Computer Science Technical Report TR-08-13
July 18, 2008

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ACHIEVING VERY HIGH ORDER FOR IMPLICIT EXPLICIT TIME STEPPING: EXTRAPOLATION METHODS *

EMIL M. CONSTANTINESCU† AND ADRIAN SANDU‡

Abstract. In this paper we construct extrapolated implicit-explicit time stepping methods that allow to efficiently solve problems with both stiff and non-stiff components. The proposed methods can provide very high order discretizations of ODEs, index-1 DAEs, and PDEs in the method of lines framework. These methods are simple to construct, easy to implement and parallelize. We establish the existence of perturbed asymptotic expansions of global errors, explain the convergence orders of these methods, and explore their linear stability properties. Numerical results with stiff ODEs, DAEs, and PDEs illustrate the theoretical findings and the potential of these methods to solve multiphysics multiscale problems.

Key words. extrapolation methods, implicit explicit methods, ODE, DAE index-1, PDE

AMS subject classifications.

1. Introduction. Models described by processes that have multiple physics and scale components are pervasive in numerical simulations. Typical applications include mechanical and chemical engineering, aeronautics, astrophysics, meteorology and oceanography, financial modeling, environmental sciences, which are modeled by Navier-Stokes [Bramkampa et al., 2004], convection-diffusion-reaction [Ascher et al., 1995; Ruuth, 1995; Constantinescu et al., 2008], or Black-Scholes. The individual physics or scale components typically have very different properties that are reflected in their discretization; e.g., for advection-diffusion-reaction systems, the discrete advection has a relatively slow dynamics, while the diffusion and chemistry are typically fast evolving [Gebhardt et al., 2002; Ruuth, 1995; Verwer et al., 1996]. The dynamics of a process can be categorized in the relative fast and slow terms. The informal expressions stiff and non-stiff are commonly associated with the fast and slow evolution, respectively.

The discretization in time of slow processes with an explicit method is typically more efficient, due to its low cost, than using an implicit scheme, whereas implicit methods are more appropriate for stiff processes due to their favorable stability properties [Hairer and Lubich, 1988; Hairer et al., 1988]. For multiscale processes, purely explicit or implicit methods are not efficient because in general, explicit methods require prohibitively small time steps and implicit methods are either too difficult to implement or too expensive to compute [Hairer et al., 1993a; Lambert, 1991].

An approach to solve problems with both stiff and non-stiff components that has gained widespread popularity is called implicit-explicit (IMEX) method. In the IMEX approach one uses an implicit scheme for the stiff components and an explicit integrator for the slow dynamics such that the combined method has the desired stability and accuracy properties. IMEX linear multistep methods have been investigated in [Ascher et al., 1995; Frank et al., 1997; Hundsdorfer and Ruuth, 2007] and IMEX Runge-Kutta schemes have been developed in [Ascher et al., 1997; Boscarino, 2007; Pareschi and Russo, 2000; Verwer and Sommeijer, 2004]. These methods are generally limited to low consistency orders (typically, lower than five). High order IMEX Runge-Kutta methods are difficult to construct due to a large number of order

*This work was supported by the National Science Foundation through award NSF CCF-0515170.

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conditions and IMEX linear multistep methods have increasing stability restrictions with increasing the order of accuracy.

In this study we propose a new family of IMEX methods using extrapolation. In the extrapolation approach several numerical approximations using the same method but different fractions of the step size are used to eliminate truncation error terms. The proposed methods have a very simple construction procedure, can attain very high consistency orders, and are parallelizable.

We are concerned with solving the following problem

$$y'(x) = F(x, y)\,,\ F(x, y) = f(x, y) + g(x, y)\,,\ x > x_0\,,\ y(x_0) = y_0\,, \tag{1.1}$$

where f represents the non-stiff part and g the stiff component of the problem. We seek to apply an explicit method to f and an implicit method to g. We consider the extrapolation methods [Deuflhard, 1985; Hairer et al., 1993a,b] for the efficient integration of (1.1) and extend the pioneering work of Deuflhard [1985]; Deuflhard et al. [1987] on extrapolated linearly implicit and mid-point rule to extrapolated IMEX methods.

The contributions of this paper are the following. We propose three novel implicit-explicit methods. In contrast with IMEX Runge-Kutta and linear multistep strategies, the proposed methods have a very simple construction, implementation, can attain very high orders of accuracy, and are parallelizable. We investigate the linear stability properties and show the existence of perturbed asymptotic expansions of the global discretization errors. We illustrate these theoretical considerations on ODEs, DAEs, and PDEs examples.

The rest of the paper is organized as follows. In Section 2 we review the extrapolation methods along with their consistency and linear stability properties; in Section 3 we investigate the asymptotic error expansion for the extrapolated IMEX methods applied to index-1 differential algebraic problems [Hairer et al., 1993b], and in Section 4 we illustrate the theoretical findings on two numerical examples. In Section 5 we study the error expansion for the extrapolated IMEX schemes applied to stiff ODEs and in Section 6 we show numerical evidence that supports the theory. In Section 7 we present a typical PDE example and give some implementation considerations in Section 8. The conclusions follow in Section 9.

2. Extrapolation Methods. Consider a sequence n_j of positive integers with $n_j < n_{j+1}$, $1 \le j < M$ and define corresponding step sizes $h_1, h_2, h_3, \ldots$ by $h_j = H/n_j$. Further, define the numerical approximation of (1.1) at $x_0 + H$ using the step size h_j by

$$T_{j,1} := y_{h_j}(x_0 + H)\,,\ 1 \le j \le M\,. \qquad [\textit{Base method}] \tag{2.1}$$

Historically, the notation T comes from the trapezoidal rule, albeit now it is used in place of a generic discretization method. Let us assume that the local error of the p^{th} order method employed to solve (2.1) has an asymptotic expansion of the form

$$y(x) - y_h(x) = e_{p+1}(x)\, h^{p+1} + \cdots + e_N(x)\, h^N + E_h(x)\, h^{N+1}\,, \tag{2.2}$$

where $e_i(x)$ are errors that do not depend on h, and E_h is bounded for $x_0 \le x \le x_{\text{end}}$. This is true for the methods discussed in this paper (see Theorem 2.1 and Section 2.1). By using M approximations to (2.1) with different h_j's one can eliminate the error terms in the global error asymptotic expansion (2.2) by employing the same

T_{11}				p			
T_{21}	T_{22}			p	$p+1$		
T_{31}	T_{32}	T_{33}		p	$p+1$	$p+2$	
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$

(a) $T_{i,k}$ tableau (b) Classical orders

TABLE 2.1

Tableaux with (a) the $T_{i,k}$ solutions and (b) their corresponding classical orders for a p^{th} order base method.

procedure as in Richardson extrapolation (see [Hairer et al., 1993a, Chap. II.9]). High order approximations of the numerical solution of (1.1) can be determined by solving a linear system with M equations. Then the k^{th} solution represents a numerical method of order $p + k - 1$ [Hairer et al., 1993a, Chap. II, Thm. 9.1]. The most economical solution to this set of linear equations is given by the Aitken-Neville formula [Aitken, 1932; Neville, 1934; Gasca and Sauer, 2000]:

$$T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j/n_{j-1}\right) - 1}\,,\ j \le M\,,\ k < j. \tag{2.3a}$$

If the numerical method (2.1) is symmetric, then the Aitken-Neville formula yields

$$T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j/n_{j-1}\right)^2 - 1}\,,\ j \le M\,,\ k < j. \tag{2.3b}$$

Scheme (2.1), (2.3) is called the *extrapolation method*. For illustration purposes, the $T_{j,k}$ solutions can be represented in a tableau; e.g., see Table 2.1.a. As it can be seen in Table 2.1.b, the method is represented by a sequence of lower order embedded methods. This fact and the methods's easy construction can be used for (macro-) step size (H) control and variable order approaches. There are several choices for the sequences n_j; however, Deuflhard [1983] showed that the harmonic sequence $n_j = 1, 2, 3, 4, \ldots$ is the most economical one. This sequence will be used for the rest of this study.

2.1. Base Methods . Typical base methods used to compute (2.1) include the forward Euler method

$$y^{n+1} = y^n + h\left(f(y^n) + g(y^n)\right), \qquad [\textit{Explicit Euler}]$$

and the linearly implicit Euler method (see Appendix A)

$$y^{n+1} = y^n + \left[I - h\,(f+g)'(y^n)\right]^{-1}\left(h\,f(y^n) + h\,g(y^n)\right). \qquad [\textit{Linearly implicit}] \tag{2.4a}$$

Method (2.4a) has been used in [Deuflhard, 1985; Deuflhard et al., 1987] as the base method, for solving stiff ODEs of type (1.1) with (2.1), (2.3). Symmetric base methods have also been considered. This class includes implicit mid-point rule and GBS [Deuflhard, 1985; Hairer et al., 1993a]. Explicit Euler and the symmetric methods are not addressed further in this study.

In this paper we consider $J = F'(y) \approx \tilde{J} = (g(y))'$ and extend the analysis done by Deuflhard et al. [1987] to problems that have components treated implicitly and explicitly such as in the generic representation given in (1.1). We propose the following base methods for the extrapolation algorithm (2.1), (2.3): the *W-IMEX* scheme

$$y^{n+1} = y^n + [I - h\,g'(y^n)]^{-1}\left(h\,f(y^n) + h\,g(y^n)\right), \qquad [\textit{W-IMEX}] \tag{2.4b}$$

the *Pure-IMEX* method

$$y^{n+1} = y^n + h\,f(y^n) + [I - h\,g'(y^n)]^{-1}\left(h\,g(y^n)\right), \qquad [\textit{Pure-IMEX}] \tag{2.4c}$$

and the *Split-IMEX* scheme

$$y^{n+1} = y^* + [I - h\,g'(y^n)]^{-1}\left(h\,g(y^*)\right); \;\; y^* = y^n + h\,f(y^n)\,. \qquad [\textit{Split-IMEX}] \tag{2.4d}$$

The W-IMEX scheme is essentially the same as the linearly implicit method except for the Jacobian, which is approximated by using only the stiff part of the problem, which is typically required for the stability of the numerical algorithm. This makes the W-IMEX method computationally cheaper than the linearly implicit one. The Pure-IMEX and Split-IMEX schemes use the same approximation of the Jacobian (as in the W-IMEX); however, the explicit and implicit parts are treated separately, making them truly IMEX schemes. The Split-IMEX scheme evolves the explicit part first and then the implicit one.

2.2. Consistency of the Extrapolation Methods. In Henrici's notation [Henrici, 1962], one step methods are expressed as

$$y^{n+1} = y^n + h\,\Phi\left(x^n, y^n, h\right)\,. \tag{2.5}$$

Methods (2.4) can be represented in Henrici's notation in the following way

$$\begin{aligned}
\Phi\left(x^n, y^n, h\right) &= \left[I - h\,(f+g)'(y^n)\right]^{-1}\left(h\,f(y^n) + h\,g(y^n)\right), && [\textit{implicit Euler}]\\
\Phi\left(x^n, y^n, h\right) &= \left[I - h\,g'(y^n)\right]^{-1}\left(h\,f(y^n) + h\,g(y^n)\right), && [\textit{W-IMEX}]\\
\Phi\left(x^n, y^n, h\right) &= h\,f(y^n) + \left[I - h\,g'(y^n)\right]^{-1}\left(h\,g(y^n)\right), && [\textit{Pure-IMEX}]\\
\Phi\left(x^n, y^n, h\right) &= h\,f(y^n) + \left[I - h\,g'\,(y^n)\right]^{-1}\left(h\,g\!\left(y^n + h\,f(y^n)\right)\right). && [\textit{Split-IMEX}]
\end{aligned}$$

A method of order p applied to a differential equation with each term being sufficiently differentiable possesses an expansion of the *local error* of the form

$$y(x+h) - y(x) - h\,\Phi\left(x, y(x), h\right) = d_{p+1}(x)\,h^{p+1} + \cdots + d_{p+N}(x)\,h^{N+1} + O\left(h^{N+2}\right)\,. \tag{2.6}$$

Following [Gragg and Stetter, 1964; Hairer et al., 1993a] we consider discretization methods that have a global error function $e_p(x)$ that satisfies (see [Hairer et al., 1993a, Chp. II, Thm. 3.6])

$$y(x) - y_h(x) = e_p(x)\,h^p + O(h^{p+1})\,. \tag{2.7}$$

Methods (2.4) are of this type with $p = 1$. Then we have the following result due to Gragg and Stetter [1964].

Theorem 2.1 ([Gragg and Stetter, 1964]). *Suppose that a given method with sufficiently smooth increment function Φ satisfies the consistency condition $\Phi\left(x, y, 0\right) = f(x, y)$ and*

2					1			
2	3				1	2		
2	3	4			1	2	3	
...	...	...	...		...	...	...	...

(a) Local orders (b) Global orders

TABLE 2.2

The classical (a) local and (b) global orders for the extrapolation methods with first order base methods.

possesses an expansion (2.6) for the local error. Then the global error has an asymptotic expansion of the form

$$y(x) - y_h(x) = e_p(x)\, h^p + \cdots + e_N(x)\, h^N + E_h(x)\, h^{N+1} \tag{2.8}$$

where $e_j(x)$, $j = p, p+1, \ldots N$, *satisfies (2.7) with* $e_j(x_0) = 0$ *and* $E_h(x)$ *is bounded for* $x_0 \le x \le x_{\text{end}}$ *and* $0 \le h \le h_0$.

Proof. See Gragg [1965] and [Hairer et al., 1993b, Chp. II, Thm. 8.1]. □

Methods (2.4) possess the local error expansion (2.6) and global error expansion (2.8), and therefore can be extrapolated using (2.1),(2.3a). It follows that the classical orders of accuracy of the extrapolation methods (2.4) are the ones given in Table 2.2.

Next we discuss the linear stability properties of IMEX methods (2.4b, 2.4c, 2.4d) and of their extrapolations.

2.3. Linear Stability Analysis of the Extrapolated IMEX Methods. In this section we investigate the linear stability properties of extrapolated (2.4) and follow the analysis done by Frank et al. [1997]. Consider methods (2.4) applied to the following linear scalar test problem

$$y(t)' = \lambda y(t) + \mu y(t)\,, \tag{2.9}$$

where $\lambda,\ \mu \in \mathbb{C}$; e.g., $\lambda,\ \mu$ can be the eigenvalues of the non-stiff (f) and stiff (g) parts in a PDE application, respectively.

The transfer or stability functions $R(z, w)$ defined by

$$y^{n+1} = R(\lambda h, \mu h) y^n\,, \tag{2.10}$$

for (2.4) are given by (see Appendix B)

$$y^{n+1} = \left(\frac{1}{1-(\lambda h + \mu h)}\right) y^n;\ R(z,w) = \frac{1}{1-(z+w)} \qquad [\textit{Linearly implicit}] \tag{2.11a}$$

$$y^{n+1} = \left(\frac{1+\lambda h}{1-\mu h}\right) y^n;\ R(z,w) = \frac{1+z}{1-w} \qquad [\textit{W-IMEX}] \tag{2.11b}$$

$$y^{n+1} = \left(\frac{1+\lambda h - \lambda h\, \mu h}{1-\mu h}\right) y^n;\ R(z,w) = \frac{1+z-zw}{1-w} \qquad [\textit{Pure-IMEX}] \tag{2.11c}$$

$$y^{n+1} = \left(\frac{1+\lambda h(1-\mu h(1-\lambda h))}{1-\mu h - \lambda h\, \mu h}\right) y^n;\ R(z,w) = \frac{1+z}{1-w} \qquad [\textit{Split-IMEX}] \tag{2.11d}$$

The stability region $\mathcal{S}$ is defined by

$$\mathcal{S} = \{z \in \mathcal{S}_z, w \in \mathcal{S}_w; \|R(z,w)\| \le 1, (\mathcal{S}_z \times \mathcal{S}_w) \subset (\mathbb{C}\times\mathbb{C})\}\ .$$

A method with a transfer function $R(\dots)$ defined by (2.10) is stable if $R(\dots) \subseteq \mathcal{S}$. In other words, for scalar problems, linear stability requires that $|R(z,w)| \le 1$. As expected, the linearly implicit Euler method has the same transfer function as implicit Euler. Incidentally, the W-IMEX method has the same transfer function as the Split-IMEX scheme. The stability function of the extrapolated methods are calculated from the extrapolation formula (2.3a) as [Hairer et al., 1993b, Chap. IV]:

$$R_{j,k+1}(z,w) = R_{j,k}(z,w) + \frac{R_{j,k}(z,w) - R_{j-1,k}(z,w)}{(n_j/n_{j-k}) - 1}\,,$$

where $R(\dots)$ is the one-step transfer function for a specific base method and the subscripts denote the corresponding position in the extrapolation tableau.

In practice implicit methods that are A-stable or $A(\alpha)$-stable [Hairer et al., 1993b] are desirable for problems with stiff solution components. We take a practical approach and ask the following question: To ensure $A(\alpha)$-stability of the stiff part, what is the necessary restriction on the non-stiff part? We consider three stability regions for the stiff part: A-stable and $A(\alpha)$-stable, $\alpha = 30^\circ, 60^\circ$. In Figure 2.1 we show the stability regions for the implicit part (left column) and the corresponding stability regions of the explicit part of extrapolated (2.4) methods for several (T_{jk}) entries in the extrapolation tableau (see Table 2.1.a).

We remark that the stability region of the implicit parts can easily accommodate the typical stiff problems encountered in practice. Depending on the problem, the implicit stability region can be relaxed by decreasing α and as a result the explicit stability region grows, relaxing the step size restriction for the entire method. Moreover, the stability regions of the extrapolated explicit parts encompass a section of the imaginary axis, which is a desirable property when solving certain PDEs via the method of lines [Hundsdorfer and Verwer, 2003]. We also note that the explicit stability regions grow as more T_{jk} terms are computed.

In practice, the fast process represented by μ has large values on the negative real axis whereas the slow process represented by λ sits close to the origin in the negative real half plane. The stability regions presented in Figure 2.1 illustrate the relationship between the IMEX solver and the physical process properties. Next we investigate the accuracy of the extrapolated IMEX methods.

3. Global Error Expansion for Extrapolated IMEX Methods applied to DAEs. Consider the following test problem

$$\begin{aligned} &u' = f(x,u) + g(x,u) \\ &\text{with } u = y + \varepsilon\, z\,. \end{aligned} \tag{3.1}$$

The y component is associated with the slow evolving and z with the stiff part of u. The stiffness is controlled by ε; i.e., the problem is stiffer as $0 \le \varepsilon \ll 1$ shrinks. This problem can be reformulated to obtain two processes: f, the slow and g, the fast process

$$\left\{ \begin{array}{l} y' = \widehat{f}(y,z) = f(y + \varepsilon\, z) \\ \varepsilon\, z' = \widehat{g}(y,z) = g(y + \varepsilon\, z) \end{array} \right. \quad \text{with} \left\{ \begin{array}{l} y^0 + \varepsilon\, z^0 = u^0 \\ y + \varepsilon\, z = u \\ (y + \varepsilon\, z)' = u' \end{array} \right. . \tag{3.2}$$

Then we have

$$\begin{pmatrix} y \\ \varepsilon\, z \end{pmatrix}' = \begin{pmatrix} f(y,z) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ g(y,z) \end{pmatrix}. \tag{3.3}$$

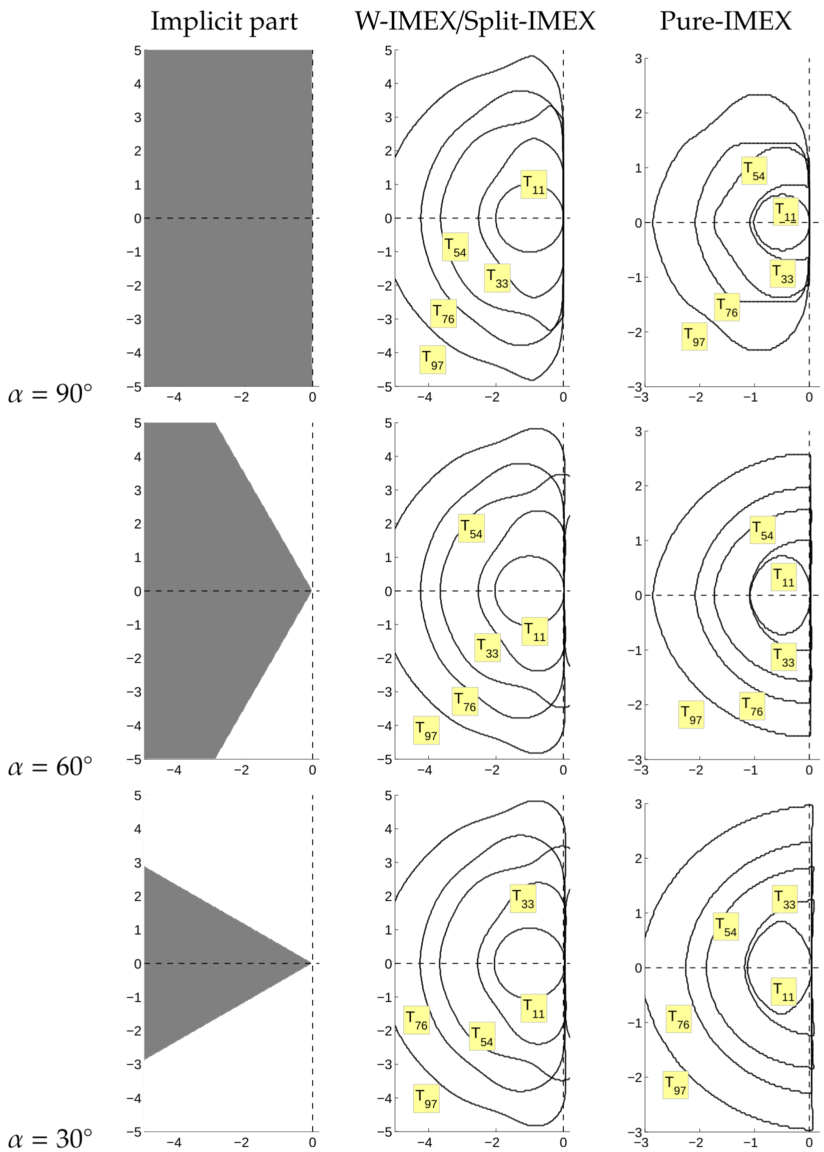


FIG. 2.1. *Stability region of the implicit part for A-stability and $A(\alpha)$-stability, $\alpha = 30°, 60°$ and the corresponding stability region of the explicit part for several extrapolated IMEX terms with base methods (2.4).*

This system can be analyzed in a singular perturbation problem (SPP) setting and obtain the reduced differential algebraic (DAE) form by taking $\varepsilon \to 0$:

$$\begin{pmatrix} y \\ 0 \end{pmatrix}' = \begin{pmatrix} f(y,z) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ g(y,z) \end{pmatrix}, \tag{3.4}$$

where $g(0) = g(y_0, z_0)$ and we assume

$$g_z \text{ is invertible}, \tag{3.5}$$

and hence (3.4) is an index-1 DAE.

In order to assess the accuracy of the extrapolated methods we first analyze the discretization of the reduced system (3.4) with the proposed extrapolated IMEX methods and then address the discretization of the full problem (3.3). We next discuss the consistency properties of extrapolated (2.4). We start with W-IMEX and continue with Pure-IMEX (sec. 3.2) and Split-IMEX (sec. 3.3).

