hold at the first grid points but is valid as soon as R_ν and $R_\nu^{[0]}$ are sufficiently damped.

Obviously, a *global connection strategy* (cf. [6], (2.9)) is advisable in the mildly stiff case, similarly as for extrapolation (see Subsection 2.2). Local connection should only be used after a change of stepsize where the re-occurrence of the 'irregular' error terms at the h^2-level is unavoidable.

IDeC based on the ITR can be analyzed analogously.

3.2. *Numerical Examples, Discussion*

We now present some results[13] obtained for IDeC based on the IMR and ITR, applied to test problem (1.1) with $A(t)$ from (2.21), $\varepsilon = 10^{-5}$, full coupling ($\alpha = \beta = 1$), $\varphi(t, y)$ from (2.23) and initial condition (2.27). Table 3.1 shows the L_2-norm of the global error at $t = 2$. Piecewise polynomial interpolation (degree 8) at even grid points was used. For the finer stepsizes $h = 1/32, \ldots$, global connection was applied.

In Table 3.1, all stepsizes satisfy $\varepsilon \leq Ch^2$, i.e. the assumptions of Proposition 3.1 are satisfied. The predicted orders 2, 4, ... are observed with decreasing h. On the

[13] High accuracy arithmetic ($\approx$29 decimal digits) was used.

Table 3.1

h	IMR	1st DC	2nd DC	3rd DC	ITR	1st DC	2nd DC	3rd DC
DEFECT CORRECTION	EPSILON = 1E−5							
1/16	6.812D−03	4.776D−04	5.996D−04	6.054D−04	3.534D−04	1.732D−04	1.603D−04	1.602D−04
1/32	1.680D−03	3.649D−06	3.095D−06	3.125D−06	8.842D−05	2.482D−06	2.267D−06	2.271D−06
1/64	4.006D−04	6.425D−08	2.865D−09	2.941D−09	2.211D−05	1.203D−08	3.973D−09	4.039D−09
1/128	8.500D−05	3.949D−09	8.171D−12	9.166D−12	5.528D−06	4.651D−10	5.611D−12	6.340D−12
1/256	1.520D−05	2.422D−10	1.834D−14	3.175D−14	1.382D−06	2.862D−11	1.137D−14	2.220D−14
1/512	3.425D−06	1.528D−11	1.944D−16	5.538D−17	3.455D−07	1.787D−12	8.596D−17	8.131D−17
	OBSERVED ORDER							
	2.02	7.03	7.60	7.60	2.00	6.12	6.14	6.14
	2.07	5.83	10.08	10.05	2.00	7.69	9.16	9.14
	2.24	4.02	8.45	8.33	2.00	4.69	9.47	9.32
	2.48	4.03	8.80	8.17	2.00	4.02	8.95	8.16
	2.15	3.99	6.52	9.16	2.00	4.00	7.05	8.09

coarsest grids, however, the IDeC steps show an increased order, and the level of accuracy actually achieved is rather low. Obviously, the convergence towards the fixed point of the IDeC iteration[14] is very fast; at the same time the approximation quality of this fixed point is very good on the finer grids (due to its high order) but only moderate on the coarser grids—a phenomenon not uncommon for higher order methods in cases where the true solution is not 'very smooth'.[15]

For this example the efficiency of defect correction compared with extrapolation can be estimated on the basis of Tables 2.2, 2.9 and 3.1:

- IMR: For $h = 1/6$, extrapolation yields the smaller error $1 * 10^{-5}$ (Table 2.2) compared with $6 * 10^{-4}$ (coarsest grid in Table 3.1). For finer and finer grids, defect correction turns out to be superior.
- ITR: A comparison of Tables 2.9 and 3.1 shows that only on very fine grid defect correction yields a smaller error. For moderate accuracy requirements, extrapolation appears to be more promising.

For a further comparison we now consider an example with a very smooth solution:

$$y' = A(t)(y - g(t)) + g'(t), \qquad y(0) = g(0) \tag{3.32}$$

with $A(t)$ from (2.21), $\varepsilon = 10^{-5}$, full coupling and the true solution $g(t) = \begin{pmatrix} e^{-t} \\ e^{-t} \end{pmatrix}$. In Table 3.2 we contrast the resp. results (L_2-norm of the global error at $t = 1$) for defect correction (polynomials of degree 8, interpolation at even grid points, global connection) and extrapolation based on the ITR.