3.1. W-IMEX. Applying the W-IMEX method (2.4b) with y the non-stiff and z the stiff components to (3.3) yields

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ 0 \end{pmatrix} + h \begin{pmatrix} 0 \\ g(y_i, z_i) \end{pmatrix} \text{ or}$$
$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix}, \tag{3.6}$$

Then the reduced form of (3.6) given by $\varepsilon \to 0$ is

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix}. \tag{3.7}$$

In order to assess the accuracy of the W-IMEX scheme we first analyze the reduced system (3.7) and then address the full problem (3.6) in Section 5.1. The following theorems and their proofs follow the ones for the extrapolated linearly implicit Euler method developed by Deuflhard et al. [1987] and briefly described in [Hairer et al., 1993b, chap. VI.5]. We start with the reduced problem (DAE) and give the following result.

Theorem 3.1 (Global error expansion of the extrapolated W-IMEX method applied to DAEs). *Consider problem (3.4) with consistent initial values* (y_0, z_0)*, and suppose that (3.5) is satisfied. The global error of the IMEX scheme (3.7) then has an asymptotic h-expansion of the form*

$$\begin{aligned} y_i - y(x_i) &= \sum_{j=1}^{M} h^j \left(a^{(j)}(x_i) + \alpha_i^{(j)} \right) + O\left(h^{M+1}\right) \\ z_i - z(x_i) &= \sum_{j=1}^{M} h^j \left(b^{(j)}(x_i) + \beta_i^{(j)} \right) + O\left(h^{M+1}\right) \end{aligned}, \tag{3.8}$$

where $a^{(j)}(x)$ *and* $b^{(j)}(x)$ *are smooth functions and the perturbations satisfy*

$$\alpha_i^{(1)} = 0\,,\ \alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 0\,, \tag{3.9a}$$
$$\alpha_i^{(3)} = 0\,,\ \alpha_i^{(4)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 1\,, \tag{3.9b}$$
$$\alpha_i^{(j)} = 0\,,\ \forall i \geq j-3\,,\ j \geq 5\,, \tag{3.9c}$$
$$\beta_i^{(j)} = 0\,,\ \forall i \geq j-2\,,\ j \geq 3\,. \tag{3.9d}$$

The error terms in (3.8) are uniformly bounded for $x_i = ih \le H$, if H is sufficiently small.

Proof. Following Deuflhard et al. [1987], the proof consists of two parts: in the first part (a) truncated expansions are constructed and in the second one (b) an error bound is obtained from a stability estimate.

a). Consider the truncated expansions of the numerical solution

$$\begin{aligned} \widehat{y_i} &= y(x_i) + \sum_{j=1}^{M} h^j \left(a^{(j)}(x_i) + \alpha_i^{(j)}\right) \\ \widehat{z_i} &= z(x_i) + \sum_{j=1}^{M} h^j \left(b^{(j)}(x_i) + \beta_i^{(j)}\right) \end{aligned} \tag{3.10}$$

such that the defect of $\widehat{y_i}$, $\widehat{z_i}$ inserted in the method (3.7) is small (see [Hairer and Lubich, 1984]):

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y_i} \\ \widehat{z}_{i+1} - \widehat{z_i} \end{pmatrix} = h \begin{pmatrix} f(\widehat{y_i}, \widehat{z_i}) \\ g(\widehat{y_i}, \widehat{z_i}) \end{pmatrix} + O\left(h^{M+2}\right). \tag{3.11}$$

The initial values are the exact solution ($\widehat{y_0} = y_0, \widehat{z_0} = z_0$) and we also assume that the perturbation terms (α, β) satisfy

$$a^{(j)}(0) + \alpha_0^{(j)} = 0\,, \qquad b^{(j)}(0) + \beta_0^{(j)} = 0\,, \tag{3.12a}$$

$$\alpha_i^{(j)} \to 0\,, \qquad \beta_i^{(j)} \to 0\,, \qquad \text{for } i \to \infty\,. \tag{3.12b}$$

The Taylor expansions for $f(\widehat{y_i}, \widehat{z_i})$ and $g(\widehat{y_i}, \widehat{z_i})$ about $(y(x_i), z(x_i))$ give

$$\begin{aligned} f\left(\widehat{y_i}, \widehat{z_i}\right) = {} & f\left(y(x_i), z(x_i)\right) + \\ & + f_y\left(x_i\right)\left(ha^{(1)}(x_i) + h\alpha_i^{(1)} + \dots\right) + f_z\left(x_i\right)\left(hb^{(1)}(x_i) + h\beta_i^{(1)} + \dots\right) + \\ & + f_{yy}\left(x_i\right)\left(ha^{(1)}(x_i) + h\alpha_i^{(1)} + \dots\right)^2 + \dots\,, \\ g\left(\widehat{y_i}, \widehat{z_i}\right) = {} & g\left(y(x_i), z(x_i)\right) + \\ & + g_y\left(x_i\right)\left(ha^{(1)}(x_i) + h\alpha_i^{(1)} + \dots\right) + g_z\left(x_i\right)\left(hb^{(1)}(x_i) + h\beta_i^{(1)} + \dots\right) + \\ & + g_{yy}\left(x_i\right)\left(ha^{(1)}(x_i) + h\alpha_i^{(1)} + \dots\right)^2 + \dots\,. \end{aligned}$$

Similarly,

$$\begin{aligned} \widehat{y}_{i+1} - \widehat{y_i} &= \underbrace{y(x_{i+1}) - y(x_i)}_{hy'(x_i) + \frac{h^2}{2}y''(x_i) + \dots} + h\Big(\underbrace{a^{(1)}(x_{i+1}) - a^{(1)}(x_i)}_{h\left(a^{(1)}\right)'(x_i) + \dots} + \alpha_{i+1}^{(1)} - \alpha_i^{(1)}\Big) + \dots \\ &= hy'(x_i) + \frac{h^2}{2}y''(x_i) + \dots + h^2\left(a^{(1)}\right)'(x_i) + h\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) + \dots \\ \widehat{z}_{i+1} - \widehat{z_i} &= z(x_{i+1}) - z(x_i) + h\left(b^{(1)}(x_{i+1}) - b^{(1)}(x_i) + \beta_{i+1}^{(1)} - \beta_i^{(1)}\right) + \dots \\ &= hz'(x_i) + \frac{h^2}{2}z''(x_i) + \dots + h^2\left(b^{(1)}\right)'(x_i) + h\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) + \dots \end{aligned}$$

Replacing the above in (3.11) yields

$$
\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \cdot
$$
$$
\cdot \begin{pmatrix} hy'(x_i) + \frac{h^2}{2}y''(x_i) + \cdots + h^2\left(a^{(1)}\right)'(x_i) + h\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) + h^3\left(a^{(2)}\right)'(x_i) + h^2\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) + \ldots \\ hz'(x_i) + \frac{h^2}{2}z''(x_i) + \cdots + h^2\left(b^{(1)}\right)'(x_i) + h\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) + \ldots \end{pmatrix} =
$$
$$
= \begin{pmatrix} hf\left(y(x_i), z(x_i)\right) + f_y(x_i)\left(h^2a^{(1)}(x_i) + h^2\alpha_i^{(1)} + \ldots\right) \\ hg\left(y(x_i), z(x_i)\right) + g_y(x_i)\left(h^2a^{(1)}(x_i) + h^2\alpha_i^{(1)} + \ldots\right) \end{pmatrix} +
$$
$$
+ \begin{pmatrix} f_z(x_i)\left(h^2b^{(1)}(x_i) + h^2\beta_i^{(1)} + \ldots\right) + \ldots \\ g_z(x_i)\left(h^2b^{(1)}(x_i) + h^2\beta_i^{(1)} + \ldots\right) + \ldots \end{pmatrix} + O\left(h^{M+2}\right). \tag{3.13}
$$

Equating coefficients of h^1 in (3.13) gives

$$
\begin{pmatrix} y'(x_i) + \left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) \\ 0 \end{pmatrix} = \begin{pmatrix} f\left(y(x_i), z(x_i)\right) \\ g\left(y(x_i), z(x_i)\right) \end{pmatrix}.
$$

Using the consistency requirement (3.12b) gives $\alpha_{i+1}^{(1)} = \alpha_i^{(1)}$ which verifies (3.4) and thus we have $\alpha_i^{(1)} = 0$, $\forall i \geq 0$. Next we consider the coefficients of h^2 in (3.13):

$$
\begin{pmatrix} \frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) + \left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) \\ -g_y(0)\,y'(x) - g_z(0)\,z'(x) - g_y(0)\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) - g_z(0)\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) \end{pmatrix} =
$$
$$
= \begin{pmatrix} f_y(x)\left(a^{(1)}(x) + \alpha_i^{(1)}\right) + f_z(x)\left(b^{(1)}(x) + \beta_i^{(1)}\right) \\ g_y(x)\left(a^{(1)}(x) + \alpha_i^{(1)}\right) + g_z(x)\left(b^{(1)}(x) + \beta_i^{(1)}\right) \end{pmatrix}
$$

or, by separating the smooth terms and the perturbations yields

$$
\begin{aligned}
&\frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) = f_y(x)\,a^{(1)}(x) + f_z(x)\,b^{(1)}(x)\,, \\
&-g_y(0)\,y'(x) - g_z(0)\,z'(x) = g_y(x)\,a^{(1)}(x) + g_z(x)\,b^{(1)}(x)\,, \\
&\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) = f_y(x)\,\alpha_i^{(1)} + f_z(x)\,\beta_i^{(1)}\,, \\
&-g_y(0)\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) - g_z(0)\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) = g_y(x)\,\alpha_i^{(1)} + g_z(x)\,\beta_i^{(1)}\,.
\end{aligned}
$$

These conditions can be simplified by using the consistency requirement $\alpha_i^{(1)} = 0$, $\forall i \geq 0$, and the fact that α and β do not depend on h (i.e., $f_z(x) \to f_z(0)$ and $g_z(x) \to g_z(0)$: The terms of $O(h)$ are considered in (3.14c) - (3.14d)), yields

$$
\frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) = f_y(x)\,a^{(1)}(x) + f_z(x)\,b^{(1)}(x)\,, \tag{3.14a}
$$
$$
-g_y(0)\,y'(x) - g_z(0)\,z'(x) = g_y(x)\,a^{(1)}(x) + g_z(x)\,b^{(1)}(x)\,, \tag{3.14b}
$$
$$
\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) = f_z(0)\,\beta_i^{(1)} + \gamma_i^{(2)}\,h\,, \tag{3.14c}
$$
$$
-g_z(0)\left(\beta_{i+1}^{(1)} - \cancel{\beta_i^{(1)}}\right) = \cancel{g_z(0)\,\beta_i^{(1)}} + \eta_i^{(2)}\,h\,. \tag{3.14d}
$$

The terms $\gamma_i^{(j)}$ and $\eta_i^{(j)}$, $\forall i, j$ are neglected for the rest of the proof. The system (3.14a)-(3.14b) can be solved in the following way. Compute $b^{(1)}(x)$ in (3.14b) using (3.5) to give

$$b^{(1)}(x) = -g_z(x)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) + g_y(x)\,a^{(1)}(x)\right],$$

and replace it in (3.14a):

$$\frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) = f_y(x)\,a^{(1)}(x) - f_z(x)\,g_z(x)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) + g_y(x)\,a^{(1)}(x)\right],$$

which leads to the following ODE in $a^{(1)}$

$$\left(a^{(1)}\right)'(x) + \left(f_z(x)\,g_z(x)^{-1}g_y(x) - f_y(x)\right)a^{(1)}(x) = -\frac{1}{2}y''(x) - f_z(x)\,g_z(x)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x)\right].$$

Using (3.12a); i.e., $a^{(1)}(0)+\alpha_0^{(1)} = 0$, and the fact that $\alpha_0^{(1)} = 0$ gives $a^{(1)}(0) = 0$. Therefore $a^{(1)}(x)$ and $b^{(1)}(x)$ are uniquely determined by (3.14a) and (3.14b). We continue with (3.14c) and (3.14d) and use $0 = g(y,z)$ for $x = 0$:

$$\frac{dg}{dx}\left(y(x), z(x)\right) = \frac{\partial g}{\partial y}\frac{\partial y}{\partial x}(x) + \frac{\partial g}{\partial z}\frac{\partial z}{\partial x}(x) = g_y y' + g_z z'.$$

The above expression is true for $x = 0$ and hence the left hand side of (3.14b) vanishes:

$$g_y(0)\,a^{(1)}(0) + g_z(0)\,b^{(1)}(0) = 0 \Rightarrow g_z(0)\,b^{(1)}(0) = 0 \Rightarrow b^{(1)}(0) = 0.$$

By (3.12a) we have that $\beta_0^{(1)} = 0$. In general, we have $\beta_i^{(1)} = 0$, $\forall i \geq 0$ due to (3.14d) and together with (3.14c) we obtain $\alpha_i^{(2)} = 0$, $\forall i \geq 0$.

To compare the coefficients of h^3 it is useful to extend (3.11) with one more term:

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \cdot \tag{3.15}$$
$$\cdot \begin{pmatrix} \frac{h^2}{2}y''(x_i) + \frac{h^3}{6}y'''(x_i) + h^2\left(a^{(1)}\right)'(x_i) + h^3\left(a^{(2)}\right)'(x_i) + h^2\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) + h^4\left(a^{(3)}\right)'(x_i) + h^3\left(\alpha_{i+1}^{(3)} - \alpha_i^{(3)}\right)\dots \\ \dots + \frac{h^2}{2}z''(x_i) + \frac{h^3}{6}z'''(x_i) + \dots + h^2\left(b^{(1)}\right)'(x_i) + h\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) + h^3\left(b^{(2)}\right)'(x_i) + h^2\left(\beta_{i+1}^{(2)} - \beta_i^{(2)}\right) + \dots \end{pmatrix} =$$
$$= \begin{pmatrix} \dots + hf_y(x_i)\left(\dots + h^2a^{(2)}(x_i) + h^2\alpha_i^{(2)} + \dots\right) + \frac{h}{2}f_{yy}(x_i)\left(\dots + h^2a^{(1)}(x_i) + h^2\alpha_i^{(1)} + \dots\right) \\ \dots + hg_y(x_i)\left(\dots + h^2a^{(2)}(x_i) + h^2\alpha_i^{(2)} + \dots\right) + \frac{h}{2}g_{yy}(x_i)\left(\dots + h^2a^{(1)}(x_i) + h^2\alpha_i^{(1)} + \dots\right) \end{pmatrix} +$$
$$+ \begin{pmatrix} hf_z(x_i)\left(\dots + h^2b^{(2)}(x_i) + h^2\beta_i^{(2)} + \dots\right) + \frac{h}{2}f_{zz}(x_i)\left(\dots + h^2b^{(1)}(x_i) + h^2\beta_i^{(1)} + \dots\right) + \dots \\ hg_z(x_i)\left(\dots + h^2b^{(2)}(x_i) + h^2\beta_i^{(2)} \dots\right) + \frac{h}{2}g_{zz}(x_i)\left(\dots + h^2b^{(1)}(x_i) + h^2\beta_i^{(1)} \dots\right) + \dots \end{pmatrix},$$

where some contributions of the derivatives f_{yy}, f_{zz}, and f_{yz} are zero due to the fact that their factors are ($\alpha_i^{(1)}$, $\alpha_i^{(2)}$, and $\beta_i^{(1)}$, $\forall i \geq 0$) zero. Then the coefficients of h^3 in (3.15) give

$$\left(a^{(2)}\right)'(x) = f_y(x)\,a^{(2)}(x) + f_z(x)\,b^{(2)}(x) + r^{(2)}(x), \tag{3.16a}$$
$$0 = g_y(x)\,a^{(2)}(x) + g_z(x)\,b^{(2)}(x) + s^{(2)}(x), \tag{3.16b}$$

where $r^{(2)}(x)$ and $s^{(2)}(x)$ are known functions which depend on the derivatives of $y(x)$,

$z(x)$, $a^{(1)}(x)$, $b^{(1)}(x)$, and can be shown to be

$$r^{(2)}(x) = -\frac{1}{6}y'''(x) + \tag{3.17a}$$
$$+ \frac{1}{2}f_{yy}(x)\left(a^{(1)}\right)^2(x) + \frac{1}{2}f_{zz}(x)\left(b^{(1)}\right)^2(x) + f_{yz}(x)a^{(1)}(x)b^{(1)}(x)\,,$$
$$s^{(2)}(x) = \frac{1}{2}g_y(0)y''(x) + \frac{1}{2}g_z(0)z''(x) + g_y(0)\left(a^{(1)}\right)'(x) + g_z(0)\left(b^{(1)}\right)'(x) + \tag{3.17b}$$
$$+ \frac{1}{2}g_{yy}(x)\left(a^{(1)}\right)^2(x) + \frac{1}{2}g_{zz}(x)\left(b^{(1)}\right)^2(x) + g_{yz}(x)a^{(1)}(x)b^{(1)}(x)\,.$$

The perturbations can be expressed as

$$\alpha_{i+1}^{(3)} - \alpha_i^{(3)} = f_y(0)\alpha_i^{(2)} + f_z(0)\beta_i^{(2)}\,,$$
$$-g_y(0)\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) - g_z(0)\left(\beta_{i+1}^{(2)} - \beta_i^{(2)}\right) = g_y(0)\alpha_i^{(2)} + g_z(0)\beta_i^{(2)}\,,$$

with additional cancellations of terms that have coefficients $\alpha_i^{(1)} = 0$ and $\beta_i^{(1)} = 0$, $\forall i$, and using $\alpha_i^{(2)} = 0$, $\forall i$ lead to

$$\alpha_{i+1}^{(3)} - \alpha_i^{(3)} = f_z(0)\beta_i^{(2)}\,, \tag{3.18a}$$
$$0 = g_z(0)\beta_{i+1}^{(2)}\,. \tag{3.18b}$$

Terms $a^{(2)}(x)$ and $b^{(2)}(x)$ are determined in the same way as $a^{(1)}(x)$ and $b^{(1)}(x)$. Now we have

$$b^{(2)}(x) = -g_z(x)^{-1}\left[g_y(x)\,a^{(2)}(x) + s^{(2)}(x)\right]\,, \tag{3.19a}$$

which can be inserted in (3.16a) to give the following linear differential equation

$$\left(a^{(2)}\right)'(x) + \left(f_z(x)\,g_z(x)^{-1}g_y(x) - f_y(x)\right)a^{(2)}(x) = -f_z(x)\,g_z(x)^{-1}g_y(x)\,s^{(2)}(x) + r^{(2)}(x)\,. \tag{3.19b}$$

Since $\alpha_i^{(2)} = 0$, $\forall i$ we have $a^{(2)}(0) = 0$ and thus expressions (3.19) determine $a^{(2)}(x)$ and $b^{(2)}(x)$ uniquely. However, $b^{(2)}(0) \neq 0$ in general and by (3.12a) we have that $\beta_0^{(2)} \neq 0$. From (3.18b) we get $\beta_i^{(2)} = 0$, $\forall i \geq 1$, and together with (3.18a) we obtain that $\alpha_i^{(3)} = 0$, $\forall i \geq 1$.

For the coefficients of h^4 we obtain a similar result as in the previous step:

$$\left(a^{(3)}\right)'(x) = f_y(x)\,a^{(3)}(x) + f_z(x)\,b^{(3)}(x) + r^{(3)}(x)\,, \tag{3.20a}$$
$$0 = g_y(x)\,a^{(3)}(x) + g_z(x)\,b^{(3)}(x) + s^{(3)}(x)\,, \tag{3.20b}$$
$$\alpha_{i+1}^{(4)} - \alpha_i^{(4)} = f_z(0)\beta_i^{(3)} + f_y(0)\alpha_i^{(3)}\,, \tag{3.20c}$$
$$0 = g_z(0)\beta_{i+1}^{(3)} + g_y(0)\alpha_{i+1}^{(3)}\,. \tag{3.20d}$$

The expressions for $r^{(3)}(x)$ and $s^{(3)}(x)$ are more complicated (depending on derivatives of $y(x)$, $z(x)$, $a^{(\ell)}(x)$, $b^{(\ell)}(x)$, $\ell = 1\,,2$) and their representation is not shown here. Using (3.12b), the conclusions, however, are that $\beta_i^{(3)} = 0$, $\forall i \geq 1$, and $\alpha_i^{(4)} = 0$, $\forall i \geq 1$.

$\alpha_i^{(j)}$	$i=0$	1	2	3	4	5	6
	y_0	y_1	y_2	y_3	y_4	y_5	y_6
$j=1$	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	•	0	0	0	0	0	0
4	•	0	0	0	0	0	0
5	•	•	0	0	0	0	0
6	•	•	•	0	0	0	0
7	•	•	•	•	0	0	0

$\beta_i^{(j)}$	$i=0$	1	2	3	4	5	6
	z_0	z_1	z_2	z_3	z_4	z_5	z_6
-							
$j=1$	0	0	0	0	0	0	0
2	•	0	0	0	0	0	0
3	•	0	0	0	0	0	0
4	•	•	0	0	0	0	0
5	•	•	•	0	0	0	0
6	•	•	•	•	0	0	0

TABLE 3.1
Non-zero α and β values represented with "•" marker.

A general recurrence formula can be constructed for the coefficients of h^{j+1}, $\forall j \geq 4$:

$$\left(a^{(j)}\right)'(x) = f_y(x)\, a^{(j)}(x) + f_z(x)\, b^{(j)}(x) + r^{(j)}(x)\,, \tag{3.21a}$$

$$0 = g_y(x)\, a^{(j)}(x) + g_z(x)\, b^{(j)}(x) + s^{(j)}(x)\,, \tag{3.21b}$$

$$\alpha_{i+1}^{(j+1)} - \alpha_i^{(j+1)} = f_z(0)\beta_i^{(j)} + \varrho_i^{(j)}\,, \tag{3.21c}$$

$$0 = g_z(0)\beta_{i+1}^{(j)} + \sigma_i^{(j)}\,, \tag{3.21d}$$

where $\varrho_i^{(j)}$ and $\sigma_i^{(j)}$ are linear combinations of expressions which contain as factors $\alpha_{i+1}^{(\ell)}, \alpha_{i+1}^{(\ell-1)}, \beta_{i+1}^{(\ell-1)}, \ell \leq j$. For instance, we have

$$\begin{aligned}
\varrho_i^{(3)} &= \alpha_i^{(3)} f_y(0) \text{ and } \sigma_i^{(3)} = \cancel{\alpha_{i+1}^{(3)} g_y(0)}\,,\\
\varrho_i^{(4)} &= \alpha_i^{(4)} f_y(0) + \frac{1}{2} f_{zz}(0)\left(\beta_i^{(2)}\right)^2 \text{ and } \sigma_i^{(4)} = \cancel{\alpha_{i+1}^{(4)} g_y(0)} + \frac{1}{2} g_{zz}(0)\left(\beta_i^{(2)}\right)^2\,,\\
\varrho_i^{(5)} &= \alpha_i^{(5)} f_y(0) + f_{zz}(0)\beta_i^{(2)}\beta_i^{(3)} + f_{yz}(0)\alpha_i^{(3)}\beta_i^{(2)} \text{ and } \sigma_i^{(5)} = \alpha_{i+1}^{(5)} g_y(0) + g_{zz}(0)\beta_i^{(2)}\beta_i^{(3)}\,,\\
\varrho_i^{(6)} &= \alpha_i^{(6)} f_y(0) + \frac{1}{2}\alpha_i^{(3)^2} f_{yy}(0) + \left(\alpha_i^{(4)}\beta_i^{(2)} + \alpha_i^{(3)}\beta_i^{(3)}\right) f_{yz}(0) +\\
&\quad + \frac{1}{2}\left(\beta_i^{(3)^2} + 2\beta_i^{(2)}\beta_i^{(4)}\right) f_{zz}(0) + \frac{1}{6}\beta_i^{(2)^3} f_{zzz}(0) \text{ and}\\
\sigma_i^{(6)} &= \alpha_{i+1}^{(6)} g_y(0) + \frac{1}{2}\alpha_i^{(3)^2} g_{yy}(0) + \left(\alpha_i^{(4)}\beta_i^{(2)} + \alpha_i^{(3)}\beta_i^{(3)}\right) g_{yz}(0) +\\
&\quad + \frac{1}{2}\left(\beta_i^{(3)^2} + 2\beta_i^{(2)}\beta_i^{(4)}\right) g_{zz}(0) + \frac{1}{6}\beta_i^{(2)^3} g_{zzz}(0)\,.
\end{aligned}$$

To conclude, let us consider the ϱ and σ values for i and j in Table 3.2 based on the values of α and β in Table 3.1. Here we show the non-zero coefficients of h^j, $1 \leq j \leq 7$.

Finally, we use induction on j with the hypothesis that $\varrho_i^{(j)} = 0$ and $\sigma_i^{(j)} = 0$ for $i \geq j-3$. Equation (3.21d) implies that $\beta_{i+1}^{(j)} = 0$, $i \geq j-3$ and then relations (3.12b) and (3.21c) give $\alpha_{i+1}^{(j+1)} = 0$, $i \geq j-3$. This concludes the proof for (3.9c) and (3.9d).

b). The second part of this proof consists in estimating a bound on the reminder term; i.e., differences $\Delta y_i = y_i - \widehat{y_i}$ and $\Delta z_i = z_i - \widehat{z_i}$. Subtracting (3.11) from (3.7) and eliminating Δy_i and Δz_i yields

$\varrho_i^{(j)}$	$i=0$	1	2	3	4	5	6
	y_0	y_1	y_2	y_3	y_4	y_5	y_6
$j=1$	0	0	0	0	0	0	0
$2(h^2)$	0	0	0	0	0	0	0
$3(h^3)$	•	0	0	0	0	0	0
$4(h^4)$	•	0	0	0	0	0	0
$5(h^5)$	•	•	0	0	0	0	0
$6(h^6)$	•	•	0	0	0	0	0

$\sigma_i^{(j)}$	$i=0$	1	2	3	4	5	6
	z_0	z_1	z_2	z_3	z_4	z_5	z_6
$j=1$	0	0	0	0	0	0	0
$2(h^2)$	0	0	0	0	0	0	0
$3(h^3)$	0	0	0	0	0	0	0
$4(h^4)$	•	0	0	0	0	0	0
$5(h^5)$	•	0	0	0	0	0	0
$6(h^6)$	•	0	0	0	0	0	0

Table 3.2

Non-zero ϱ and σ values represented with "•" marker.

$$
\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1}-y_i \\ z_{i+1}-z_i \end{pmatrix} - \begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1}-\widehat{y}_i \\ \widehat{z}_{i+1}-\widehat{z}_i \end{pmatrix} =
$$

$$
= h \begin{pmatrix} f(y_i,z_i) \\ g(y_i,z_i) \end{pmatrix} - h \begin{pmatrix} f(\widehat{y}_i,\widehat{z}_i) \\ g(\widehat{y}_i,\widehat{z}_i) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+2}\right) \end{pmatrix},
$$

$$
\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} - \begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} =
$$

$$
= h \begin{pmatrix} f(y_i,z_i) - f(\widehat{y}_i,\widehat{z}_i) \\ g(y_i,z_i) - g(\widehat{y}_i,\widehat{z}_i) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+2}\right) \end{pmatrix},
$$

$$
\begin{pmatrix} I & 0 \\ -g_y(0) & -g_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} = \begin{pmatrix} I & 0 \\ -g_y(0) & -g_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} +
$$

$$
+ \begin{pmatrix} h\left(f(y_i,z_i) - f(\widehat{y}_i,\widehat{z}_i)\right) \\ g(y_i,z_i) - g(\widehat{y}_i,\widehat{z}_i) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix},
$$

$$
\begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} = \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} + \begin{pmatrix} I & 0 \\ -g_y(0) & -g_z(0) \end{pmatrix}^{-1} \begin{pmatrix} h\left(f(y_i,z_i) - f(\widehat{y}_i,\widehat{z}_i)\right) \\ g(y_i,z_i) - g(\widehat{y}_i,\widehat{z}_i) \end{pmatrix} +
$$

$$
+ \begin{pmatrix} I & 0 \\ -g_y(0) & -g_z(0) \end{pmatrix}^{-1} \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix},
$$

$$
\begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} = \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} + \begin{pmatrix} I & 0 \\ \mathcal{O}(1) & -g_z(0)^{-1} \end{pmatrix} \begin{pmatrix} h\left(f(y_i,z_i) - f(\widehat{y}_i,\widehat{z}_i)\right) \\ g(y_i,z_i) - g(\widehat{y}_i,\widehat{z}_i) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix}.
$$

The application of the Lipschitz condition on $f(y,z)$ and $g(y,z)$ gives

$$
\begin{pmatrix} \left\|\Delta y_{i+1}\right\| \\ \left\|\Delta z_{i+1}\right\| \end{pmatrix} \le \begin{pmatrix} I & 0 \\ \mathcal{O}(1) & \zeta \end{pmatrix} \begin{pmatrix} \left\|\Delta y_i\right\| \\ \left\|\Delta z_i\right\| \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix}, \tag{3.22}
$$

where $|\zeta| < 1$ if H is sufficiently small. Using Lemma C.1 (see Appendix C) gives $\left\|\Delta y_i\right\| + \left\|\Delta z_i\right\| = \mathcal{O}\left(h^{M+1}\right)$. □

Next we continue to investigate the orders for the extrapolation with base method (3.7). The following (harmonic) sequence is considered $n_j = \{1, 2, 3, \ldots\}$ and $h_j = H/n_j$. We define the components

$$
Y_{jk} = y_{h_j}(x_0 + H), \qquad Z_{jk} = z_{h_j}(x_0 + H), \tag{3.23}
$$

$\alpha^{(1)}_{\{1\}}$	$\cancel{a^{(2)}(\cdot)}$	$\cancel{a^{(3)}(\cdot)}$	$\cancel{a^{(4)}(\cdot)}$	$\cancel{a^{(5)}(\cdot)}$	$\cancel{a^{(6)}(\cdot)}$	$\cancel{a^{(7)}(\cdot)}$
$\alpha^{(1)}_{\{2\}}$	$\alpha^{(2)}_{\{1,2\}}$					
$\alpha^{(1)}_{\{3\}}$	$\alpha^{(2)}_{\{2,3\}}$	$\alpha^{(3)}_{\{1,2,3\}}$				
$\alpha^{(1)}_{\{4\}}$	$\alpha^{(2)}_{\{3,4\}}$	$\alpha^{(3)}_{\{2,3,4\}}$	$\alpha^{(4)}_{\{1,2,3,4\}}$			
$\alpha^{(1)}_{\{5\}}$	$\alpha^{(2)}_{\{4,5\}}$	$\alpha^{(3)}_{\{3,4,5\}}$	$\alpha^{(4)}_{\{2,3,4,5\}}$	$\alpha^{(5)}_{\{1,2,3,4,5\}}$		
$\alpha^{(1)}_{\{6\}}$	$\alpha^{(2)}_{\{5,6\}}$	$\alpha^{(3)}_{\{4,5,6\}}$	$\alpha^{(4)}_{\{3,4,5,6\}}$	$\alpha^{(5)}_{\{2,3,4,5,6\}}$	$\alpha^{(6)}_{\{1,2,3,4,5,6\}}$	
$\alpha^{(1)}_{\{7\}}$	$\alpha^{(2)}_{\{6,7\}}$	$\alpha^{(3)}_{\{5,6,7\}}$	$\alpha^{(4)}_{\{4,5,6,7\}}$	$\alpha^{(5)}_{\{3,4,5,6,7\}}$	$\alpha^{(6)}_{\{2,3,4,5,6,7\}}$	$\alpha^{(7)}_{\{1,2,3,4,5,6,7\}}$

Perturbation coefficients for y_{jk}

$\beta^{(1)}_{\{1\}}$	$\cancel{b^{(2)}(\cdot)}$	$\cancel{b^{(3)}(\cdot)}$	$\cancel{b^{(4)}(\cdot)}$	$\cancel{b^{(5)}(\cdot)}$	$\cancel{b^{(6)}(\cdot)}$	$\cancel{b^{(7)}(\cdot)}$
$\beta^{(1)}_{\{2\}}$	$\beta^{(2)}_{\{1,2\}}$					
$\beta^{(1)}_{\{3\}}$	$\beta^{(2)}_{\{2,3\}}$	$\beta^{(3)}_{\{1,2,3\}}$				
$\beta^{(1)}_{\{4\}}$	$\beta^{(2)}_{\{3,4\}}$	$\beta^{(3)}_{\{2,3,4\}}$	$\beta^{(4)}_{\{1,2,3,4\}}$			
$\beta^{(1)}_{\{5\}}$	$\beta^{(2)}_{\{4,5\}}$	$\beta^{(3)}_{\{3,4,5\}}$	$\beta^{(4)}_{\{2,3,4,5\}}$	$\beta^{(5)}_{\{1,2,3,4,5\}}$		
$\beta^{(1)}_{\{6\}}$	$\beta^{(2)}_{\{5,6\}}$	$\beta^{(3)}_{\{4,5,6\}}$	$\beta^{(4)}_{\{3,4,5,6\}}$	$\beta^{(5)}_{\{2,3,4,5,6\}}$	$\beta^{(6)}_{\{1,2,3,4,5,6\}}$	
$\beta^{(1)}_{\{7\}}$	$\beta^{(2)}_{\{6,7\}}$	$\beta^{(3)}_{\{5,6,7\}}$	$\beta^{(4)}_{\{4,5,6,7\}}$	$\beta^{(5)}_{\{3,4,5,6,7\}}$	$\beta^{(6)}_{\{2,3,4,5,6,7\}}$	$\beta^{(7)}_{\{1,2,3,4,5,6,7\}}$

Perturbation coefficients for z_{jk}

Table 3.3

Extrapolated perturbation error propagation. The entries represent the perturbations that affect the solutions in the extrapolation tableau.

which represent the numerical solution of (3.4) after j steps with step size h_j, extrapolated with (2.3a); i.e., on the k^{th} column of the extrapolation tableau. We make the following remarks that will aid the understanding of the next result.

1. Each extrapolation step (2.3a) cancels one smooth term ($\{a, b\}^{(j)}$) from the error expansion (3.8).
2. The perturbations α and β propagate through the extrapolation steps (2.3a) in the form described by Table 3.3. Furthermore, we note that the accuracy of the solution on the extrapolation tableau diagonal is affected by terms $\{\alpha, \beta\}_1^{(j)}$.
3. Nonzero smooth terms $a(0)$ and $b(0)$ affect the perturbations α_0 and β_0 through (3.12a); e.g., $b^{(2)}(0) \neq 0 \Rightarrow \beta_0^{(2)} \neq 0$.

We prove the following result which follows the theorems presented in [Hairer et al., 1993b, chap. VI, Thm. 5.4] or in [Deuflhard et al., 1987].

Theorem 3.2 (Accuracy for the extrapolated W-IMEX applied to DAEs). *If we consider the harmonic sequence $\{1, 2, 3, \dots\}$, then the extrapolated values Y_{jk} and Z_{jk} satisfy*

$$Y_{jk} - y(x_0 + h) = O\left(H^{r_{jk}}\right), \qquad Z_{jk} - z(x_0 + h) = O\left(H^{s_{jk}}\right), \tag{3.24}$$

where the differential-algebraic orders r_{jk} and s_{jk} are given in Table 3.4 up to $j = 12$, $k = 12$.

<table>
<tr><td>1</td><td>**2**|**2**|**2**|**2**</td><td>$\cancel{a^{(2)}(\cdot)}$</td><td>$\cancel{a^{(3)}(\cdot)}$</td><td>$\cancel{a^{(4)}(\cdot)}$</td><td>$\cancel{a^{(5)}(\cdot)}$</td><td>$\cancel{a^{(6)}(\cdot)}$</td><td>$\cancel{a^{(7)}(\cdot)}$</td><td>$\cancel{a^{(8)}(\cdot)}$</td><td>$\cancel{a^{(9)}(\cdot)}$</td><td>$\cancel{a^{(10)}(\cdot)}$</td><td>$\cancel{a^{(11)}(\cdot)}$</td><td>$\cancel{a^{(12)}(\cdot)}$</td></tr>
<tr><td>2</td><td>2|2|2|2</td><td>**3**|**3**|**2**|**3**</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>3</td><td>2|2|2|2</td><td>3|3|2|3</td><td>**4**|**3**|**3**|**3**</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>4</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|**3**|3</td><td>**5**|**4**|3|**4**</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>5</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|**3**|3</td><td>5|4|4|**4**</td><td>**5**|**5**|3|4</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>6</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|**4**|4</td><td>**5**|**5**|4|**5**</td><td>6|5|3|4</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>7</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|**4**|4</td><td>5|5|5|**5**</td><td>**6**|**6**|4|5</td><td>6|5|3|4</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>8</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|**5**|5</td><td>**6**|**6**|5|**6**</td><td>7|6|4|5</td><td>6|5|3|4</td><td></td><td></td><td></td><td></td></tr>
<tr><td>9</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|**5**|5</td><td>6|6|6|**6**</td><td>**7**|**7**|5|6</td><td>7|6|4|4</td><td>6|5|3|4</td><td></td><td></td><td></td></tr>
<tr><td>10</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|**6**|6</td><td>**7**|**7**|6|**7**</td><td>8|7|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td><td></td><td></td></tr>
<tr><td>11</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|**6**|6</td><td>7|7|7|**7**</td><td>**8**|**8**|6|7</td><td>8|7|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td><td></td></tr>
<tr><td>12</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|6|6</td><td>7|7|**7**|7</td><td>**8**|**8**|7|**8**</td><td>9|8|6|7</td><td>8|7|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td></tr>
<tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td><td>6</td><td>7</td><td>8</td><td>9</td><td>10</td><td>11</td><td>12</td></tr>
</table>

Orders (r_{jk}) for component y_{jk} for Linearly implicit|W-IMEX|Pure-IMEX|Split-IMEX

<table>
<tr><td>1</td><td>**2**|**2**|**1**|**2**</td><td>$\cancel{b^{(2)}(\cdot)}$</td><td>$\cancel{b^{(3)}(\cdot)}$</td><td>$\cancel{b^{(4)}(\cdot)}$</td><td>$\cancel{b^{(5)}(\cdot)}$</td><td>$\cancel{b^{(6)}(\cdot)}$</td><td>$\cancel{b^{(7)}(\cdot)}$</td><td>$\cancel{b^{(8)}(\cdot)}$</td><td>$\cancel{b^{(9)}(\cdot)}$</td><td>$\cancel{b^{(10)}(\cdot)}$</td><td>$\cancel{b^{(11)}(\cdot)}$</td><td>$\cancel{b^{(12)}(\cdot)}$</td></tr>
<tr><td>2</td><td>2|2|1|2</td><td>**2**|**2**|**2**|**2**</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>3</td><td>2|2|1|2</td><td>2|2|2|2</td><td>**3**|**3**|**2**|**3**</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>4</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|**3**|3</td><td>**4**|**4**|2|**3**</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>5</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|**3**|3</td><td>4|4|3|**4**</td><td>**4**|**4**|2|3</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>6</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|**4**|4</td><td>**5**|**5**|3|**4**</td><td>4|4|2|3</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>7</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|**4**|4</td><td>5|5|4|**5**</td><td>**5**|**5**|3|4</td><td>4|4|2|3</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>8</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|4|4</td><td>5|5|**5**|5</td><td>**6**|**6**|4|**5**</td><td>5|5|3|4</td><td>4|4|2|3</td><td></td><td></td><td></td><td></td></tr>
<tr><td>9</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|4|4</td><td>5|5|**5**|5</td><td>6|6|5|**6**</td><td>**6**|**6**|4|5</td><td>5|5|3|4</td><td>4|4|2|3</td><td></td><td></td><td></td></tr>
<tr><td>10</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|4|4</td><td>5|5|5|5</td><td>6|6|**6**|6</td><td>**7**|**7**|5|**6**</td><td>6|6|4|5</td><td>5|5|3|4</td><td>4|4|2|3</td><td></td><td></td></tr>
<tr><td>11</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|4|4</td><td>5|5|5|5</td><td>6|6|**6**|6</td><td>7|7|6|**7**</td><td>**7**|**7**|5|6</td><td>6|6|4|5</td><td>5|5|3|4</td><td>4|4|2|3</td><td></td></tr>
<tr><td>12</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|3|3</td><td>4|4|4|4</td><td>5|5|5|5</td><td>6|6|6|6</td><td>7|7|**7**|7</td><td>**8**|**8**|6|**7**</td><td>7|7|5|6</td><td>6|6|4|5</td><td>5|5|3|4</td><td>4|4|2|3</td></tr>
<tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td><td>6</td><td>7</td><td>8</td><td>9</td><td>10</td><td>11</td><td>12</td></tr>
</table>

Orders (s_{jk}) for component z_{jk} for Linearly implicit|W-IMEX|Pure-IMEX|Split-IMEX

TABLE 3.4

Theoretical local extrapolation orders for linearly implicit, W-IMEX, Pure-IMEX, and Split-IMEX methods for index-1 DAEs. Bold face fonts represent the "best" or optimal choice for a given number of steps.

Proof. We use the expansion (3.8). It follows from (3.9a) (i.e., $\alpha_i^{(1)} = \beta_i^{(1)} = 0$) and from (3.12a) that $a(x_0) = 0$ and $b(x_0) = 0$. Since $a^{(j)}(x)$ and $b^{(j)}(x)$ are smooth functions, we obtain $a^{(1)}(x_0+H) = O(H)$ and $b^{(1)}(x_0+H) = O(H)$ and thus the errors in Y_{j1} and Z_{j1} are of $O(H^2)$, which gives the first column entries in Table 3.4 for the W-IMEX scheme. In the same way we deduce that $a^{(2)}(x_0 + h) = O(H)$; however, since $\beta_0^{(2)} \neq 0$, by (3.12a) we have that $b^{(2)}(0) \neq 0$ (in general), and $b^{(2)}(x_0 + h) = O(1)$. One extrapolation of the numerical method eliminates the terms with $j = 1$ in (3.8). The error is thus $O(H^3)$ for Y_{j2} and $O(H^2)$ for Z_{j2}. Equivalently, if we expand (3.8) to

$$\begin{cases} y_1 - y(x_1) = h^1 \left(a^{(1)}(x_1) + \alpha_1^{(1)}\right) + h^2 \left(a^{(2)}(x_1) + \alpha_1^{(2)}\right) + \ldots \\ z_1 - z(x_1) = h^1 \left(b^{(1)}(x_1) + \beta_1^{(1)}\right) + h^2 \left(b^{(2)}(x_1) + \beta_1^{(2)}\right) + \ldots \end{cases},$$

which gives

$$\begin{cases} y_1 - y(x_1) = h^1 \left(O(H) + 0\right) + \cdots = O\left(H^2\right) \\ z_1 - z(x_1) = h^1 \left(O(H) + 0\right) + \cdots = O\left(H^2\right) \end{cases}.$$

However, for $j = 2$ we have $a^{(2)}(x_0 + h) = O(H)$ and $b^{(2)}(x_0 + h) = O(1)$, and thus

$$\begin{cases} y_1 - y(x_1) = h^2 \left(O(H) + 0\right) + \cdots = O\left(H^3\right) \\ z_1 - z(x_1) = h^2 \left(O(1) + 0\right) + \cdots = O\left(H^2\right) \end{cases}.$$

If we continue, the smooth parts of (3.8) are eliminated one by one; however, the perturbations are not, and the approximation orders are reduced as follows. One order is "lost" on columns y_{j3} and z_{j2} due to $O(1)$ smooth part expansion, however, thereafter the orders are increasing by using the extrapolation formula (2.3a) that cancels the smooth terms. The nonzero perturbation terms affect the orders of the extrapolation method by propagating through (2.3a) as shown in Table 3.3. Specifically, for y_{jk} components we have: $\alpha_1^{(5)} \neq 0$ which limits the order on the diagonal for y_{jj}, $j \geq 6$ to 4. Using the same argument, it can be shown that the first sub-diagonal $y_{j\,j-1}$, $j \geq 8$ is limited to 5 and the second one $y_{j\,j-2}$, $j \geq 10$ is limited to 6 due to $\alpha_2^{(6)} \neq 0$ and $\alpha_3^{(7)} \neq 0$, respectively, and so on. Similarly, for z_{jk} components we have z_{jj}, $j \geq 5$ to 3; $z_{j\,j-1}$, $j \geq 7$ to 4; and $z_{j\,j-2}$, $j \geq 9$ to 5, due to $\beta_1^{(4)} \neq 0$, $\beta_2^{(5)} \neq 0$, and $\beta_3^{(6)} \neq 0$, respectively. This process can be continued to find all the entries in Table 3.4. □

Of particular interest is the location of the term in the extrapolation tableau that yields the maximum order of accuracy for a given number of steps j; i.e., the column that has the highest power of H for a given row number. A quick inspection of Table 3.4 reveals that the best choice is $T_{j,j}$ for $j \leq 4$; $T_{j,(j-1)/2+3}$ for $j \geq 5$ and odd; and $T_{j,\,j/2+2}$ for $j \geq 6$ and even. We used bold face fonts to identify the location of the most accurate yielding extrapolation tableau term. In Table 3.4 we also show the theoretical orders for the extrapolated linearly implicit Euler method (2.4a) as described in [Hairer et al., 1993b; Deuflhard et al., 1987]. The "best" terms are selected by first identifying the most accurate stiff components and then matching them with the best non-stiff counterparts.

We next investigate the error expansion for the other two proposed extrapolated methods.

3.2. Pure-IMEX Method. Applying the Pure-IMEX method (2.4c) to (3.3) yields

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} f(y_i, z_i) + hg(y_i, z_i) \text{ or}$$
$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) - hg_y(0) f(y_i, z_i) \end{pmatrix}, \tag{3.25}$$

The reduced form given by $\varepsilon \to 0$ is

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) - hg_y(0) f(y_i, z_i) \end{pmatrix}, \tag{3.26}$$

or

$$\begin{pmatrix} I & 0 \\ 0 & -hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix}. \tag{3.27}$$

We next formulate a similar pair of theorems (error expansions and extrapolated orders) for the extrapolated Pure-IMEX method.

Theorem 3.3 (Global error expansion of the extrapolated Pure-IMEX method applied to DAEs). *Consider problem (3.4) with consistent initial values* (y_0, z_0), *and suppose that (3.5) is satisfied. The global error of the Pure-IMEX scheme (3.26) then has an asymptotic h-expansion of the form (3.8) with* $a^{(j)}(x)$ *and* $b^{(j)}(x)$ *are smooth functions and the perturbations satisfy*

$$\alpha_i^{(1)} = 0\,,\ \forall i \geq 0\,, \tag{3.28a}$$
$$\alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 1\,,\ \alpha_i^{(3)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 2\,, \tag{3.28b}$$
$$\alpha_i^{(j)} = 0\,,\ \forall i \geq j-1\,,\ j \geq 4\,, \tag{3.28c}$$
$$\beta_i^{(j)} = 0\,,\ \forall i \geq j\,,\ j \geq 3\,. \tag{3.28d}$$

The error terms in (3.8) are uniformly bounded for $x_i = ih \leq H$, *if H is sufficiently small.*

Proof. This proof follows the same ideas used in the proof of Theorem 3.1. We begin with part (a) in which the truncated expansions are constructed. The second part can be shown easily following the same steps as in the W-IMEX method. We shall focus on the first part only.