Table 3.2(a)

h	ITR	1st DC	2nd DC	3rd DC
DEFECT CORRECTION	EPSILON = 1E−5			
1/16	2.178D−04	7.474D−08	3.659D−11	1.178D−10
1/32	5.450D−05	4.779D−09	2.518D−12	4.029D−13
1/64	1.363D−05	2.983D−10	3.161D−14	1.579D−15
1/128	3.408D−06	1.864D−11	4.747D−16	6.152D−18
1/256	8.519D−07	1.165D−12	7.344D−18	2.402D−20
	OBSERVED ORDER			
	2.00	3.97	3.86	8.19
	2.00	4.00	6.32	8.00
	2.00	4.00	6.06	8.00
	2.00	4.00	6.01	8.00

[14] The fixed point of an IDeC iteration can be characterized as the solution of a certain collocation method (cf. [8]).

[15] The true solution of this problem is smooth in the sense that there are no transient terms like $e^{-t/\varepsilon}$; however, it shows a significant variation on the interval [1, 2] and the higher derivatives are not moderate.

Table 3.2(b)

EXTRAPOLATION EPSILON = 1E − 5

h	ITR	1st EX	2nd EX	3rd EX	4th EX	5th EX	6th EX
1/4	3.412D − 03						
1/8	8.675D − 04	1.927D − 05					
1/16	2.178D − 04	1.215D − 06	1.104D − 08				
1/32	5.450D − 05	7.608D − 08	1.688D − 10	8.338D − 12			
1/64	1.363D − 05	4.761D − 09	9.580D − 12	8.033D − 12	8.048D − 12		
1/128	3.408D − 06	3.006D − 10	6.562D − 12	6.518D − 12	6.512D − 12	6.511D − 12	
1/256	8.519D − 07	2.007D − 11	2.912D − 12	2.854D − 12	2.840D − 12	2.837D − 12	2.836D − 12
	OBSERVED ORDER						
	1.98						
	1.99	3.99					
	2.00	4.00	6.03				
	2.00	4.00	4.14	0.05			
	2.00	3.99	0.55	0.30	0.31		
	2.00	3.90	1.17	1.19	1.20	1.20	

Since the true solution is very smooth, IDeC yields a high increase of accuracy already on the coarsest grid. Furthermore, the accuracy level achieved by IDeC is throughout better than for extrapolation, especially on the finer grids (where extrapolations shows the usual 'stagnations'). Analogous comparisons based on the IMR show again that IDeC yields a higher accuracy; the difference is even more significant. However, if the extrapolated IMR is combined with smoothing then the situation turns out to be similar as in Table 3.2.

In all these examples, IDeC was based on interpolation at even grid points. However, interpolation at all grid points will also work successfully in all those cases where the oscillating global error components have an additional factor ε, e.g. for semilinear problems (cf. [3]). This can be confirmed by numerical experiments.

References

[1] U. Ascher, On symmetric schemes and differential-algebraic equations, SIAM J. Sci. Stat. Comp. *10*, 937–949 (1989).

[2] W. Auzinger, R. Frank, F. Macsek, Asymptotic error expansions for stiff equations: The implicit Euler scheme, to appear in SIAM J. Numer. Anal. 27 (1990).

[3] W. Auzinger, R. Frank, Asymptotic error expansions for stiff equations: An analysis for the implicit midpoint and trapezoidal rules in the strongly stiff case, to appear in Numer. Math.

[4] W. Auzinger, R. Frank, Asymptotic error expansions for stiff equations: The implicit midpoint rule, Report Nr. 77/88, Institut für Angewandte und Numerische Mathematik, TU Wien, 1988 (submitted).

[5] G. Bader, P. Deuflhard, A semi-implicit midpoint rule for stiff systems of ordinary differential equations, Numer. Math. *41*, 373–398 (1983).

[6] R. Frank, J. Hertling, H. Lehner, B-Convergence properties of Defect Correction methods I, Numer. Math. *49*, 139–162 (1986).

[7] R. Frank, J. Hertling, H. Lehner, B-Convergence properties of Defect Correction methods II, Numer. Math. *49*, 163–188 (1986).

[8] R. Frank, C. W. Ueberhuber, Iterated Defect Correction for the efficient solution of stiff systems of ordinary differential equations, BIT *17*, 146–159 (1977).

[9] E. Hairer, Ch. Lubich, Extrapolation at stiff differential equations, Numer. Math. *52*, 377–400 (1988).

W. Auzinger
R. Frank
G. Kirlinger
Institut für Angewandte und
Numerische Mathematik
Technische Universität Wien
Wiedner Hauptstrasse 6-10
A-1040 Wien
Austria