We consider again the truncated expansions (3.10) with small defects

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y}_i \\ \widehat{z}_{i+1} - \widehat{z}_i \end{pmatrix} = h \begin{pmatrix} f(\widehat{y}_i, \widehat{z}_i) \\ g(\widehat{y}_i, \widehat{z}_i) - hg_y(0) f(\widehat{y}_i, \widehat{z}_i) \end{pmatrix} + O\left(h^{M+1}\right). \tag{3.29}$$

The initial values are exact and the perturbation terms satisfy (3.12). Replacing the

Taylor expansion for $f(\widehat{y_i},\widehat{z_i})$ and $g(\widehat{y_i},\widehat{z_i})$ about $(y(x_i),z(x_i))$ in (3.29) yields

$$
\begin{aligned}
&\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \cdot \qquad (3.30)\\
&\cdot \begin{pmatrix} hy'(x_i) + \frac{h^2}{2}y''(x_i) + \cdots + h^2\left(a^{(1)}\right)'(x_i) + h\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) + h^3\left(a^{(2)}\right)'(x_i) + h^2\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) + \dots \\ hz'(x_i) + \frac{h^2}{2}z''(x_i) + \cdots + h^2\left(b^{(1)}\right)'(x_i) + h\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) + \dots \end{pmatrix} = \\
&= \begin{pmatrix} hf\left(y(x_i),z(x_i)\right) + f_y\left(x_i\right)\left(h^2 a^{(1)}(x_i) + h^2\alpha_i^{(1)} + \dots\right) \\ hg\left(y(x_i),z(x_i)\right) + g_y\left(x_i\right)\left(h^2 a^{(1)}(x_i) + h^2\alpha_i^{(1)} + \dots\right) \end{pmatrix} + \\
&+ \begin{pmatrix} f_z\left(x_i\right)\left(h^2 b^{(1)}(x_i) + h^2\beta_i^{(1)} + \dots\right) + \dots \\ g_z\left(x_i\right)\left(h^2 b^{(1)}(x_i) + h^2\beta_i^{(1)} + \dots\right) + \dots \end{pmatrix} + \begin{pmatrix} 0 \\ -h^2 g_y(0) f\left(y(x_i),z(x_i)\right) \end{pmatrix} + O\left(h^{M+2}\right).
\end{aligned}
$$

The coefficients of h^1 in (3.30) give

$$
\begin{pmatrix} y'(x_i) + \left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) \\ 0 \end{pmatrix} = \begin{pmatrix} f\left(y(x_i),z(x_i)\right) \\ g\left(y(x_i),z(x_i)\right) \end{pmatrix}.
$$

Using the consistency requirements (3.12b) gives (3.4) and hence $\alpha_i^{(1)} = 0, \forall i \geq 0$. The coefficients of h^2 give the following equations

$$
\frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) = f_y\left(x\right)a^{(1)}(x) + f_z\left(x\right)b^{(1)}(x)\,, \tag{3.31a}
$$

$$
-\, g_y(0)\,y'(x) - g_z(0)\,z'(x) = g_y\left(x\right)a^{(1)}(x) + g_z\left(x\right)b^{(1)}(x) - f(x)g_y(0)\,, \tag{3.31b}
$$

$$
\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) = f_z\left(0\right)\beta_i^{(1)}\,, \tag{3.31c}
$$

$$
-\, g_z(0)\left(\beta_{i+1}^{(1)} - \cancel{\beta_i^{(1)}}\right) = \cancel{g_z\left(0\right)\beta_i^{(1)}}. \tag{3.31d}
$$

This system can be solved by using (3.5) and computing $b^{(1)}(x)$ in (3.31b) to give

$$
b^{(1)}(x) = -g_z\left(x\right)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) + g_y\left(x\right)a^{(1)}(x) - f(x)g_y(0)\right],
$$

then we replace it into (3.31a) to yield

$$
\begin{aligned}
&\frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) = \\
&\quad = f_y\left(x\right)a^{(1)}(x) - f_z\left(x\right)g_z\left(x\right)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) + g_y\left(x\right)a^{(1)}(x) - f(x)g_y(0)\right], \\
&\left(a^{(1)}\right)'(x) + \left(f_z\left(x\right)g_z\left(x\right)^{-1}g_y\left(x\right) - f_y\left(x\right)\right)a^{(1)}(x) = \\
&\quad = -\frac{1}{2}y''(x) - f_z\left(x\right)g_z\left(x\right)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) - f(x)g_y(0)\right].
\end{aligned}
$$

Using (3.12a) and $\alpha_0^{(1)} = 0$ we have again that $a^{(1)}(0) = 0$. Therefore $a^{(1)}(x)$ and $b^{(1)}(x)$ are uniquely determined by (3.31a) and (3.31b). In contrast with the W-IMEX method (3.14b), the left hand side of (3.31b) does not vanish anymore:

$$
g_y\left(0\right)a^{(1)}(0) + g_z\left(0\right)b^{(1)}(0) = f(0)g_y(0) \Rightarrow g_z\left(0\right)b^{(1)}(0) = f(0)g_y(0) \Rightarrow b^{(1)}(0) \neq 0\,.
$$

By (3.12a) we also have that $\beta_0^{(1)} \neq 0$. In general we have that $\beta_i^{(1)} = 0, \forall i \geq 1$ due to (3.31d) and together with (3.31c) and (3.12b) we obtain $\alpha_i^{(2)} = 0, \forall i \geq 1$.

Next we investigate the coefficients of h^3 which for the smooth part give

$$\left(a^{(2)}\right)'(x) = f_y(x)\, a^{(2)}(x) + f_z(x)\, b^{(2)}(x) + r^{(2)}(x)\,, \tag{3.32a}$$
$$0 = g_y(x)\, a^{(2)}(x) + g_z(x)\, b^{(2)}(x) + s^{(2)}(x)\,, \tag{3.32b}$$

where $r^{(2)}(x)$ and $s^{(2)}(x)$ are known functions which depend on derivatives of $y(x)$, $z(x)$, $a^{(1)}(x)$, $b^{(1)}(x)$, and can be shown to be

$$r^{(2)}(x) = -\frac{1}{6}y'''(x) + \tag{3.33a}$$
$$+\frac{1}{2}f_{yy}(x)\left(a^{(1)}\right)^2(x) + \frac{1}{2}f_{zz}(x)\left(b^{(1)}\right)^2(x) + f_{yz}(x)a^{(1)}(x)b^{(1)}(x)\,,$$
$$s^{(2)}(x) = \frac{1}{2}g_y(0)y''(x) + \frac{1}{2}g_z(0)z''(x) + g_y(0)\left(a^{(1)}\right)'(x) + g_z(0)\left(b^{(1)}\right)'(x) + \tag{3.33b}$$
$$+\frac{1}{2}g_{yy}(x)\left(a^{(1)}\right)^2(x) + \frac{1}{2}g_{zz}(x)\left(b^{(1)}\right)^2(x) + g_{yz}(x)a^{(1)}(x)b^{(1)}(x) - \left(f_y(x)a^{(1)}(x) + f_z(x)b^{(1)}(x)\right)g_y(0)\,.$$

The perturbations can be expressed as

$$\alpha_{i+1}^{(3)} - \alpha_i^{(3)} = f_y(0)\alpha_i^{(2)} + \cancel{f_{yz}(0)\alpha_i^{(1)}\beta_i^{(1)}} + f_z(0)\beta_i^{(2)} + \cancel{\frac{1}{2}(\alpha_i^{(1)})^2 f_{yy}(0)} + \frac{1}{2}(\beta_i^{(1)})^2 f_{zz}(0) -$$
$$-\left(\cancel{f_y(0)\alpha_i^{(1)}} + f_z(0)\beta_i^{(1)}\right)g_y(0) + \beta_i^{(1)}b^{(1)}(0)f_{zz}(0)\cdots\,,$$
$$-g_y(0)\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) - g_z(0)\left(\beta_{i+1}^{(2)} - \beta_i^{(2)}\right) = \cancel{g_y(0)\alpha_i^{(2)}} + \cancel{g_{yz}(0)\alpha_i^{(1)}\beta_i^{(1)}} + g_z(0)\beta_i^{(2)} +$$
$$+\cancel{\frac{1}{2}(\alpha_i^{(1)})^2 g_{yy}(0)} + \frac{1}{2}(\beta_i^{(1)})^2 g_{zz}(0) + \beta_i^{(1)}b^{(1)}(0)g_{zz}(0) + \cdots\,,$$

where the vanishing terms have been canceled. It follows that

$$\alpha_{i+1}^{(3)} - \alpha_i^{(3)} = f_y(0)\alpha_i^{(2)} + \beta_i^{(1)}(\ldots) + f_z(0)\beta_i^{(2)}\,, \tag{3.34a}$$
$$0 = g_z(0)\beta_{i+1}^{(2)} + \beta_i^{(1)}(\ldots) + \alpha_i^{(2)}(\ldots)\,. \tag{3.34b}$$

From (3.34) we have that $\beta_i^{(2)} = 0$, $\forall i \geq 2$ and $\alpha_i^{(3)} = 0$, $\forall i \geq 2$. This concludes the proof for hypotheses (3.28a) and (3.28b). The general recurrence follows

$$\left(a^{(j)}\right)'(x) = f_y(x)\, a^{(j)}(x) + f_z(x)\, b^{(j)}(x) + r_j(x)\,, \tag{3.35a}$$
$$0 = g_y(x)\, a^{(j)}(x) + g_z(x)\, b^{(j)}(x) + s_j(x)\,, \tag{3.35b}$$
$$\alpha_{i+1}^{(j+1)} - \alpha_i^{(j+1)} = f_z(0)\beta_i^{(j)} + \varrho_i^{(j)}\,, \tag{3.35c}$$
$$0 = g_z(0)\beta_{i+1}^{(j)} + \sigma_i^{(j)}\,, \tag{3.35d}$$

where the smooth terms are determined by (3.35a) and (3.35b). Hypotheses (3.28c) and (3.28d) can be easily verified following the same type of induction on (3.35a) and (3.35b) as in the proof of Theorem 3.1. □

Theorem 3.4 (Accuracy for the extrapolated Pure-IMEX method applied to DAEs). *If we consider the harmonic sequence* $\{1, 2, 3, \ldots\}$, *then the extrapolated values* Y_{jk} *and* Z_{jk} *satisfy*

$$Y_{jk} - y(x_0 + h) = \mathcal{O}(H^{r_{jk}})\,, \qquad Z_{jk} - z(x_0 + h) = \mathcal{O}(H^{s_{jk}})\,, \tag{3.36}$$

where the differential-algebraic orders r_{jk} and s_{jk} are given in Table 3.4.

Proof. The orders in Table 3.4 for the Pure-IMEX method can be recovered by using the same procedure as in the proof of Theorem 3.2 with the error expansion given by Theorem 3.3. The major differences are given by the fact that now $\alpha_0^{(2)}$ is nonzero and thus one classical order is "lost" on the second column of the y component. Then $\alpha_1^{(3)}$ gives the third order on the diagonal. For the z component, $\beta_0^{(1)}$ is nonzero and hence the first column of the z component is 1. Furthermore, $\beta_1^{(2)}$ does not vanish and thus the diagonal T_{kk} is 2 for $k \geq 2$. The rest follows from the propagation of error terms as described by Table 3.3. □

3.3. Split-IMEX Method. The Split-IMEX method (2.4d) applied to (3.3) yields

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} f(y_i, z_i) \\ 0 \end{pmatrix} + \\ + h \begin{pmatrix} 0 \\ g\big(y_i + hf(y_i, z_i), z_i\big) \end{pmatrix} \text{ or}$$

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g\big(y_i + hf(y_i, z_i), z_i\big) - hg_y(0) f(y_i, z_i) \end{pmatrix}, \tag{3.37}$$

The DAE reduced form given by $\varepsilon \to 0$ is

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = h \begin{pmatrix} f(y_i, z_i) \\ g\big(y_i + hf(y_i, z_i), z_i\big) - hg_y(0) f(y_i, z_i) \end{pmatrix}. \tag{3.38}$$

We continue with a similar pair of theorems (error expansions and extrapolated orders) for the extrapolated Split-IMEX method.

Theorem 3.5 (Global error expansion of the extrapolated Split-IMEX method applied to DAEs). *Consider problem (3.4) with consistent initial values (y_0, z_0), and suppose that (3.5) is satisfied. The global error of the Split-IMEX scheme (3.38) then has an asymptotic h-expansion of the form (3.8) with $a^{(j)}(x)$ and $b^{(j)}(x)$ are smooth functions and the perturbations satisfy*

$$\alpha_i^{(1)} = 0\,, \alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 0\,, \tag{3.39a}$$

$$\alpha_i^{(3)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 1\,, \tag{3.39b}$$

$$\alpha_i^{(j)} = 0\,,\ \forall i \geq j-2\,,\ j \geq 4\,, \tag{3.39c}$$

$$\beta_i^{(j)} = 0\,,\ \forall i \geq j-1\,,\ j \geq 3\,. \tag{3.39d}$$

The error terms in (3.8) are uniformly bounded for $x_i = ih \leq H$, if H is sufficiently small.

Proof. This proof follows the same ideas used in the proof of Theorem 3.1. We begin with part (a) in which the truncated expansions are constructed. The second part can be shown easily following the same steps as in the W-IMEX case.

We consider again the truncated expansions (3.10) with defects

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y}_i \\ \widehat{z}_{i+1} - \widehat{z}_i \end{pmatrix} = \tag{3.40}$$
$$= h \begin{pmatrix} f(\widehat{y}_i, \widehat{z}_i) \\ g\left(\widehat{y}_i + hf(\widehat{y}_i, \widehat{z}_i), \widehat{z}_i\right) - hg_y(0) f(\widehat{y}_i, \widehat{z}_i) \end{pmatrix} + O\left(h^{M+1}\right).$$

The initial values are exact and the perturbation terms satisfy (3.12). Replacing the Taylor expansion for $f(\widehat{y}_i, \widehat{z}_i)$ and $g(\widehat{y}_i, \widehat{z}_i)$ about $(y(x_i), z(x_i))$ in (3.40) yields

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix} \cdot \tag{3.41}$$
$$\cdot \begin{pmatrix} hy'(x_i) + \frac{h^2}{2} y''(x_i) + h^2 \left(a^{(1)}\right)'(x_i) + h\left(\alpha^{(1)}_{i+1} - \alpha^{(1)}_i\right) + h^3 \left(a^{(2)}\right)'(x_i) + h^2 \left(\alpha^{(2)}_{i+1} - \alpha^{(2)}_i\right) + \dots \\ hz'(x_i) + \frac{h^2}{2} z''(x_i) + \dots + h^2 \left(b^{(1)}\right)'(x_i) + h\left(\beta^{(1)}_{i+1} - \beta^{(1)}_i\right) + \dots \end{pmatrix} =$$
$$= \begin{pmatrix} hf\left(y(x_i), z(x_i)\right) + f_y(x_i)\left(h^2 a^{(1)}(x_i) + h^2 \alpha^{(1)}_i + \dots\right) \\ hg\left(y(x_i), z(x_i)\right) + g_y(x_i)\left(h^2 a^{(1)}(x_i) + h^2 \alpha^{(1)}_i + \dots\right) \end{pmatrix} +$$
$$+ \begin{pmatrix} f_z(x_i)\left(h^2 b^{(1)}(x_i) + h^2 \beta^{(1)}_i + \dots\right) + \dots \\ g_z(x_i)\left(h^2 b^{(1)}(x_i) + h^2 \beta^{(1)}_i + \dots\right) + \dots \end{pmatrix} +$$
$$+ \begin{pmatrix} 0 \dots \\ -h^2 g_y(0) f\left(y(x_i), z(x_i)\right) + h^2 g_y(x_i) f\left(y(x_i), z(x_i)\right) + \dots \end{pmatrix} + O\left(h^{M+2}\right).$$

The coefficients of h^1 in (3.41) give

$$\begin{pmatrix} y'(x_i) + \left(\alpha^{(1)}_{i+1} - \alpha^{(1)}_i\right) \\ 0 \end{pmatrix} = \begin{pmatrix} f\left(y(x_i), z(x_i)\right) \\ g\left(y(x_i), z(x_i)\right) \end{pmatrix}.$$

Using the consistency requirements (3.12b) gives (3.4) and hence $\alpha^{(1)}_i = 0$, $\forall i \geq 0$. The h^2 terms give the following system:

$$\frac{1}{2} y''(x) + \left(a^{(1)}\right)'(x) = f_y(x)\, a^{(1)}(x) + f_z(x)\, b^{(1)}(x)\,, \tag{3.42a}$$
$$- g_y(0)\, y'(x) - g_z(0)\, z'(x) = g_y(x)\, a^{(1)}(x) + g_z(x)\, b^{(1)}(x) + f(x) g_y(x) - f(x) g_y(0)\,, \tag{3.42b}$$
$$\left(\alpha^{(2)}_{i+1} - \alpha^{(2)}_i\right) = f_z(0)\, \beta^{(1)}_i\,, \tag{3.42c}$$
$$- g_z(0)\left(\beta^{(1)}_{i+1} - \cancel{\beta^{(1)}_i}\right) = \cancel{g_z(0)\, \beta^{(1)}_i}. \tag{3.42d}$$

The differential equation (3.42a-3.42b) can be solved by using (3.5) and computing $b^{(1)}(x)$ in (3.31b) to give

$$b^{(1)}(x) = -g_z(x)^{-1}\left[g_y(0)\, y'(x) + g_z(0)\, z'(x) + g_y(x)\, a^{(1)}(x) + f(x) g_y(x) - f(x) g_y(0)\right],$$

and then by replacing it into (3.14a) yields

$$
\begin{aligned}
&\frac{1}{2}y''(x) + \left(a^{(1)}\right)'(x) = \\
&= f_y(x)\,a^{(1)}(x) - f_z(x)\,g_z(x)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) + g_y(x)\,a^{(1)}(x) + f(x)g_y(x) - f(x)g_y(0)\right], \\
&\left(a^{(1)}\right)'(x) + \left(f_z(x)\,g_z(x)^{-1}g_y(x) - f_y(x)\right)a^{(1)}(x) = \\
&= -\frac{1}{2}y''(x) - f_z(x)\,g_z(x)^{-1}\left[g_y(0)\,y'(x) + g_z(0)\,z'(x) + f(x)g_y(x) - f(x)g_y(0)\right].
\end{aligned}
$$

Using (3.12a) and $\alpha_0^{(1)} = 0$ we have again that $a^{(1)}(0) = 0$. Therefore $a^{(1)}(x)$ and $b^{(1)}(x)$ are uniquely determined by (3.42a) and (3.42b). The left hand side of (3.42b) at $x = 0$ gives:

$$g_y(0)\,a^{(1)}(0) + g_z(0)\,b^{(1)}(0) + f(0)g_y(0) - f(0)g_y(0) = 0 \Rightarrow g_z(0)\,b^{(1)}(0) = 0 \Rightarrow b^{(1)}(0) = 0\,.$$

By (3.12a) and (3.42d) we also have that $\beta_0^{(1)} = 0$ and in general $\beta_i^{(1)} = 0$, $\forall i \geq 0$ due to (3.42d). Further, by using (3.42c) and (3.12b) we obtain $\alpha_i^{(2)} = 0$, $\forall i \geq 0$.

Next we investigate the coefficients of h^3 which for the smooth part give

$$\left(a^{(2)}\right)'(x) = f_y(x)\,a^{(2)}(x) + f_z(x)\,b^{(2)}(x) + r^{(2)}(x)\,, \tag{3.43a}$$

$$0 = g_y(x)\,a^{(2)}(x) + g_z(x)\,b^{(2)}(x) + s^{(2)}(x)\,, \tag{3.43b}$$

where $r^{(2)}(x)$ and $s^{(2)}(x)$ are known functions which depend on derivatives of $y(x)$, $z(x)$, $a^{(1)}(x)$, $b^{(1)}(x)$, and can be shown to be

$$
\begin{aligned}
r^{(2)}(x) &= -\frac{1}{6}y'''(x) + \qquad\qquad (3.44a)\\
&+ \frac{1}{2}f_{yy}(x)\left(a^{(1)}\right)^2(x) + \frac{1}{2}f_{zz}(x)\left(b^{(1)}\right)^2(x) + f_{yz}(x)a^{(1)}(x)b^{(1)}(x)\,, \\
s^{(2)}(x) &= \frac{1}{2}g_y(0)y''(x) + \frac{1}{2}g_z(0)z''(x) + g_y(0)\left(a^{(1)}\right)'(x) + g_z(0)\left(b^{(1)}\right)'(x) + \qquad\qquad (3.44b)\\
&+ \left(f_y(x)a^{(1)}(x) + f_z(x)b^{(1)}(x)\right)g_y(x) + \frac{1}{2}g_{yy}(x)\left(a^{(1)}(x) + f(x)\right)^2 + \\
&+ \frac{1}{2}g_{zz}(x)\left(b^{(1)}\right)^2(x) + g_{yz}(x)\left(a^{(1)}(x) + f(x)\right)b^{(1)}(x) - \left(f_y(x)a^{(1)}(x) + f_z(x)b^{(1)}(x)\right)g_y(0)\,.
\end{aligned}
$$

The perturbations can be expressed as

$$
\begin{aligned}
&\alpha_{i+1}^{(3)} - \alpha_i^{(3)} = \cancel{f_y(0)\alpha_i^{(2)}} + \cancel{f_{yz}(0)\alpha_i^{(1)}\beta_i^{(1)}} + f_z(0)\beta_i^{(2)} + \cancel{\frac{1}{2}(\alpha_i^{(1)})^2 f_{yy}(0)} + \cancel{\frac{1}{2}(\beta_i^{(1)})^2 f_{zz}(0)} - \\
&\quad - \cancel{\left(f_y(0)\alpha_i^{(1)} + f_z(0)\beta_i^{(1)}\right)g_y(0)} + \cancel{\beta_i^{(1)}b^{(1)}(0)f_{zz}(0)} + \cdots\,, \\
&\cancel{-g_y(0)\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right)} - g_z(0)\left(\beta_{i+1}^{(2)} - \beta_i^{(2)}\right) = \cancel{g_y(0)\alpha_i^{(2)}} + \cancel{g_{yz}(0)\alpha_i^{(1)}\beta_i^{(1)}} + g_z(0)\beta_i^{(2)} + \\
&\quad + \cancel{\frac{1}{2}(\alpha_i^{(1)})^2 g_{yy}(0)} + \cancel{\frac{1}{2}(\beta_i^{(1)})^2 g_{zz}(0)} + \cancel{\beta_i^{(1)}b^{(1)}(0)g_{zz}(0)} + \cdots\,,
\end{aligned}
$$

where the vanishing terms have been canceled. It follows that

$$\alpha_{i+1}^{(3)} - \alpha_i^{(3)} = f_z(0)\beta_i^{(2)}\,, \tag{3.45a}$$

$$0 = g_z(0)\beta_{i+1}^{(2)}\,. \tag{3.45b}$$

From (3.45) we have that $\beta_i^{(2)} = 0$, $\forall i \geq 1$ and $\alpha_i^{(3)} = 0$, $\forall i \geq 1$.

The coefficients in h^4 reveal that the perturbations satisfy

$$\alpha_{i+1}^{(4)} - \alpha_i^{(4)} = f_y(0)\alpha_i^{(3)} + f_z(0)\beta_i^{(3)}\,, \tag{3.46a}$$

$$0 = g_z(0)\beta_{i+1}^{(3)} + g_y(0)\alpha_{i+1}^{(3)} + f(0)g_{yz}(0)\beta_i^{(2)}\,. \tag{3.46b}$$

From (3.46) we have that $\beta_i^{(3)} = 0$, $\forall i \geq 2$ and $\alpha_i^{(4)} = 0$, $\forall i \geq 2$. This concludes the proof for hypotheses (3.39a) and (3.39b). The general recurrence formula follows as

$$\left(a^{(j)}\right)'(x) = f_y(x)\,a^{(j)}(x) + f_z(x)\,b^{(j)}(x) + r_j(x)\,, \tag{3.47a}$$

$$0 = g_y(x)\,a^{(j)}(x) + g_z(x)\,b^{(j)}(x) + s_j(x)\,, \tag{3.47b}$$

$$\alpha_{i+1}^{(j+1)} - \alpha_i^{(j+1)} = f_z(0)\beta_i^{(j)} + \varrho_i^{(j)}\,, \tag{3.47c}$$

$$0 = g_z(0)\beta_{i+1}^{(j)} + \sigma_i^{(j)}\,, \tag{3.47d}$$

where the smooth terms are determined by (3.47a) and (3.47b). Hypotheses (3.39c) and (3.39d) can be easily verified following the same type of induction on (3.47a) and (3.47b) as in the proof of Theorem 3.1. □

Theorem 3.6 (Accuracy for the extrapolated Split-IMEX method applied to DAEs). *If we consider the harmonic sequence* $\{1, 2, 3, \dots\}$, *then the extrapolated values* Y_{jk} *and* Z_{jk} *satisfy*

$$Y_{jk} - y(x_0 + h) = O\left(H^{r_{jk}}\right)\,, \qquad Z_{jk} - z(x_0 + h) = O\left(H^{s_{jk}}\right)\,, \tag{3.48}$$

where the differential-algebraic orders r_{jk} *and* s_{jk} *are given in Table 3.4.*

Proof. The orders in Table 3.4 for the Split-IMEX method can be recovered by using the same procedure as in the proof of Theorem 3.2 with the error expansion given by Theorem 3.5. In contrast with the proof of Theorem 3.4, $\alpha_0^{(3)}$ is non-zero and thus one classical order is "lost" on the third column of the y component. Then $\alpha_1^{(4)}$ gives the fourth order on the diagonal. For the z component, $\beta_1^{(2)}$ is nonzero and hence the second column of the z component is 2. Furthermore, $\beta_1^{(3)}$ does not vanish and thus the diagonal T_{kk} is 3 for $k \geq 3$. The rest follows from the propagation of error terms as described by Table 3.3. □

The previous theorem concludes the set of theoretical results for the proposed three extrapolation IMEX methods applied to DAEs. The results point to the W-IMEX scheme as being the most accurate; however, from the implementation point of view, the Split-IMEX scheme is superior. The Split-IMEX method gives a good balance between accuracy and computational cost.

4. Numerical Results for Extrapolated IMEX Applied to DAEs. We illustrate the theoretical findings using two DAE examples: the reduced van der Pol equation and a trigonometric problem developed by us. The reduced van der Pol equation comes from the stiff van der Pol ODE with $\varepsilon \to 0$ which is a typical example for numerical stiffness analysis. In this case the numerical results using Split-IMEX have a slightly higher order than what the theory predicts. We explain this phenomenon and use the trigonometric equation to illustrate that the numerical orders concur with the theoretical ones.

Schemes (2.4) are implemented in Matlab® using variable precision arithmetic with 64 digits of accuracy. For van der Pol a reference solution is computed with very high accuracy.

Methods (2.4) are implemented in the following way:

$$\begin{pmatrix} y_{i+1} \\ z_{i+1} \end{pmatrix} = \begin{pmatrix} y_i \\ z_i \end{pmatrix} + h \begin{pmatrix} I - hf_y(0) & -hf_z(0) \\ -hg_y(0) & -hg_z(0) \end{pmatrix}^{-1} \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix} \qquad \begin{bmatrix} \textit{linearly} \\ \textit{implicit} \end{bmatrix} \tag{4.1a}$$

$$\begin{pmatrix} y_{i+1} \\ z_{i+1} \end{pmatrix} = \begin{pmatrix} y_i \\ z_i \end{pmatrix} + h\tilde{J}^{-1} \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix} \qquad [\textit{W-IMEX}] \tag{4.1b}$$

$$\begin{pmatrix} y_{i+1} \\ z_{i+1} \end{pmatrix} = \begin{pmatrix} y_i \\ z_i \end{pmatrix} + h \begin{pmatrix} f(y_i, z_i) \\ 0 \end{pmatrix} + h\tilde{J}^{-1} \begin{pmatrix} 0 \\ g(y_i, z_i) \end{pmatrix} \qquad [\textit{Pure-IMEX}] \tag{4.1c}$$

$$\begin{pmatrix} y_{i+1} \\ z_{i+1} \end{pmatrix} = \begin{pmatrix} \overline{y}_{i+1} \\ \overline{z}_{i+1} \end{pmatrix} + h\tilde{J}^{-1} \begin{pmatrix} 0 \\ g\left(\overline{y}_i, \overline{z}_i\right) \end{pmatrix} \qquad \begin{bmatrix} \textit{Split-} \\ \textit{IMEX} \end{bmatrix} \tag{4.1d}$$

where

$$\tilde{J} = \begin{pmatrix} I & 0 \\ -hg_y(0) & -hg_z(0) \end{pmatrix}, \qquad \begin{pmatrix} \overline{y}_{i+1} \\ \overline{z}_{i+1} \end{pmatrix} = \begin{pmatrix} y_i \\ z_i \end{pmatrix} + h \begin{pmatrix} f(y_i, z_i) \\ 0 \end{pmatrix}.$$

The experiments consist in integrating the problem by taking successively smaller steps H while using the same sequence n_j.

4.1. Experiments with the Van Der Pol Equation. The reduced van der Pol equation is given by

$$\begin{array}{rcll} y' & = & -z & = f(y,z) \\ 0 & = & y - \left(\frac{z^3}{3} - z\right) & = g(y,z) \end{array} . \tag{4.2}$$

We take $y(0) = -2$ and $z(0) = -2.35530139760811990992528773586425095191\ldots$ which satisfies $g(y(0), z(0)) = 0$. The values of H range from 10^{-1} to $10^{-4.5}$.

The orders based on the local errors are given in Table 4.1. The experimental orders should be compared with the theoretical ones given in Table 3.4. We note that the experimental orders verify the theoretical conclusions for the linearly implicit, W-IMEX, and the Pure-IMEX method.

1	2	3	4	5	6	7	8	9
2.0|2.0|2.0|2.0								
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0							
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0						
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0	5.0|4.0|3.0|4.0					
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0	5.0|4.0|4.0|4.0	5.1|5.0|3.0|5.0				
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0	5.0|4.0|4.0|4.0	5.1|5.0|4.0|5.0	6.1|5.1|3.0|5.1			
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0	5.0|4.0|4.0|4.0	5.1|5.0|5.0|5.0	6.2|6.0|4.0|6.0	5.9|5.0|3.0|5.0		
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0	5.0|4.0|4.0|4.0	5.2|5.0|5.0|5.0	6.2|6.0|5.0|6.0	8.4|5.8|4.0|5.8	5.9|5.0|3.0|5.0	
2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0	4.0|3.0|3.0|3.0	5.0|4.0|4.0|4.0	5.2|5.0|5.0|5.0	6.2|6.0|6.0|6.0	7.3|7.0|5.0|7.0	7.0|6.0|4.0|6.0	(6)|4.9|2.9|4.9

Orders component y_{jk} (linearly implicit|W-IMEX|Pure-IMEX|Split-IMEX)

1	2	3	4	5	6	7	8	9
2.0|2.0|1.0|2.0								
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0							
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|2.0|3.0						
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|3.0|3.0	4.0|4.0|2.0|4.0					
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|3.0|3.0	4.0|4.0|3.0|4.0	4.1|4.1|2.0|4.1				
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|3.0|3.0	4.0|4.0|4.0|4.0	5.0|5.0|3.0|5.0	3.9|4.0|2.0|4.0			
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|3.0|3.0	4.0|4.0|4.0|4.0	5.0|5.0|4.0|5.0	4.6|4.8|3.0|4.8	3.9|4.0|2.0|4.0		
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|3.0|3.0	4.0|4.0|4.0|4.0	5.0|5.0|5.0|5.0	6.0|6.0|4.0|6.0	5.0|5.0|3.0|5.0	3.8|3.9|1.9|3.9	
2.0|2.0|1.0|2.0	2.0|2.0|2.0|2.0	3.0|3.0|3.0|3.0	4.0|4.0|4.0|4.0	5.0|5.0|5.0|5.0	6.0|6.0|5.0|6.0	6.2|6.1|4.0|6.1	4.9|5.0|3.0|5.0	(4)|(4)|(2)|(4)

Orders component z_{jk} (linearly implicit|W-IMEX|Pure-IMEX|Split-IMEX)

Table 4.1

Numerical local extrapolation orders for linearly implicit, W-IMEX, Pure-IMEX, and Split-IMEX methods for index-1 DAEs (based on L_1 error norm). These results can be compared with the theoretical ones presented in Table 3.4.

The experimental orders for the Split-IMEX method are higher than the orders predicted by the theory. We can explain this disagreement by paying a closer attention at equation (4.2) and note that g_{yz} is zero. If we factor this in (3.46b) we find that the perturbation factor $\beta_2^{(3)}$ is zero and leads to $\alpha_2^{(4)} = 0$. This effectively increases the order by one on the diagonal terms corresponding to the y and z components.

Next we explore an example that has g_{yz} non-zero in order to illustrate the theoretical findings for the Split-IMEX method.

4.2. Experiments with a Trigonometric Equation. We next investigate the numerical solution of the following DAE discretized using the Split-IMEX method

$$\begin{array}{rcll} y' & = & \dfrac{y^2}{z\sqrt{\frac{y^2}{z^2}-1}} & = f(y,z) \\ 0 & = & z^2 - \dfrac{1}{1+y^2} - y^2\left(\dfrac{1}{z^2}-1\right) & = g(y,z) \end{array} . \tag{4.3}$$

The exact solution is $y(t) = \sinh(t)$, $z(t) = \tanh(t)$. We start with $t_0 = 0.5$ and note that g_{yz} is nonzero. The experimental orders for Split-IMEX are shown in Table 4.2. The orders can be verified to be the same as the theoretical ones given in Table 3.4. We note that the results are harvested automatically and some entries are not integers. This happens due to some variation of the convergence slope which is either due to linearly unstable results or round-off. The edited places are marked in parentheses.

5. Global Error Expansion for Extrapolated IMEX Methods Applied to stiff ODEs. In this section we extend the theoretical results for the global error expansion of extrapolated implicit-explicit methods applied to stiff ODEs. For this analysis we consider the following singular perturbation system [Hairer and Lubich, 1988; Auzinger et al., 1990]

$$\begin{array}{rcll} y' & = & f(y,z)\,, & y(0) = y_0 \\ \varepsilon z' & = & g(y,z)\,, & z(0) = z_0\,,\ 0 < \varepsilon \ll 1\,, \end{array} \tag{5.1}$$

which is solved using the W-IMEX (3.6), Pure-IMEX (3.25), and Split-IMEX (3.37) schemes. The favorable convergence results obtained for DAEs in the previous sections do not extend directly to the stiff ODEs ($\varepsilon \neq 0\,,\ \varepsilon \leq h$). In this case, the asymptotic expansions of the global error is more complicated, especially for "small" values of H. Moreover, different convergence regimes can be identified for the numerical approximations in the extrapolation tableau that depend on H/ε. We study the asymptotic behavior of the global error for the proposed IMEX methods and explore the reasons for the changes in their convergence slope.

5.1. W-IMEX. We start with the W-IMEX method and consider equations of the following form (in line with (3.16))

$$\begin{array}{rcl} a' & = & f_y(x)a + f_z(x)b + c(x,\varepsilon)\,, \\ \varepsilon b' & = & g_y(x)a + g_z(x)b + d(x,\varepsilon)\,. \end{array} \tag{5.2}$$

Their solution described by Lemma C.2 will be the basis for proving the next theorems which are the second set of main results of this paper.

Theorem 5.1 (Global error expansion for the extrapolated W-IMEX applied to stiff ODEs). *Assume that the solution of (5.1) is smooth. Under the condition (given by (C.3))*

$$\left\|(I-\gamma g_z(0))^{-1}\right\| \leq \frac{1}{1+\gamma} \quad \text{for} \quad \gamma \geq 1\,, \tag{5.3}$$

1	2.0											
2	1.9	3.0										
3	1.9	3.0	3.0									
4	2.0	3.0	2.9	4.0								
5	2.0	3.0	3.0	4.0	4.0							
6	2.0	3.0	3.0	3.9	4.9	4.0						
7	2.0	3.0	3.0	4.0	4.9	4.9	4.1					
8	2.0	3.0	3.0	4.0	4.9	5.9	4.9	(4)				
9	2.0	3.0	3.0	4.0	4.9	5.9	5.9	5.0	(4)			
10	2.0	3.0	3.0	4.0	4.9	5.9	6.9	5.9	5.0	(4)		
11	2.0	3.0	3.0	4.0	4.9	5.9	6.8	6.9	5.9	5.1	(4)	
12	2.0	3.0	3.0	4.0	4.9	5.9	6.8	8.1	6.9	6.0	5.2	(4)
	1	2	3	4	5	6	7	8	9	10	11	12

Orders component y_{jk}

1	2.0											
2	2.0	2.0										
3	2.2	2.0	3.0									
4	1.8	2.0	2.9	3.0								
5	1.9	2.0	2.9	4.0	3.0							
6	1.9	2.0	2.9	3.9	4.0	3.1						
7	1.9	2.0	2.9	3.9	5.0	4.0	3.2					
8	1.9	2.0	2.9	3.9	4.9	4.9	4.0	(3)				
9	2.0	2.0	2.9	3.9	4.9	6.0	5.0	4.0	(3)			
10	2.0	2.0	2.9	3.9	4.9	5.9	5.9	5.0	4.1	(3)		
11	2.0	2.0	3.0	3.9	4.9	5.9	7.0	5.9	5.0	4.2	(3)	
12	2.0	2.0	3.0	3.9	4.9	5.9	6.9	6.9	6.0	5.0	4.3	(3)
	1	2	3	4	5	6	7	8	9	10	11	12

Orders component z_{jk}

Table 4.2

Numerical approximation of the extrapolated local orders for the trigonometric DAE using the Split-IMEX scheme (based on L_1 error norm).

the numerical solution of (3.6) possesses for $\varepsilon \leq h$ a perturbed asymptotic expansion of the form

$$
\begin{aligned}
y_i &= y(x_i) + ha^{(1)}(x_i) + h^2 a^{(2)}(x_i) + \mathcal{O}(h^3) - && (5.4a)\\
&\quad - \varepsilon f_z(0) g_z^{-1}(0) \left(I - \frac{h}{\varepsilon} g_z(0) \right)^{-i+1} \left(hb^{(1)}(0) + h^2 b^{(2)}(0) \right), \\
z_i &= z(x_i) + hb^{(1)}(x_i) + h^2 b^{(2)}(x_i) + \mathcal{O}(h^3) - && (5.4b)\\
&\quad - \left(I - \frac{h}{\varepsilon} g_z(0) \right)^{-i+1} \left(hb^{(1)}(0) + h^2 b^{(2)}(0) \right),
\end{aligned}
$$

where $x_i = ih \le H$ with H sufficiently small independent of ε. The smooth functions $a^{(1)}(0) = \mathcal{O}(\varepsilon h)$, $a^{(2)}(0) = \mathcal{O}(h)$, $b^{(1)}(0) = \mathcal{O}(\varepsilon)$, $b^{(2)}(0) = \mathcal{O}(1)$.

Proof. The proof goes along the lines of Theorem 3.1 also [Hairer et al., 1993b, chap. VI, Thm. 5.6] and [Hairer and Lubich, 1988]. See also a similar approach for implicit Euler [Auzinger et al., 1990]. We start by considering the truncated expansions

$$\begin{aligned} \widehat{y_i} &= y(x_i) + \sum_{j=1}^{M} h^j \left(a^{(j)}(x_i) + \alpha_i^{(j)}\right) \\ \widehat{z_i} &= z(x_i) + \sum_{j=1}^{M} h^j \left(b^{(j)}(x_i) + \beta_i^{(j)}\right) \end{aligned} , \tag{5.5}$$

such that

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y_i} \\ \widehat{z}_{i+1} - \widehat{z_i} \end{pmatrix} = h \begin{pmatrix} f\left(\widehat{y_i}, \widehat{z_i}\right) \\ g\left(\widehat{y_i}, \widehat{z_i}\right) \end{pmatrix} + \mathcal{O}\left(h^{M+2}\right), \tag{5.6}$$

is satisfied.

a). The smooth functions $a(x)$ and $b(x)$ depend on ε, but are independent of h. The perturbation terms $\alpha_i^{(j)}$ and $\beta_i^{(j)}$, $\forall i \ge 1$ depend smoothly on ε and ε/h. We also consider (3.12a) and (3.12b) satisfied.

$M = 0$. This case is easily verified.

$M = 1$. We insert (5.5) in (5.6) and compare the smooth coefficients of h^2:

$$\left(a^{(1)}\right)'(x) + \frac{1}{2} y''(x) = f_y(x)\, a^{(1)}(x) + f_z(x)\, b^{(1)}(x), \tag{5.7a}$$

$$\frac{1}{2}\varepsilon\, z''(x) - g_y(0)\, y'(x) - g_z(0)\, z'(x) + \varepsilon \left(b^{(1)}\right)'(x) = g_y(x)\, a^{(1)}(x) + g_z(x)\, b^{(1)}(x), \tag{5.7b}$$

By Lemma C.2, the initial value $b^{(1)}(0)$ is uniquely determined by $a^{(1)}(0)$. Differentiating $\varepsilon z'(x) = g(y(x), z(x))$ gives

$$\varepsilon z''(x) = g_y(x)\, y'(x) + g_z(x)\, z'(x),$$

and inserting it in (5.7b) at $x = 0$ yields

$$\begin{aligned} g_y(0)\ a^{(1)}(0) + g_z(0)\ b^{(1)}(0) &= -\frac{1}{2}\underbrace{\left(g_y(0)\ y'(0) + g_z(0)\ z'(0)\right)}_{\varepsilon z''(0)} + \varepsilon \left(b^{(1)}\right)'(0), \\ g_y(0)\ a^{(1)}(0) + g_z(0)\ b^{(1)}(0) &= \mathcal{O}(\varepsilon) \end{aligned} \tag{5.8}$$

with known right-hand side. The perturbation terms up to $\mathcal{O}(h^2)$ give

$$\alpha_{i+1}^{(1)} - \alpha_i^{(1)} = hf_y(x_i)\alpha_i^{(1)} + hf_z(x_i)\beta_i^{(1)}, \tag{5.9a}$$

$$\varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) - hg_y(0)\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) - hg_z(0)\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) = hg_y(x_i)\alpha_i^{(1)} + hg_z(x_i)\beta_i^{(1)}. \tag{5.9b}$$

Next we try to eliminate as many terms in (5.9) as possible by replacing $f_y(x_i)$ with $f_y(0)$, $g_y(x_i)$ with $g_y(0)$, and so on. With $x_i = ih$, the following substitution is of order h: $f_y(x_i) - f_y(0) = O(h)$ due to $i \leq 1$. Then we are left with

$$\begin{cases} \alpha_{i+1}^{(1)} - \alpha_i^{(1)} = hf_y(0)\alpha_i^{(1)} + hf_z(0)\beta_i^{(1)} + O(h^2) \\ \varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) - hg_y(0)\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) - hg_z(0)\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) = hg_y(0)\alpha_i^{(1)} + hg_z(0)\beta_i^{(1)} \end{cases}.$$

After further cancellations we obtain

$$\begin{cases} \alpha_{i+1}^{(1)} - \alpha_i^{(1)} = hf_y(0)\alpha_i^{(1)} + hf_z(0)\beta_i^{(1)} + O(h^2) \\ \varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) - hg_y(0)\alpha_{i+1}^{(1)} - hg_z(0)\beta_{i+1}^{(1)} = O(h^2) \end{cases}. \tag{5.10}$$

In (5.10), second expression, we note that $\beta_{i+1}^{(1)}$ is multiplied by ε whereas $\alpha_{i+1}^{(1)}$ is not and thus can be ignored (for $\varepsilon \ll h$). Then we get

$$\alpha_{i+1}^{(1)} - \alpha_i^{(1)} = hf_z(0)\beta_i^{(1)} \tag{5.11a}$$

$$\varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right) = hg_z(0)\beta_{i+1}^{(1)}, \tag{5.11b}$$

We next analyze the solutions of (5.7), (5.11) when substituted in (5.6). From (5.11b) we obtain

$$\beta_{i+1}^{(1)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-1} \beta_i^{(1)},$$

$$\beta_1^{(1)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-1} \beta_0^{(1)},$$

$$\beta_2^{(1)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-1} \beta_1^{(1)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-1} \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-1} \beta_0^{(1)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-2} \beta_0^{(1)},$$

with

$$\beta_i^{(1)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i} \beta_0^{(1)}. \tag{5.12}$$

Substituting (5.12) in (5.11a) and using (3.12b) gives

$$\alpha_{i+1}^{(1)} - \alpha_i^{(1)} = hf_z(0)\beta_i^{(1)} = hf_z(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i} \beta_0^{(1)},$$

$$\alpha_i^{(1)} = \alpha_{i+1}^{(1)} - hf_z(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i} \beta_0^{(1)}, \ \alpha_{i+1}^{(1)} = \alpha_{i+2}^{(1)} - hf_z(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-(i+1)} \beta_0^{(1)}$$

$$\alpha_i^{(1)} = \alpha_{i+2}^{(1)} - hf_z(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-(i+1)} \beta_0^{(1)} - hf_z(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i} \beta_0^{(1)}$$

$$\alpha_i^{(1)} = \alpha_{i+2}^{(1)} - hf_z(0)\left(\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-(i+1)} + \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i}\right)\beta_0^{(1)},$$

$$\alpha_i^{(1)} = \alpha_\infty^{(1)} - hf_z(0)\sum_{k=1}^{\infty}\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-k} \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i+1} \beta_0^{(1)},$$

$$\alpha_i^{(1)} = -hf_z(0)\left(-\frac{h}{\varepsilon}g_z(0)\right)^{-1} \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i+1} \beta_0^{(1)} = \varepsilon f_z(0)g_z^{-1}(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i+1} \beta_0^{(1)}. \tag{5.13}$$

Expression (5.13) at $i = 0$ with $\varepsilon \le h$ yields

$$\alpha_0^{(1)} = \varepsilon f_z(0) g_z^{-1}(0) \left(I - \frac{h}{\varepsilon} g_z(0) \right) \beta_0^{(1)} = O(h)\, \beta_0^{(1)} = O(\varepsilon h)\,. \tag{5.14}$$

In the previous relation we used (5.8) and (3.12a) to bound $\beta_0^{(1)}$. The consistency assumptions (3.12a); i.e., $a^{(j)}(0) + \alpha_0^{(j)} = 0$, $b^{(j)}(0) + \beta_0^{(j)} = 0$, with (5.8) and (5.14) and by using Lemma C.2 guarantee that the coefficients $a^{(1)}(0)$, $b^{(1)}(0)$, $\alpha_0^{(1)}$, $\beta_0^{(1)}$ are uniquely determined; moreover, we have $a^{(1)}(0) = O(\varepsilon h)$ and $b^{(1)}(0) = O(\varepsilon)$ ($\alpha_i^{(1)} = O(\varepsilon h)$, $\beta_i^{(1)} = O(\varepsilon)$). Now the relation (5.6) can be verified for $M = 1$, $\varepsilon \le h$ as follows. Replacing (5.5) in (5.6) gives

$$\begin{aligned}
&h\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)} + y'\right) + h^2\left(\frac{1}{2}y'' + \left(a^{(1)}\right)'(x)\right) = \\
&\quad = h\left(f(x)\right) + h^2\left(\left(\alpha_i^{(1)} + a^{(1)}(x)\right) f_y(x) + \left(\beta_i^{(1)} + b^{(1)}(x)\right) f_y(x)\right) + O\left(h^3\right) ,\\
&h\varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)} + z'\right) + h^2\left(\frac{1}{2}\varepsilon z'' + g_y(0)\left(\alpha_i^{(1)} - \alpha_{i+1}^{(1)}\right) + g_z(0)\left(\beta_i^{(1)} - \beta_{i+1}^{(1)}\right) - z' g_z(0) - y' g_y(0) + \varepsilon\left(b^{(1)}\right)'(x)\right) = \\
&\quad = h\left(g(x)\right) + h^2\left(\left(\alpha_i^{(1)} + a^{(1)}(x)\right) g_y(x) + \left(\beta_i^{(1)} + b^{(1)}(x)\right) g_z(x)\right) + O\left(h^3\right) .
\end{aligned}$$

Smooth terms $a^{(1)}(x)$, $\left(a^{(1)}\right)'(x)$, $b^{(1)}(x)$, $\left(b^{(1)}\right)'(x)$ will cancel all $O(1)$ terms according to (5.7) except for the perturbation terms which require $\alpha_i^{(1)} = O(h^2)$ and $\beta_i^{(1)} = O(h)$. It follows that relation (5.6) is satisfied for $\alpha_i^{(1)} = O(\varepsilon h)$ and $\beta_i^{(1)} = O(\varepsilon)$, $\varepsilon \le h$.

$M = 2$. We again insert (5.5) in (5.6) and compare the smooth coefficients of h^3:

$$\begin{aligned}
&\left(a^{(2)}\right)'(x) + \frac{1}{6}y'''(x) = \qquad (5.16a)\\
&\quad = a^{(2)}(x) f_y(x) + \frac{1}{2}a_1^2(x) f_{yy}(x) + a^{(1)}(x) b^{(1)}(x) f_{yz}(x) + f_z(x)\, b^{(2)}(x) + \frac{1}{2}b_1^2(x) f_{zz}(x) ,\\
&\frac{1}{6}\varepsilon\, z'''(x) - \frac{1}{2}g_y(0)\, y''(x) - \frac{1}{2}g_z(0)\, z''(x) - g_y(0)\left(a^{(1)}\right)'(x) - g_z(0)\left(b^{(1)}\right)'(x) + \varepsilon\left(b^{(2)}\right)'(x) = \qquad (5.16b)\\
&\quad = g_y(x)\, a^{(2)}(x) + g_z(x)\, b^{(2)}(x) + \frac{1}{2}g_{yy}(x)\, a_1^2(x) + g_{yz}(x)\, a^{(1)}(x) b^{(1)}(x) + \frac{1}{2}g_{zz}(x)\, (b^{(1)}(x))^2 ,
\end{aligned}$$

which has the same form as (5.2): Equation (5.16a) gives

$$\begin{aligned}
&\left(a^{(2)}\right)'(x) = a^{(2)}(x) f_y(x) + f_z(x)\, b^{(2)}(x) + c(x,\varepsilon) ,\\
&c(x,\varepsilon) = -\frac{1}{6}y'''(x) + \frac{1}{2}a_1^2(x) f_{yy}(x) + a^{(1)}(x) b^{(1)}(x) f_{yz}(x) + \frac{1}{2}b_1^2(x) f_{zz}(x) .
\end{aligned}$$

Using $\varepsilon z'(x) = g(y(x), z(x))$ yields

$$\begin{aligned}
\varepsilon z'''(x) = {}& g_y(x)\, y''(x) + g_z(x)\, z''(x) + \\
&+ \left(g_{yz}(x) z'(x) + g_{yy}(x) y'(x)\right) y'(x) + \left(g_{zz}(x) z'(x) + g_{yz}(x) y'(x)\right) z'(x) ,
\end{aligned}$$

and then inserting it in (5.16b) gives

$$
\begin{aligned}
&\varepsilon\, \left(b^{(2)}\right)'(x) = g_y\,(x)\, a^{(2)}(x) + g_z\,(x)\, b^{(2)}(x) + d(x,\varepsilon)\,,\\
&d(x,\varepsilon) = -\frac{1}{6}\Big[\left(g_{yz}(x)z'(x) + g_{yy}(x)y'(x)\right)y'(x) + \left(g_{zz}(x)z'(x) + g_{yz}(x)y'(x)\right)z'(x)\Big]\\
&\quad + \frac{1}{2}g_y(0)\, y''(x) + \frac{1}{2}g_z(0)\, z''(x) + g_y(0)\left(a^{(1)}\right)'(x) + g_z(0)\left(b^{(1)}\right)'(x)\\
&\quad - \frac{1}{6}\left(g_y(x)\, y''(x) + g_z(x)\, z''(x)\right) + \frac{1}{2}g_{yy}\,(x)\, a_1^2(x) + g_{yz}\,(x)\, a^{(1)}(x)b^{(1)}(x) + \frac{1}{2}g_{zz}\,(x)\,(b^{(1)}(x))^2
\end{aligned}
$$

Further, by evaluating at $x = 0$ we obtain

$$
\begin{aligned}
&\varepsilon\, \left(b^{(2)}\right)'(0) = g_y\,(0)\, a^{(2)}(0) + g_z\,(0)\, b^{(2)}(0) + d(0,\varepsilon)\,,\\
&d(0,\varepsilon) = -\frac{1}{6}\Big[\left(g_{yz}(0)z'(0) + g_{yy}(0)y'(0)\right)y'(0) + \left(g_{zz}(0)z'(0) + g_{yz}(0)y'(0)\right)z'(0)\Big] +\\
&\qquad + \frac{1}{3}g_y(0)\, y''(0) + \frac{1}{3}g_z(0)\, z''(0) + g_y(0)\left(a^{(1)}\right)'(0) + g_z(0)\left(b^{(1)}\right)'(0) +\\
&\qquad + \frac{1}{2}g_{yy}\,(0)\, a_1^2(0) + g_{yz}\,(0)\, a^{(1)}(0)b^{(1)}(0) + \frac{1}{2}g_{zz}\,(0)\,(b^{(1)}(0))^2\,.
\end{aligned}
$$

It follows from Lemma C.2 and $d(0,\varepsilon) = O(1)$ that

$$
g_y\,(0)\, a^{(2)}(0) + g_z\,(0)\, b^{(2)}(0) = O(1)\,. \tag{5.17}
$$

Just as in the $M = 1$ case, for the perturbations we require

$$
\alpha_{i+1}^{(2)} - \alpha_i^{(2)} = h f_z(0)\beta_i^{(2)} \tag{5.18a}
$$

$$
\varepsilon\left(\beta_{i+1}^{(2)} - \beta_i^{(2)}\right) = h g_z(0)\beta_{i+1}^{(2)}\,, \tag{5.18b}
$$

and

$$
\beta_i^{(2)} = \left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i}\beta_0^{(2)}\,, \tag{5.19a}
$$

$$
\alpha_i^{(2)} = \varepsilon f_z(0) g_z^{-1}(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)^{-i+1}\beta_0^{(2)}\,, \tag{5.19b}
$$

$$
\alpha_0^{(2)} = \varepsilon f_z(0) g_z^{-1}(0)\left(I - \frac{h}{\varepsilon}g_z(0)\right)\beta_0^{(2)}\,, \tag{5.19c}
$$

are obtained just as for (5.12), (5.13), and (5.14), respectively. The values $a^{(1)}(0)$, $b^{(1)}(0)$, $\alpha_0^{(1)}$, $\beta_0^{(1)}$ are uniquely determined by (3.12a), (5.17) and (5.19c). We again remark that by using Lemma C.2 together with (5.16) gives $a^{(2)}(0) = O(h)$ and $b^{(1)}(0) = O(1)$; moreover, by using (3.12a) we obtain that $\alpha_i^{(2)} = O(h)$ for $\varepsilon \leq h$. The verification of (5.6) for $M = 2$ is very tedious, but it can be shown to be satisfied in general using the following remarks. The coefficients of h^1 can be ignored since they vanish for large i's. The assumption (5.3) gives $\beta_i^{(1)} = O\left(\varepsilon 2^{-i}\right)$ and $\beta_i^{(2)} = O\left(2^{-i}\right)$. These terms can also be neglected; however, in practice, they can give additional convergence regimes that quickly vanish. The convergence ($H \to 0$, $H/\varepsilon \to \infty$) will have different slopes that are determined by the ratio of H and ε.

This analysis gets very complicated for $M \geq 3$; however, we do not need to go any further to understand the error behavior in practical applications.

b). The second part of the proof consists in estimating a bound on the reminder term just as we did for the proof of Theorem 3.1; i.e., differences $\Delta y_i = y_i - \widehat{y_i}$ and $\Delta z_i = z_i - \widehat{z_i}$. Subtracting (5.6) from (3.6) and eliminating Δy_i and Δz_i gives

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} - \begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y_i} \\ \widehat{z}_{i+1} - \widehat{z_i} \end{pmatrix} =$$

$$= h \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix} - h \begin{pmatrix} f(\widehat{y_i}, \widehat{z_i}) \\ g(\widehat{y_i}, \widehat{z_i}) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+2}\right) \end{pmatrix},$$

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} - \begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} =$$

$$= h \begin{pmatrix} f(y_i, z_i) - f(\widehat{y_i}, \widehat{z_i}) \\ g(y_i, z_i) - g(\widehat{y_i}, \widehat{z_i}) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+2}\right) \end{pmatrix},$$

$$\begin{pmatrix} I & 0 \\ -g_y(0) & \frac{\varepsilon}{h} I - g_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} = \begin{pmatrix} I & 0 \\ -g_y(0) & \frac{\varepsilon}{h} I - g_z(0) \end{pmatrix} \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} +$$

$$+ \begin{pmatrix} h\left(f(y_i, z_i) - f(\widehat{y_i}, \widehat{z_i})\right) \\ g(y_i, z_i) - g(\widehat{y_i}, \widehat{z_i}) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix},$$

$$\begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} = \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} + \begin{pmatrix} I & 0 \\ -g_y(0) & \frac{\varepsilon}{h} I - g_z(0) \end{pmatrix}^{-1} \begin{pmatrix} h\left(f(y_i, z_i) - f(\widehat{y_i}, \widehat{z_i})\right) \\ g(y_i, z_i) - g(\widehat{y_i}, \widehat{z_i}) \end{pmatrix} +$$

$$+ \begin{pmatrix} I & 0 \\ -g_y(0) & \frac{\varepsilon}{h} I - g_z(0) \end{pmatrix}^{-1} \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix}.$$

Finally, we obtain

$$\begin{pmatrix} \Delta y_{i+1} \\ \Delta z_{i+1} \end{pmatrix} = \begin{pmatrix} \Delta y_i \\ \Delta z_i \end{pmatrix} +$$

$$+ \begin{pmatrix} I & 0 \\ \mathcal{O}(1) & \left(\frac{\varepsilon}{h} I - g_z(0)\right)^{-1} \end{pmatrix} \begin{pmatrix} h\left(f(y_i, z_i) - f(\widehat{y_i}, \widehat{z_i})\right) \\ g(y_i, z_i) - g(\widehat{y_i}, \widehat{z_i}) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+1}\right) \end{pmatrix}.$$

Due to (5.3) and $\varepsilon \le h$ we have

$$\left\| I + \left(\frac{\varepsilon}{h} I - g_z(0)\right)^{-1} g_z(0) \right\| = \left\| \left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-1} \right\| \le \frac{\varepsilon}{\varepsilon + h} \le \frac{1}{2}. \tag{5.20}$$

We therefore obtain (3.22) with $|\zeta| < 1$ and H is sufficiently small. Using the same procedure as in in the proof of Theorem 3.1 we obtain $\left\|\Delta y_i\right\| + \|\Delta z_i\| = \mathcal{O}\left(h^{M+1}\right)$.
□

A close inspection of (5.4) reveals that the global error has different regimes when $\varepsilon \le h$. We now focus on the global error expansion of the stiff component (5.4) which gives the following leading term

$$Z_{j1} = \left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-n_j+1} \left(hb^{(1)}(0) + h^2 b^{(2)}(0)\right),$$

$$Z_{j1} = h^2 \left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-n_j+1} b^{(2)}(0).$$

We further consider $g_z(0) \propto -1$ and with $H = h/n_j$ we have

$$
\begin{aligned}
T_{j1} &= \left(\frac{H}{\varepsilon n_j}\right)^2 \left(1 + \frac{H}{\varepsilon n_j}\right)^{-n_j+1} b^{(2)}(0) \text{ and} \\
Z_{j1} &= \varepsilon^2 T_{j1} b^{(2)}(0) .
\end{aligned}
$$

The error propagates through the extrapolation tableau through (2.3a). Similar to the behavior of the global error for the linearly implicit method [Hairer et al., 1993b, pp. 438], the first sub-diagonal ($T_{j\,j-1}$) with $n_1 = 1$ gives

$$
T_{j\,j-1} = \text{const.} \left(\frac{H}{\varepsilon}\right)^{2-n_2} + O\left(\left(\frac{H}{\varepsilon}\right)^{2-n_2}\right),
$$

where the constant is determined by (2.3a). This suggests a superposition of the the convergence slopes predicted for DAEs and a factor $O\left(\varepsilon^2\right)$.

5.2. Pure-IMEX Method. We now consider the Pure-IMEX method applied to SPP (5.1) to give (3.25).

Theorem 5.2 (Global error expansion for the extrapolated Pure-IMEX method applied to stiff ODEs). *Assume that the solution of (5.1) is smooth. Under the condition (5.3) the numerical solution of (3.25) possesses for $\varepsilon \leq h$ a perturbed asymptotic expansion of the form*

$$
\begin{aligned}
y_i &= y(x_i) + h a^{(1)}(x_i) + h^2 a^{(2)}(x_i) + O(h^3) - \qquad (5.21a)\\
&\quad - \varepsilon f_z(0) g_z^{-1}(0) \left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-i+1} \left(h b^{(1)}(0) + h^2 b^{(2)}(0)\right), \\
z_i &= z(x_i) + h b^{(1)}(x_i) + h^2 b^{(2)}(x_i) + O(h^3) - \qquad (5.21b)\\
&\quad - \left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-i+1} \left(h b^{(1)}(0) + h^2 b^{(2)}(0)\right),
\end{aligned}
$$

where $x_i = ih \leq H$ with H sufficiently small independent of ε. The smooth functions $a^{(1)}(0) = O(h)$, $a^{(2)}(0) = O(h)$, $b^{(1)}(0) = O(1)$, $b^{(2)}(0) = O(1)$.

Proof. The proof goes along the same lines as for Theorem 5.1. We begin with the same assumptions (5.2), (5.5), and (5.6) becomes

$$
\begin{pmatrix} I & 0 \\ -h g_y(0) & \varepsilon I - h g_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y}_i \\ \widehat{z}_{i+1} - \widehat{z}_i \end{pmatrix} = h \begin{pmatrix} f\left(\widehat{y}_i, \widehat{z}_i\right) \\ g\left(\widehat{y}_i, \widehat{z}_i\right) - h g_y(0) f\left(\widehat{y}_i, \widehat{z}_i\right) \end{pmatrix} + \begin{pmatrix} O\left(h^{M+1}\right) \\ O\left(h^{M+1}\right) \end{pmatrix}. \qquad (5.22)
$$

For $M = 1$ we obtain

$$
\left(a^{(1)}\right)'(x) + \frac{1}{2} y''(x) = f_y(x) a^{(1)}(x) + f_z(x) b^{(1)}(x), \qquad (5.23a)
$$

$$
\frac{1}{2}\varepsilon z''(x) - g_y(0) y'(x) - g_z(0) z'(x) + \varepsilon \left(b^{(1)}\right)'(x) = g_y(x) a^{(1)}(x) + g_z(x) b^{(1)}(x) - f(x) g_y(0), \qquad (5.23b)
$$

Equation (5.23b) leads to

$$g_y(0)\, a^{(1)}(0) + g_z(0)\, b^{(1)}(0) = -\frac{1}{2}\underbrace{\Big(g_y(0)\ y'(0) + g_z(0)\ z'(0)\Big)}_{\varepsilon z''(0)} + \underbrace{f(0)g_y(0)}_{O(1)} + \varepsilon \left(b^{(1)}\right)'(0)\,,$$

$$g_y(0)\, a^{(1)}(0) + g_z(0)\, b^{(1)}(0) = O(1) \tag{5.24}$$

with known right-hand side. The perturbation terms up to $O(h^2)$ give the same expression as in the W-IMEX case (5.9) that yields (5.10) and eventually (5.11). The values for $\alpha_i^{(1)}$ and $\beta_i^{(1)}$ are given by (5.13) and (5.12), respectively. By using the consistency assumptions (3.12a) and (5.12) we obtain

$$\alpha_0^{(1)} = \varepsilon f_z(0) g_z^{-1}(0)\left(I - \frac{h}{\varepsilon} g_z(0)\right)\beta_0^{(1)} = O(h)\,\beta_0^{(1)} = O(h)\,, \tag{5.25}$$

which yields $a^{(1)}(0) = O(h)$ and $b^{(1)}(0) = O(1)$ ($\alpha_i^{(1)} = O(h)$, $\beta_i^{(1)} = O(1)$). With these assumptions (5.22) can be verified.

For $M = 2$ we have the following expansions:

$$\left(a^{(2)}\right)'(x) + \frac{1}{6} y'''(x) = \tag{5.26a}$$

$$= a^{(2)}(x) f_y(x) + \frac{1}{2} a_1^2(x) f_{yy}(x) + a^{(1)}(x) b^{(1)}(x) f_{yz}(x) + f_z(x)\, b^{(2)}(x) + \frac{1}{2} b_1^2(x) f_{zz}(x)\,,$$

$$\frac{1}{6}\varepsilon\, z'''(x) - \frac{1}{2} g_y(0)\, y''(x) - \frac{1}{2} g_z(0)\, z''(x) - g_y(0)\left(a^{(1)}\right)'(x) - g_z(0)\left(b^{(1)}\right)'(x) + \varepsilon\left(b^{(2)}\right)'(x) = \tag{5.26b}$$

$$= -f_y(x) g_y(0)\, a^{(1)}(x) - f_z(x) g_y(0)\, b^{(1)}(x) +$$

$$+ g_y(x)\, a^{(2)}(x) + g_z(x)\, b^{(2)}(x) + \frac{1}{2} g_{yy}(x)\, a_1^2(x) + g_{yz}(x)\, a^{(1)}(x) b^{(1)}(x) + \frac{1}{2} g_{zz}(x)\, (b^{(1)}(x))^2\,,$$

which has the same form as (5.2). We obtain again (5.17) and (5.19). Finally, using $b^{(2)}(0) = O(1)$ yields $a^{(2)}(0) = O(h)$ and $b^{(1)}(0) = O(1)$. The rest is similar to the proof of Theorem 5.1 □ The convergence behavior of this method is very similar to the one discussed for the W-IMEX scheme (Sec. 5.1); however, in this case the superposition of the error has a factor of $O(\varepsilon)$.

5.3. Split-IMEX Method. We consider the Split-IMEX method applied to SPP (5.1) to give (3.37).

Theorem 5.3 (Global error expansion for the extrapolated Split-IMEX method applied to stiff ODEs). *Assume that the solution of (5.1) is smooth. Under the condition (5.3) the numerical solution of (3.37) possesses for $\varepsilon \leq h$ a perturbed asymptotic expansion of the form*

$$y_i = y(x_i) + h a^{(1)}(x_i) + h^2 a^{(2)}(x_i) + O(h^3) - \tag{5.27a}$$

$$- \varepsilon f_z(0) g_z^{-1}(0)\left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-i+1}\left(h b^{(1)}(0) + h^2 b^{(2)}(0)\right),$$

$$z_i = z(x_i) + h b^{(1)}(x_i) + h^2 b^{(2)}(x_i) + O(h^3) - \tag{5.27b}$$

$$- \left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-i+1}\left(h b^{(1)}(0) + h^2 b^{(2)}(0)\right),$$

where $x_i = ih \le H$ with H sufficiently small independent of ε. The smooth functions $a^{(1)}(0) = \mathcal{O}(\varepsilon h)$, $a^{(2)}(0) = \mathcal{O}(h)$, $b^{(1)}(0) = \mathcal{O}(\varepsilon)$, $b^{(2)}(0) = \mathcal{O}(1)$.

Proof. The proof goes along the same lines as for Theorem 5.1. We begin with the same assumptions (5.2), (5.5), and (5.6) becomes

$$\begin{pmatrix} I & 0 \\ -hg_y(0) & \varepsilon I - hg_z(0) \end{pmatrix} \begin{pmatrix} \widehat{y}_{i+1} - \widehat{y}_i \\ \widehat{z}_{i+1} - \widehat{z}_i \end{pmatrix} = h \begin{pmatrix} f\left(\widehat{y}_i, \widehat{z}_i\right) \\ g\Big(\widehat{y}_i + hf\left(\widehat{y}_i, \widehat{z}_i\right), \widehat{z}_i\Big) - hg_y(0) f\left(\widehat{y}_i, \widehat{z}_i\right) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(h^{M+2}\right) \\ \mathcal{O}\left(h^{M+2}\right) \end{pmatrix}. \tag{5.28}$$

For $M = 1$ we obtain

$$\left(a^{(1)}\right)'(x) + \frac{1}{2} y''(x) = f_y(x)\, a^{(1)}(x) + f_z(x)\, b^{(1)}(x)\,, \tag{5.29a}$$

$$\frac{1}{2}\varepsilon\, z''(x) - g_y(0)\, y'(x) - g_z(0)\, z'(x) + \varepsilon \left(b^{(1)}\right)'(x) = g_y(x)\, a^{(1)}(x) + g_z(x)\, b^{(1)}(x) + f(x)\Big(g_y(x) - g_y(0)\Big)\,, \tag{5.29b}$$

Equation (5.29b) leads to

$$\begin{aligned} g_y(0)\; a^{(1)}(0) + g_z(0)\; b^{(1)}(0) &= -\frac{1}{2}\underbrace{\Big(g_y(0)\; y'(0) + g_z(0)\; z'(0)\Big)}_{\varepsilon z''(0)} + \varepsilon \left(b^{(1)}\right)'(0)\,, \\ g_y(0)\; a^{(1)}(0) + g_z(0)\; b^{(1)}(0) &= \mathcal{O}(\varepsilon) \end{aligned} \tag{5.30}$$

with known right-hand side. We continue with an in-depth analysis for the rest of the proof because some derivations are not obvious. The perturbation terms up to $\mathcal{O}(h^2)$ give the same expression as in the W-IMEX case (5.34) that yields (5.10) and eventually (5.11):

$$\underbrace{\alpha_{i+1}^{(1)} - \alpha_i^{(1)}}_{(5.11a)} = \cancel{hf_y(x_i)\alpha_i^{(1)}} + \underbrace{hf_z(x_i)\beta_i^{(1)}}_{(5.11a)}\,, \tag{5.31a}$$

$$\begin{aligned} &\underbrace{\varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right)}_{(5.11b)} + h\left(-\cancel{\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right)}\, g_y(0) - \left(\underbrace{\beta_{i+1}^{(1)}}_{(5.11b)} - \underbrace{\cancel{\beta_i^{(1)}}}_{\mathcal{O}(h)}\right) g_z(0)\right) = \\ &\quad = h\left(\cancel{g_y(x_i)\alpha_i^{(1)}} + \cancel{g_z(x_i)\beta_i^{(1)}}\right) + h^2\left(\cancel{\alpha_i^{(2)} g_y(x)} + \cancel{\beta_i^{(2)}}\, g_z(x)\right). \end{aligned} \tag{5.31b}$$

The values for $\alpha_i^{(1)}$ and $\beta_i^{(1)}$ are given by (5.13) and (5.12), respectively. By using the consistency assumptions (3.12a) and (5.12) we obtain

$$\alpha_i^{(1)} = -hf_z(0)\left(-\frac{h}{\varepsilon} g_z(0)\right)^{-1}\left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-i+1} \beta_0^{(1)} = \varepsilon f_z(0) g_z^{-1}(0)\left(I - \frac{h}{\varepsilon} g_z(0)\right)^{-i+1} \beta_0^{(1)}.$$

and

$$\alpha_0^{(1)} = \varepsilon f_z(0) g_z^{-1}(0)\left(I - \frac{h}{\varepsilon} g_z(0)\right) \beta_0^{(1)} = \mathcal{O}(h)\, \beta_0^{(1)} = \mathcal{O}(\varepsilon h)\,, \tag{5.32}$$

which yields $a^{(1)}(0) = \mathcal{O}(\varepsilon h)$ and $b^{(1)}(0) = \mathcal{O}(\varepsilon)$ ($\alpha_i^{(1)} = \mathcal{O}(\varepsilon h)$, $\beta_i^{(1)} = \mathcal{O}(\varepsilon)$). With these assumptions (5.22) can be verified.

For $M = 2$ we have the following expansions:

$$\begin{aligned}
&\left(a^{(2)}\right)'(x) + \frac{1}{6} y'''(x) = && (5.33a)\\
&\quad = a^{(2)}(x) f_y(x) + \frac{1}{2} a_1^2(x) f_{yy}(x) + a^{(1)}(x) b^{(1)}(x) f_{yz}(x) + f_z(x)\, b^{(2)}(x) + \frac{1}{2} b_1^2(x) f_{zz}(x)\,,\\
&\frac{1}{6}\varepsilon\, z'''(x) - \frac{1}{2} g_y(0)\, y''(x) - \frac{1}{2} g_z(0)\, z''(x) - g_y(0)\left(a^{(1)}\right)'(x) - g_z(0)\left(b^{(1)}\right)'(x) + \varepsilon\left(b^{(2)}\right)'(x) = && (5.33b)\\
&\quad = -f_y(x) g_y(0)\, a^{(1)}(x) - f_z(x) g_y(0)\, b^{(1)}(x) + a^{(1)}(x) f_y(x) g_y(x) + b^{(1)}(x) f_z(x) g_y(x) +\\
&\quad + g_y(x)\, a^{(2)}(x) + g_z(x)\, b^{(2)}(x) + \frac{1}{2} g_{yy}(x)\left(a^{(1)}(x) + f(x)\right)^2 + g_{yz}(x)\left(a^{(1)}(x) + f(x)\right) b^{(1)}(x) + \frac{1}{2} g_{zz}(x)\left(b^{(1)}(x)\right)^2\,,
\end{aligned}$$

which have the same form as (5.2). We also have

$$\begin{aligned}
&\underbrace{\alpha_{i+1}^{(1)} - \alpha_i^{(1)}}_{(5.31a)} + h\underline{\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right)} = \cancel{h f_y(x_i)\alpha_i^{(1)}} + \underbrace{h f_z(x_i)\beta_i^{(1)}}_{(5.31a)} + && (5.34a)\\
&\quad + h^2\left(\cancel{f_y(x_i)\alpha_i^{(2)}} + \underline{f_z(x_i)\beta_i^{(2)}} + \frac{1}{2}\left(\alpha_i^{(1)}\right)^2 f_{yy}(x_i) + \alpha_i^{(1)}\beta_i^{(1)} f_{yz}(x_i) + \frac{1}{2}\left(\beta_i^{(1)}\right)^2 f_{zz}(x_i)\right),\\
&\underbrace{\varepsilon\left(\beta_{i+1}^{(1)} - \beta_i^{(1)}\right)}_{(5.31b)} + h\left(\underline{\varepsilon\left(\beta_{i+1}^{(2)} - \beta_i^{(2)}\right)} - \cancel{\left(\alpha_{i+1}^{(1)} - \alpha_i^{(1)}\right) g_y(0)} - \left(\underbrace{\beta_{i+1}^{(1)}}_{(5.31b)} - \underbrace{\cancel{\beta_i^{(1)}}}_{\mathcal{O}(h)}\right) g_z(0)\right) - && (5.34b)\\
&\quad - h^2\left(\cancel{\left(\alpha_{i+1}^{(2)} - \alpha_i^{(2)}\right) g_y(0)} + \left(\underline{\beta_{i+1}^{(2)}} - \underbrace{\cancel{\beta_i^{(2)}}}_{\mathcal{O}(h)}\right)\underline{g_z(0)}\right) =\\
&\quad = h\left(\cancel{g_y(x_i)\alpha_i^{(1)}} + \cancel{g_z(x_i)\beta_i^{(1)}}\right) + h^2\left(\cancel{\alpha_i^{(2)} g_y(x)} + \cancel{\beta_i^{(2)}} g_z(x)\right) +\\
&\quad + h^2\left(\alpha_i^{(1)} f_y(x)\underbrace{\left(g_y(x) - g_y(0)\right)}_{\mathcal{O}(h)} + \beta_i^{(1)} f_z(x)\underbrace{\left(g_y(x) - g_y(0)\right)}_{\mathcal{O}(h)} + \right.\\
&\quad \left. + \frac{1}{2}\left(\alpha_i^{(1)}\right)^2 g_{yy}(x_i) + \alpha_i^{(1)}\beta_i^{(1)} g_{yz}(x_i) + \frac{1}{2}\left(\beta_i^{(1)}\right)^2 g_{zz}(x)\right).
\end{aligned}$$

We obtain again (5.17) and (5.19). Finally, using $b^{(2)}(0) = \mathcal{O}(1)$ yields $a^{(2)}(0) = \mathcal{O}(h)$ and $b^{(1)}(0) = \mathcal{O}(1)$. The rest is similar to the proof of Theorem 5.1.
□

The convergence behavior of this method is asymptotically similar to the one discussed for the W-IMEX scheme (Sec. 5.1).

6. Numerical Results for Extrapolated IMEX Applied to Stiff ODEs. We investigate the numerical properties of the proposed extrapolated IMEX methods applied to stiff ODEs. We consider two stiff ordinary differential equations: stiff van der Pol and an example proposed by Hairer and Lubich [1988]. We also consider for comparison several IMEX Runge-Kutta schemes: [ARS(implicit stages, explicit (effective) stages, classical order)] (Ascher-Ruuth-Spiteri) developed by Ascher et al. [1997]; [PR(implicit stages, explicit (effective) stages, classical order)] (Pareschi and Russo) introduced by Pareschi and Russo [2000]; and the [ARK order(embedded order)stages] (Additive Runge-Kutta) methods developed by Kennedy and Carpenter [2003]. All IMEX Runge-Kutta methods require solving a (non)linear system of equations. The implicit part of the ARK methods is of ESDIRK type; i.e., explicit first stage with the same value on the diagonal of the Butcher tableau, which improves the computation efficiency.

The implementation is done in Matlab® using high (64 digits) precision arithmetic. The experiments consist in integrating the problem by taking successively smaller steps H and computing the L_1 error norm for each step size. We compare the results of the proposed IMEX methods and the above mentioned IMEX Runge-Kutta schemes with a third order reference solution computed with the stiff solver RODAS 3 [Sandu et al., 1997] and a step size of 10^{-9}. The nonlinear solver used in the computation of the reference solution and in the IMEX Runge-Kutta methods is implemented with classical Newton iterations. The process is stopped when the difference between sequential iterates is below 10^{-25}.

6.1. Van der Pol. We consider the van der Pol equation (see [Hairer et al., 1993b; Boscarino, 2007])

$$\begin{array}{rcl} y' & = & z \\ \varepsilon\, z' & = & \left(1-y^2\right)z - y \end{array} = \underbrace{\begin{pmatrix} z \\ 0 \end{pmatrix}}_{=f(y,z)} + \underbrace{\begin{pmatrix} 0 \\ \left(1-y^2\right)z - y \end{pmatrix}}_{=g(y,z)} \tag{6.1}$$

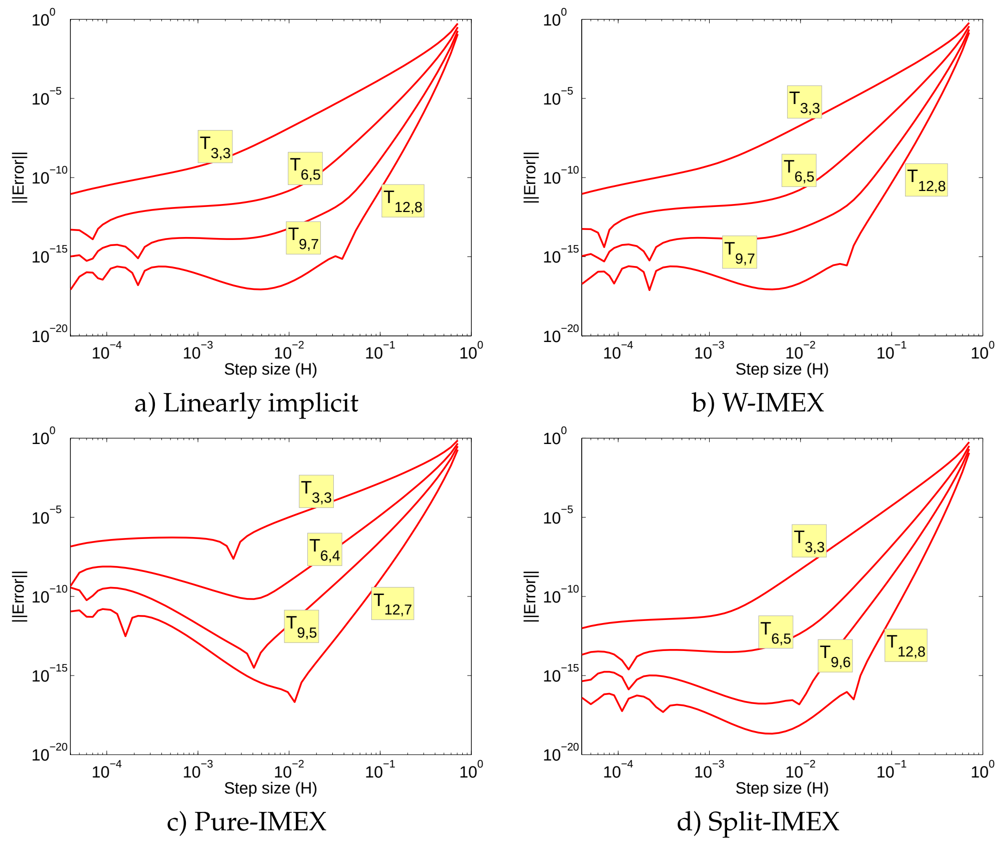
with [Boscarino, 2007]

$$y(0) = 2\,, \quad z(0) = -\frac{2}{3} + \frac{10}{81}\varepsilon - \frac{292}{2187}\varepsilon^2 - \frac{1814}{19683}\varepsilon^3 + O\left(\varepsilon^4\right)\,, \quad \varepsilon = 10^{-5}\,. \tag{6.2}$$

The stiff part is represented by z or $g(y,z)$. In Figure 6.1 we show the error for the stiff solution component (z) of the van der Pol equation using extrapolated linearly implicit and IMEX methods (2.4) for the optimal convergence rates with 3, 6, 9, and 12 extrapolation steps; i.e., optimal k for each method's $T_{3\,k}$, $T_{6\,k}$, $T_{9\,k}$, $T_{12\,k}$ extrapolation terms. The specific terms are selected from Table 3.4 for each method. The convergence rates correspond to the theoretical expectations, the error decreases until it reaches $O(\varepsilon)$ for Pure-IMEX and $O(\varepsilon^2)$ for the others.

We compare the IMEX extrapolation methods with several IMEX Runge-Kutta methods. In Figure 6.2 we show the L_1 error norm of the local errors of the stiff component for second and third order PR methods, two third order ARS methods, and third to fifth order ARK methods. The order reduction phenomenon can be clearly seen. The convergence behavior is explained in detail in [Boscarino, 2007].

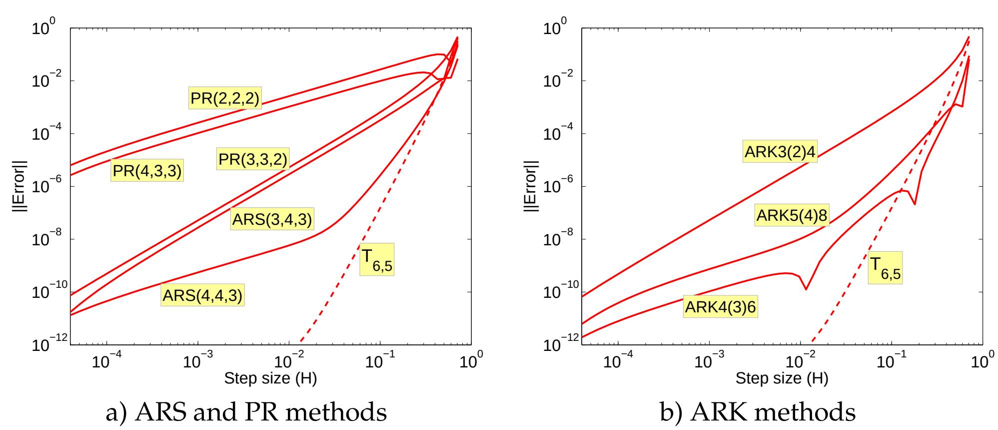
The computational cost of the IMEX extrapolation methods increases linearly with each additional extrapolation step. For T_{jk} one needs $j(j+1)/2$ right-hand-side evaluations. In contrast, for an s_i-implicit, s_e-explicit-stage IMEX Runge-Kutta scheme, one needs $\approx [(s_e - s_i) + s_i \times \#$ of Newton iterations] function evaluations. In this paper we do not focus on the actual computational cost which can change with the implementation and application, and hence we shall not present any numerical results regarding the cost.



a) Linearly implicit b) W-IMEX

c) Pure-IMEX d) Split-IMEX

FIG. 6.1. *Local error vs. step size for the stiff solution component of the van der Pol equation using extrapolated linearly implicit and IMEX methods for the optimal convergence rates with 3, 6, 9, and 12 extrapolation steps; i.e., the optimal k for each method's* T_{3k}, T_{6k}, T_{9k}, T_{12k}.



a) ARS and PR methods b) ARK methods

FIG. 6.2. *Local error vs. step size for the stiff solution component of the van der Pol equation using several IMEX Runge-Kutta methods and* $T_{6,5}$ *Split-IMEX for comparison.*

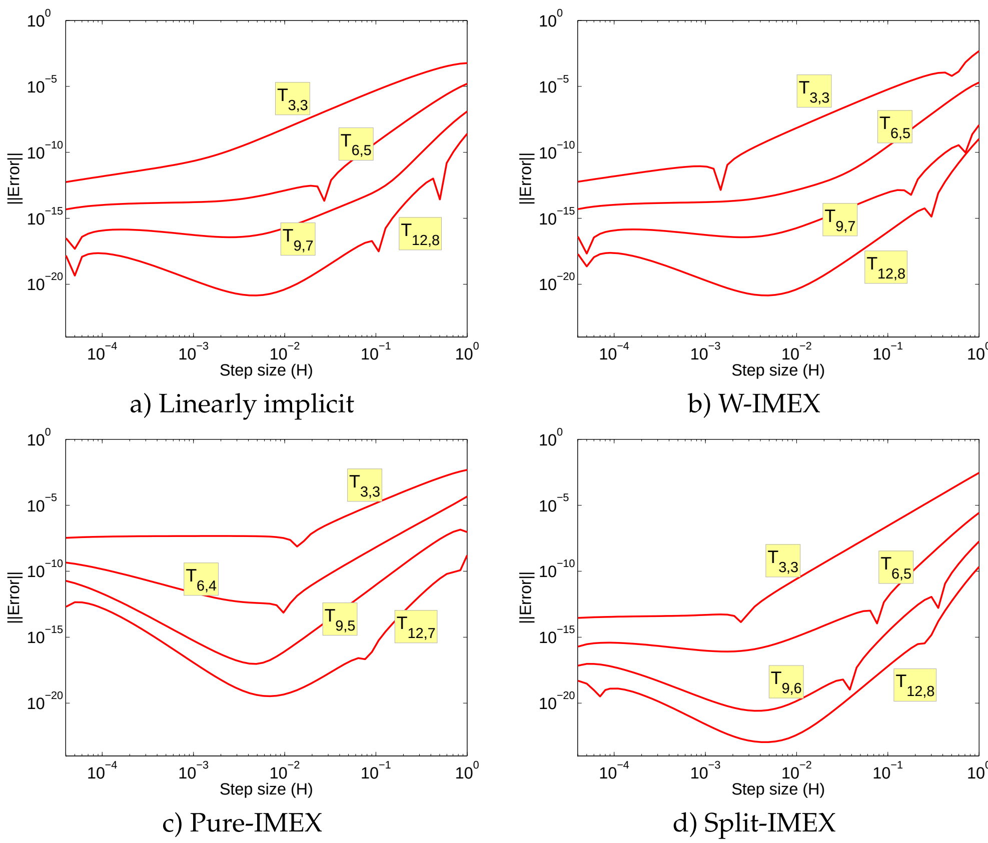


FIG. 6.3. *Local error vs. step size for the stiff solution component of equation 6.3 investigated in [Hairer and Lubich, 1988] using extrapolated linearly implicit and IMEX methods for the optimal convergence rates with 3, 6, 9, and 12 extrapolation steps.*

6.2. Example from [Hairer and Lubich, 1988]. In this section we present a second stiff differential equation example presented in [Hairer and Lubich, 1988]:

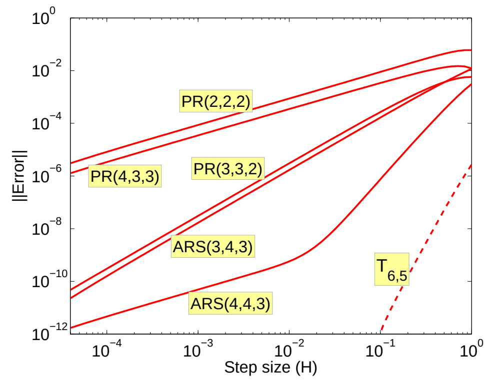
$$\begin{array}{rcl} y' & = & -y \\ \varepsilon\, z' & = & -(1+y)\,z + y^2 \end{array} = \underbrace{\begin{pmatrix} -y \\ 0 \end{pmatrix}}_{=f(y,z)} + \underbrace{\begin{pmatrix} 0 \\ -(1+y)\,z + y^2 \end{pmatrix}}_{=g(y,z)} \tag{6.3}$$

$$y(0) = 0.3\,, \quad z(0) = 0.06923086345026332\,, \quad \varepsilon = 10^{-6}\,.$$

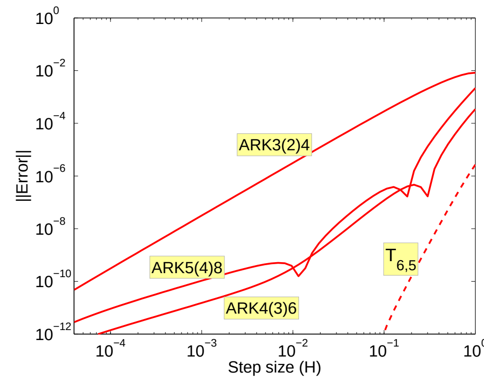
In Figure 6.3 we show the same results for the stiff solution components obtained after one step (H) with the extrapolated linearly implicit and proposed IMEX methods using the same setting as in the previous section (6.1).

In Figure 6.4 we present the stiff component local errors using several IMEX Runge-Kutta methods. The conclusions mirror the ones presented in Section 6.1.

7. Numerical Results for PDEs. We next investigate the discretization accuracy of the advection-reaction (time dependent) PDE using the W-IMEX, Pure-IMEX, and Split-IMEX schemes. In this section we use x as the spatial variable and t as the temporal variable. The implementation is carried out in Matlab® with double precision.



a) ARS and PR



b) ARK

FIG. 6.4. *Local error vs. step size for the stiff solution component of equation 6.3 proposed in [Hairer and Lubich, 1988] using several IMEX Runge-Kutta methods and $T_{6,5}$ Split-IMEX for comparison.*

The estimated numerical order of convergence is computed by using the L_1 error norm given by $L_1(= \Delta x/m \sum_{i=1}^{m} |\mathrm{Err}_i|)$, where m is the number of variables, at the final time using different step sizes (H).

We also discuss the order reduction phenomenon due to stiff boundary or source terms [Sanz-Serna et al., 1987; Sanz-Serna and Verwer, 1989; Carpenter et al., 1995] and explore numerically the behavior of the proposed IMEX methods is such cases.

7.1. Advection-Reaction Equation. We start with the advection-reaction PDE and use the setting described in Hundsdorfer and Ruuth [2007]:

$$\begin{array}{rcl} y_t + \alpha_1\, y_x & = & -k_1 y + k_2 z + s_1 \\ z_t + \alpha_2\, z_x & = & k_1 y - k_2 z + s_2 \end{array}, \quad \begin{array}{l} 0 < x < 1 \\ 0 < t \le 1 \end{array}, \quad \begin{array}{l} \alpha_1 = 1\,,\ k_1 = 10^6\,,\ s_1 = 0 \\ \alpha_2 = 0\,,\ k_2 = 2k_1\,,\ s_2 = 1 \end{array}, \tag{7.1}$$

with

$$y(x,0) = 1 + s_2 x\,, \quad z(x,0) = \frac{k_1}{k_2} y(x,0) + \frac{1}{k_2} s_2 \quad y(0,t) = 1 - \sin(12t)^4\,.$$

This example has two physics components: advection and reaction. We treat the advection term explicitly and the reaction term implicitly due to its numerical stiffness.

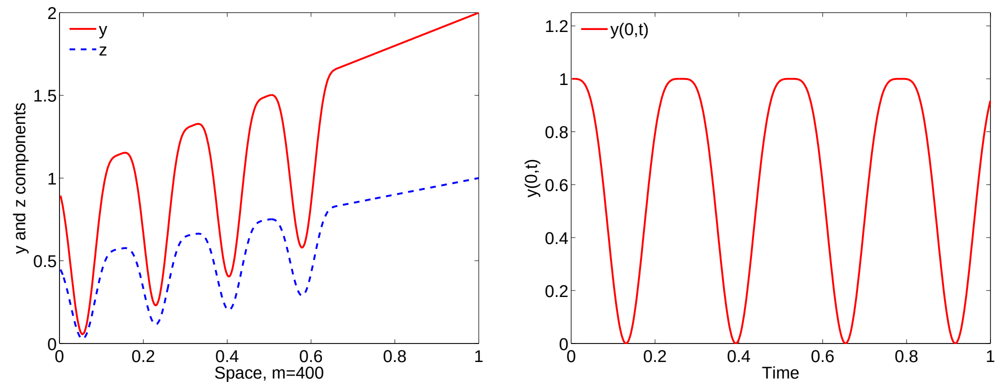
For the spatial discretization we use the fourth order central finite difference scheme for the interior points and third order biased schemes at the domain boundaries. We consider a uniform grid: $x_i = i\Delta x$, $i = 1 \ldots m$ with $\Delta x = 1/m$. The solution components for $m = 400$ at $t = 1$ and the inflow boundary condition are displayed in Figure 7.1. The inflow boundary profile is propagated inside the domain through the first component of (7.1).

The experimental orders are shown in Table 7.1. They are in accordance with the theoretical predictions with some components having slightly more optimistic results, which is expected due to the linearity of this example. The W-IMEX and the Split-IMEX schemes give the best results, while the Pure-IMEX scheme is slightly inferior. It is noteworthy that the experimental orders increase with the addition of more terms in the extrapolation tableau. Although not seen here, with a more complex example we conjecture that the W-IMEX method will have a higher order of convergence than the Split-IMEX.

<table>
<tr><td>(1)|1.0|(1)</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>(1)|1.0|(1)</td><td>2.0|1.0|2.0</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>1.0|1.0|1.0</td><td>2.0|1.0|2.0</td><td>3.0|1.9|3.0</td><td></td><td></td><td></td><td></td></tr>
<tr><td>1.2|1.0|1.2</td><td>2.0|1.0|2.0</td><td>3.0|2.0|3.0</td><td>(4)|(2)|(4)</td><td></td><td></td><td></td></tr>
<tr><td>1.0|1.0|1.0</td><td>2.0|1.0|2.0</td><td>3.0|2.0|3.0</td><td>4.0|(3)|4.0</td><td>5.0|(2)|5.0</td><td></td><td></td></tr>
<tr><td>1.0|1.0|1.0</td><td>2.0|1.0|2.0</td><td>3.0|2.0|3.0</td><td>4.0|(3)|4.0</td><td>(5)|3.0|(5)</td><td>(6)|2.3|(6)</td><td></td></tr>
<tr><td>1.0|1.0|1.0</td><td>(2)|1.0|(2)</td><td>3.0|2.0|3.0</td><td>4.0|3.1|4.0</td><td>(5)|(4)|(5)</td><td>(6)|(3)|(6)</td><td>(6)|(2)|(6)</td></tr>
</table>

TABLE 7.1

Numerical orders for the advection-reaction PDE with extrapolated W-IMEX|Pure-IMEX|Split-IMEX schemes ($t_{\text{Final}} = 1$, $m = 400$)



(a) Solution at $t = 1$ (b) Inflow function

FIG. 7.1. *Illustration of (a) the advection-reaction solution and (b) the boundary inflow term* ($y(0,t)$).

7.2. Boundary/Source Order Reduction. Extrapolation methods with explicit methods such as the treatment of f in the proposed IMEX schemes can be represented as explicit Runge-Kutta methods, which have the stage order equal to one. These methods suffer from order reduction. In order to illustrate the boundary/source order reduction phenomenon, we consider a classic test initial value problem with a nonlinear source proposed in [Sanz-Serna et al., 1987]:

$$\frac{\partial y}{\partial t} = -\frac{\partial y}{\partial x} + b(x,t)\,, \quad \begin{array}{c} 0 \le x \le 1 \\ 0 \le t \le 1 \end{array}\,, \quad \begin{array}{c} y(0,t) = b(0,t) \\ y(0,t) = y_0(x) \end{array}\,, \tag{7.2}$$

with the initial condition $y_0(x) = 1 + x$ and (left) boundary and source term defined by $b(x,t) = (t-x)/(1+t)^2$. The exact solution, $y(x,t) = (1+x)/(1+t)$, and the forcing are illustrated in Figure 7.2. Because the solution is linear in space, the first order upwind can be used in the space discretization without introducing discretization errors.

Order reduction due to stiff boundary or source terms is discussed in [Brenner et al., 1982]. Sanz-Serna et al. [1987] show that Runge-Kutta methods with $p \ge 3$ suffer from order reduction. This theoretical result is also verified in our numerical experiments. The discretization error is computed in the L_∞ norm. Special boundary/source treatment to avoid boundary/source order reduction have been discussed in [Abarbanel et al., 1996; Carpenter et al., 1993; Pathria, 1997; Calvo and Palencia, 2002; Carpenter et al., 1995; Sanz-Serna and Verwer, 1989; Sanz-Serna et al., 1987].

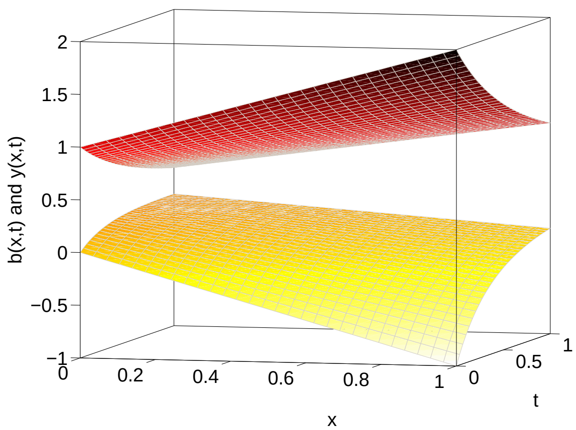


FIG. 7.2. *The exact solution (top) and the forcing (bottom) used to illustrate the order reduction phenomenon.*

Forward Euler Extrapolation					Linear Implicit Euler Extrapolation				
1.003					0.976				
1.001	2.153				0.986	1.62			
1.001	2.002	3.155			0.990	1.69	2.354		
1.001	2.001	2.862	4.325		0.992	1.71	2.449	2.851	
1.001	2.001	2.794	4.010	5.244	0.994	1.73	2.494	2.954	3.569

TABLE 7.2
Illustration of the classical order retention

Case 1: Classical order retention. Here we consider a fixed spatial resolution: $\Delta x = 1/100$. The numerical orders are displayed in Table 7.2.

Case 2: Order reduction. Here we refine in space and time maintaining a CFL of 0.5 [Laney, 1998]. In this case we notice order reduction to second order. The numerical orders are displayed in Table 7.3.

7.2.1. Avoiding Order Reduction. On way to avoid order reduction is by integrating the Dirichlet boundary condition along with the solution [Carpenter et al., 1995]. For example (7.2) we have

$$\frac{\partial \overline{y}}{\partial t} = -\left[\begin{array}{c} 0 \\ F(y) \end{array}\right] + \left[\begin{array}{c} b'(0,t) \\ b(x,t) \end{array}\right], \; F(y) \approx \frac{\partial y}{\partial x}, \; \overline{y}(x,t) = \left[\begin{array}{c} b(0,t) \\ y(x,t) \end{array}\right], \tag{7.3}$$

with the same initial condition.

The numerical orders are estimated just as before for the two settings:

Case 1: Classical order retention. Here we consider a fixed spatial resolution: $\Delta x = 1/100$. The numerical orders are displayed in Table 7.4.

Case 2: Order reduction. Here we refine both in space and time maintaining a CFL of 0.5. In this case we notice order reduction to third order. The numerical orders are displayed in Table 7.5.

The equivalence between the extrapolation methods and explicit or implicit Runge-Kutta methods has the potential to allow the strategy to avoid order reduction applied to Runge-Kutta to be applied just as well to the extrapolation methods and IMEX extrapolation methods.

Forward Euler Extrapolation					Linear Implicit Euler Extrapolation				
0.999					0.913				
0.998	1.900				0.917	1.010			
0.997	1.899	2.032			0.918	1.010	1.014		
0.997	1.898	2.032	2.006		0.919	1.010	1.014	1.015	
0.997	1.898	2.031	2.033	2.019	0.919	1.010	1.014	1.015	1.006

TABLE 7.3
Illustration of the order reduction phenomenon.

Forward Euler Extrapolation					Linear Implicit Euler Extrapolation				
1.003					1.000				
1.001	2.002				1.000	2.001			
1.001	2.001	3.003			0.999	2.002	2.461		
1.001	2.001	3.003	4.174		0.999	2.002	2.530	3.150	
1.001	2.001	3.003	3.877	4.360	0.999	2.002	2.560	3.248	3.699

TABLE 7.4
Extended system - classical order retention

8. Implementation Considerations. In this section we present a few implementation considerations for the extrapolation methods, IMEX extrapolation, and extrapolation methods applied to stiff systems.

Construction of extrapolation methods. The extrapolation methods can be described as a set of increasingly accurate composite schemes. Lower order embedded approximations are computed sequentially, which provides necessary information for a step size (H) control strategy [Hairer et al., 1993b]. Because each computational step in the extrapolation procedure is a consistent approximation of the solution, these methods do not have predetermined number of extrapolation steps (rows in extrapolation tableau), and hence one can consider an adaptive order approach based on error approximations given by the embedded lower order methods. Very high order approximations are easily obtained with no limitation on the theoretical achievable convergence order.

Cost, memory, and parallelization. In the classical setting ($\varepsilon \approx h$), the extrapolation methods are less efficient than the popular Runge-Kutta or linear multistep schemes for the same classical order of accuracy. It is not clear, however, whether the proposed IMEX methods are less efficient because that they do not necessitate nonlinear solver iterations. Moreover, the extrapolation methods can be parallelized very easily [Rauber and Rünger, 1997]. Each entry on the first extrapolation tableau column ($T_{j,1}$) can be computed independently. Moreover, the computational cost is predetermined

$$\text{Cost for } T_{jk} \propto \frac{j(j+1)}{2} \times \text{function evaluations}\,,$$

and thus each entry can be optimally scheduled on multiprocessor/multicore architectures. This could lead to more efficient overall implementations with the total computational cost $\propto j$. In contrast, the IMEX Runge-Kutta methods have a computational cost proportional to the number of implicit stages multiplied by the number of iterations required by the nonlinear solver.

The memory requirements for full extrapolation tableaux are proportional to $j(j+1)/2$, however, as we discuss below, for stiff problems, a large number of tableau

Forward Euler Extrapolation					Linear Implicit Euler Extrapolation				
0.999					0.988				
0.998	2.000				0.987	1.915			
0.997	1.999	2.893			0.987	1.915	2.006		
0.997	1.999	2.893	3.025		0.987	1.915	2.007	2.008	
0.997	1.99	2.893	3.022	2.993	0.987	1.915	2.007	2.008	2.009

TABLE 7.5
Extended system - order reduction

entries need not be computed, and thus the number of registers required in practice can be reduced.

Extrapolation methods for stiff systems. For stiff problems, the diagonal entries in the extrapolation tableau are typically not the best approximations for a given number of extrapolation steps. The theoretical results indicate that the errors propagate in the diagonal direction. In order to avoid errors represented as perturbations (in the SPP context) coming from previous extrapolation steps, and further savings are possible by not computing diagonal and sub-diagonal extrapolation terms. The optimal entries in the extrapolation tableau are emphasized in Table 3.4 given one of the three proposed IMEX methods or the linearly implicit one. This is equivalent to starting the extrapolation procedure with a shifted harmonic sequence $n_j = \ell, \ell+1, \ldots$, $j = 1, 2, \ldots$, and $\ell \geq 1$ can be chosen to include the optimal values (see Table 3.4). If a sufficiently large number of extrapolation steps is computed then the diagonal and an easy to estimate number of sub-diagonal entries need not be computed, and hence alleviating computational and memory requirements.

9. Discussion. In this paper we construct extrapolated implicit-explicit discretization methods that allow to efficiently solve problems that have both stiff and non-stiff components. These methods are well suited for the time integration of multiphysics multiscale partial differential equations. We propose three new extrapolation methods: W-IMEX, Pure-IMEX, and Split-IMEX. These methods have very low implementation costs and can reach easily very high orders of accuracy.

The W-IMEX method resembles the linearly implicit scheme in implementation and performance, however, the W-IMEX scheme does not require the evaluation of the entire Jacobian, which makes it computationally cheaper.

The closely related Pure-IMEX and Split-IMEX methods are truly implicit-explicit methods. The Split-IMEX method has the explicit part sequentially decoupled from the implicit one and has more favorable properties than the Pure-IMEX method.

The methods under investigation can attain a very high discretization order for ODEs, index-1 DAEs, and PDEs in the the method of lines framework. In this study we have not extensively assessed the efficiencies of these methods, however, the numerical tests indicate that they compare well with existing IMEX Runge-Kutta and linear multistep methods.

The proposed IMEX extrapolation methods parallelize very well and are apt to be implemented on the emerging multicore computational architectures. They have low order embedded approximations by construction, which facilitates implementations of error control mechanisms. Moreover, they do not require a predetermined number of steps, making them very robust by allowing variable order strategies.

Numerical results with stiff ODEs, DAEs, and PDEs illustrate our theoretical findings. In our numerical experiments, the Split-IMEX scheme performed best in terms of efficiency and accuracy.

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Appendix A. Linearly Implicit Euler Method.
In this section we review the linearly implicit method. Consider the implicit Euler method applied to problem (1.1) under smoothness assumptions:

$$\begin{aligned} y_{i+1} &= y_i + hF\left(x_{i+1}, y_{i+1}\right) , \\ &= y_i + h\left(J\left(y_{i+1} - y_i\right) + F\left(x_{i+1}, y_i\right)\right) + O(h^2) \\ &= y_i + h\Big(J\left(y_{i+1} - y_i\right) + F\left(x_i, y_i\right) + O(h)\Big) + O(h^2)\,, \end{aligned}$$

where J is an approximation to $\frac{\partial F}{\partial y}(x_i, y_i)$. Then the *linearly implicit Euler* method is given by

$$(I - hJ)\left(y_{i+1} - y_i\right) = hF\left(x_i, y_i\right) .$$

This method has been used in [Deuflhard, 1985; Deuflhard et al., 1987] as the "base method," for solving stiff ODEs of type (1.1) with (2.1), (2.3). In this study we consider $J = F'(y) = (f(y) + g(y))'$.

Appendix B. Transfer Functions. The stability functions for methods (2.4) applied to (2.9) are computed in the following way. For linear implicit Euler (2.4a) we have

$$\begin{aligned} y^{n+1} &= y^n + \left(1 - h\left(\lambda + \mu\right)\right)^{-1}\left(h\,\lambda y^n + h\,\mu y^n\right) , \\ y^{n+1} &= \Big(1 + \left(1 - h\left(\lambda + \mu\right)\right)^{-1} h\,\left(\lambda + \mu\right)\Big)\, y^n = \left(1 + \frac{h\,\lambda + h\,\mu}{1 - h\left(\lambda + \mu\right)}\right) y^n\,, \\ R(z, w) &= 1 + \frac{z + w}{1 - (z + w)} = \frac{1}{1 - (z + w)}\,. \end{aligned}$$

The stability function for the W-IMEX scheme (2.4b) is given by

$$y^{n+1} = y^n + \left[I - h\,g'(y^n)\right]^{-1}\left(h\,f(y^n) + h\,g(y^n)\right) ,$$

$$y^{n+1} = \Big(1 + \left(1 - h\,\mu\right)^{-1}\left(h\,\lambda + h\,\mu\right)\Big)\, y^n = \left(1 + \frac{h\,\lambda + h\,\mu}{1 - h\,\mu}\right) y^n\,, \tag{B.1}$$

$$R(z, w) = 1 + \frac{z + w}{1 - w} = \frac{1 + z}{1 - w}\,. \tag{B.2}$$

For the Pure-IMEX method (2.4c) we have

$$
\begin{aligned}
y^{n+1} &= y^n + h\, f(y^n) + \left[I - h\, g'(y^n)\right]^{-1} \, (h\, g(y^n))\,,\\
y^{n+1} &= \left(1 + h\,\lambda + (1-h\,\mu)^{-1}\,(h\,\mu)\right) y^n = \left(1 + h\,\lambda + \frac{h\,\mu}{1-h\,\mu}\right) y^n\,,\\
R(z,w) &= 1 + z + \frac{w}{1-w} = \frac{1 - w + z - zw + w}{1-w} = \frac{1+z-zw}{1-w}\,. \qquad \text{(B.3)}
\end{aligned}
$$

For the Split-IMEX (2.4d) method we obtain

$$
\begin{aligned}
y^{n+1} &= y^* + \left[I - h\, g'(y^n)\right]^{-1} \, (h\, g(y^*))\,; \qquad y^* = y^n + h\, f(y^n) = y^n + h\,\lambda\, y^n\\
y^{n+1} &= y^n + h\,\lambda\, y^n + \frac{h\, g(y^n + h\,\lambda\, y^n)}{1 - h\, g'(y^n)} = y^n + h\,\lambda\, y^n + \frac{h\,\mu(y^n + h\,\lambda\, y^n)}{1-h\,\mu}\\
y^{n+1} &= \left(1 + h\,\lambda + \frac{h\,\mu(1+h\,\lambda)}{1-h\,\mu}\right) y^n\,,\\
R(z,w) &= 1 + z + \frac{w(1+z)}{1-w} = \frac{1+z}{1-w}\,.
\end{aligned}
$$

Appendix C. Technical Lemmas. The following Lemma is adapted from [Hairer et al., 1993b, Lemma 3.9, chap. VI] and [Deuflhard et al., 1987, Lemma 2].

Lemma C.1 (Bounded series). *Let $\{u_n\}$ and $\{v_n\}$ be two sequences of non-negative numbers satisfying component-wise*

$$
\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} \le \begin{pmatrix} I & 0 \\ \mathcal{O}(1) & \alpha + \mathcal{O}(\varepsilon) \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} + M \begin{pmatrix} h \\ 1 \end{pmatrix} \qquad \text{(C.1)}
$$

with $0 \le \alpha < 1$ and $M \ge 0$. Then the following estimates hold for $\varepsilon \le ch$, $h \le h_0$ and $nh \le Const$

$$
\begin{aligned}
u_n &\le C\,(u_0 + M)\\
v_n &\le C\,(u_0 + (\varepsilon + \alpha^n) v_0 + M)
\end{aligned} \qquad \text{(C.2)}
$$

Proof. The matrix in (C.1) is transformed to diagonal form and iterate to obtain

$$
\begin{pmatrix} u_n \\ v_n \end{pmatrix} \le T^{-1} \begin{pmatrix} I & 0 \\ 0 & \lambda^n \end{pmatrix} T \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + M \sum_{j=1}^{n} T^{-1} \begin{pmatrix} I & 0 \\ 0 & \lambda^{n-j} \end{pmatrix} T \begin{pmatrix} h \\ 1 \end{pmatrix},
$$

where $\lambda = \alpha + \mathcal{O}(\varepsilon)$ are the eigenvalues and the transformation matrix T (composed of eigenvectors) satisfies

$$
T = \begin{pmatrix} 1 & 0 \\ \mathcal{O}(1) & 1 \end{pmatrix}.
$$

The statement follows from the fact that $(\alpha + \mathcal{O}(\varepsilon))^n = \mathcal{O}(\alpha^n) + \mathcal{O}(\varepsilon)$ for $\varepsilon \le ch$ and $nh \le Const$. □

We continue with the following Lemma that is first used in the proof of Theorem 5.1.

Lemma C.2 ([Hairer et al., 1993b, chap. IV, Lem. 5.5]). *Suppose that the logarithmic norm of $g_z(x)$ satisfies*

$$
\mu\left(g_z(x)\right) \le -1 \quad \text{for} \quad 0 \le x \le \overline{x}\,. \qquad \text{(C.3)}
$$

For a given value

$$a(0) = a^{(0)} + \varepsilon a^{(1)} + \cdots + \varepsilon^N a^{(N)} + \mathcal{O}\left(\varepsilon^{N+1}\right)$$

there exists a unique $\left(\text{up to } \mathcal{O}\left(\varepsilon^{N+1}\right)\right)$

$$b(0) = b^{(0)} + \varepsilon b^{(1)} + \cdots + \varepsilon^N b^{(N)} + \mathcal{O}\left(\varepsilon^{N+1}\right)$$

such that the solutions $a(x)$, $b(x)$ of (5.2) and their first N derivatives are bounded independently of ε.

Proof. The proof is discussed in [Hairer et al., 1993b] and it relies on introducing the following finite expansions

$$\widehat{a}(x) = \sum_{i=0}^{N} \varepsilon^i a^{(i)}(x), \qquad \widehat{b}(x) = \sum_{i=0}^{N} \varepsilon^i b^{(i)}(x)(x)$$

in (5.2) and compare the powers of ε. This leads to a differential-algebraic system, from which we obtain that $a^{(0)}(0)$ determines $b^{(0)}(0)$, $b^{(0)}(1)$ determines $a^{(0)}(1)$, and so on. Specifically, we have

$$\begin{aligned}
&\left(a^{(0)}\right)'(x) + \varepsilon\left(a^{(1)}\right)'(x) + \varepsilon^2\left(\left(a^{(2)}\right)'(x)\right)^2 = f_y(x)\left(a^{(0)}(x) + \varepsilon a^{(1)}(x) + \varepsilon^2\left(a^{(2)}(x)\right)^2\right) + \\
&\qquad + f_z(x)\left(b^{(0)}(x) + \varepsilon b^{(1)}(x) + \varepsilon^2\left(b^{(2)}(x)\right)^2\right) + c(x,\varepsilon) + \mathcal{O}\left(\varepsilon^3\right), \\
&\varepsilon\left(\left(b^{(0)}\right)'(x) + \varepsilon\left(b^{(1)}\right)'(x) + \varepsilon^2\left(\left(b^{(2)}\right)'(x)\right)^2\right) = g_y(x)\left(a^{(0)}(x) + \varepsilon a^{(1)}(x) + \varepsilon^2\left(a^{(2)}(x)\right)^2\right) + \\
&\qquad + g_z(x)\left(b^{(0)}(x) + \varepsilon b^{(1)}(x) + \varepsilon^2\left(b^{(2)}(x)\right)^2\right) + d(x,\varepsilon) + \mathcal{O}\left(\varepsilon^3\right).
\end{aligned}$$

By comparing the coefficients of ε^0 we obtain the following DAE:

$$\begin{aligned}
\left(a^{(0)}\right)'(x) &= f_y(x)a^{(0)}(x) + f_z(x)b^{(0)}(x) + c(x,0), \\
0 &= g_y(x)a^{(0)}(x) + g_z(x)b^{(0)}(x) + d(x,0),
\end{aligned}$$

which leads to

$$\begin{aligned}
b^{(0)}(x) &= -g_z^{-1}(x)\left(g_y(x)a^{(0)}(x) + d(x,0)\right), \\
\left(a^{(0)}\right)'(x) &= f_y(x)a^{(0)}(x) - f_z(x)\left[g_z^{-1}(x)\left(g_y(x)a^{(0)}(x) + d(x,0)\right)\right] + c(x,0).
\end{aligned}$$

The coefficients of ε^1 give

$$\begin{aligned}
\left(a^{(1)}\right)'(x) &= f_y(x)a^{(1)}(x) + f_z(x)b^{(1)}(x) + c(x,1), \\
\left(b^{(0)}\right)'(x) &= g_y(x)a^{(1)}(x) + g_z(x)b^{(1)}(x) + d(x,1),
\end{aligned}$$

which leads to

$$\begin{aligned}
b^{(1)}(x) &= -g_z^{-1}(x)\left(g_y(x)a^{(1)}(x) - \left(b^{(0)}\right)'(x) + d(x,1)\right), \\
\left(a^{(1)}\right)'(x) &= f_y(x)a^{(1)}(x) - f_z(x)\left[g_z^{-1}(x)\left(g_y(x)a^{(1)}(x) - \left(b^{(0)}\right)'(x) + d(x,0)\right)\right] + c(x,1).
\end{aligned}$$

These relations confirm that $a^{(0)}(0)$ determines $b^{(0)}(1)$, and $a^{(1)}(0)$ determine $b^{(1)}(0)$, and so on. □