The order of Runge-Kutta methods applied to semi-explicit DAEs of index 1, using Newton-type iterations to compute the internal stage values. *

Anne Kværnø †

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Abstract

This paper concerns the numerical solution of semi-explicit differential-algebraic equations of index 1, using implicit Runge-Kutta methods. The internal stage values are supposed to be computed by some Newton-type technique. By use of Butcher series and rooted trees, a complete characterization of the local error after k iterations is given.

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1 Introduction

Consider a system of differential-algebraic equations (DAEs) of index 1, given by

$$\begin{aligned} y' &= f(y,z), \qquad & y(x_0) = y_0 \\ 0 &= g(y,z), \qquad & z(x_0) = z_0 \end{aligned} \tag{1.1}$$

The index 1 condition ensures $det(\frac{\partial g}{\partial z}) \neq 0$ in some neighbourhood of the exact solution. The DAE is supposed to be solved by some implicit Runge-Kutta method:

$$Y = y_0\varepsilon_s + h\mathcal{A}f(Y,Z), \qquad g(Y,Z) = 0 \tag{1.2}$$

$$y_1 = R(\infty)y_0 + b^T\mathcal{A}^{-1}Y, \qquad z_1 = R(\infty)z_0 + b^T\mathcal{A}^{-1}Z \tag{1.3}$$

where $\mathcal{A} = (a_{ij})_{i,j}$ is the (nonsingular) coefficient matrix of the method, $b = [b_1, \cdots, b_s]^T$ is the weight vector, $\varepsilon_s = [1, \cdots, 1]^T \in I\!R^s$, the stability constant is $R(\infty) = 1 - b^T\mathcal{A}^{-1}\varepsilon_s$, and

*This work was supported by the Norwegian Research Council for Science and Humanities and NorFA.
†Division of Mathematical Sciences, Norwegian Institute of Technology, N-7034 Trondheim-NTH, Norway
E-mail: anne@imf.unit.no

the stage vectors are $Y = [Y_1^T, \cdots, Y_s^T]^T$ and $Z = [Z_1^T, \cdots, Z_s^T]^T$. For simplicity, the obvious tensor notations is omitted.

Usually, (1.2) is solved for Y and Z by some Newton-type iterations,

$$\begin{bmatrix} I - h\mathcal{A}J_{11} & -h\mathcal{A}J_{12} \\ -J_{21} & -J_{22} \end{bmatrix} \begin{bmatrix} Y^{(k+1} - Y^{(k)} \\ Z^{(k+1)} - Z^{(k)} \end{bmatrix} = \begin{bmatrix} y_0\varepsilon_s + h\mathcal{A}f(Y^{(k)}, Z^{(k)}) - Y^{(k)} \\ g(Y^{(k)}, Z^{(k)}) \end{bmatrix} \tag{1.4}$$

where J_{11} etc. are approximations to the Jacobian, and

$$y_1^{(k)} = R(\infty)y_0 + b^T\mathcal{A}^{-1}Y^{(k)}, \qquad z_1^{(k)} = R(\infty)z_0 + b^T\mathcal{A}^{-1}Z^{(k)}$$

In section 3, the theory of rooted trees and Butcher series will be used to give a complete characterization of the local errors. Three different cases of Newton iterations will be studied, the modified Newton case, where the Jacobian is updated only in the beginning of each step, the exact Newton case, and the case where the Jacobian is perturbed by some term $\mathcal{O}(h^\beta)$. The latter, with $\beta = 1$ is the case when the Jacobian is updated regularly, but not every step. The results of section 3 can be summarized as follows:

Theorem 1.1 *Let the following assumptions be satisfied:*

- *The initial values are consistent, thus* $g(y_0, z_0) = 0$.
- *The exact Runge-Kutta method is of local order* $(p_y + 1, p_z + 1)$*:*

$$y_1 - y(x_0 + h) = \mathcal{O}(h^{p_y+1}), \qquad z_1 - z(x_0 + h) = \mathcal{O}(h^{p_z+1}) \tag{1.5}$$

- *The predictor is of order* $q \geq 0$*:*

$$Y_i^{(0)} - y(x_0 + c_ih) = \mathcal{O}(h^{q+1}), \qquad Z_i^{(0)} - z(x_0 + c_ih) = \mathcal{O}(h^{q+1}) \tag{1.6}$$

- *The simplifying assumption* $C(\eta)$ *is satisfied:*

$$\sum_{j=1}^{s} a_{ij}c_j^{l-1} = \frac{c_i^l}{l}, \qquad i = 1, \cdots, s, \quad l = 1, \cdots, \eta \tag{1.7}$$

Let $r = \min(\eta, q)$. *Then the local errors after* k *iterations are given by*

$$y_1^{(k)} - y(x_0 + h) = \mathcal{O}(h^{\min(p_y, q^{(k)}+1)+1}), \qquad z_1^{(k)} - z(x_0 + h) = \mathcal{O}(h^{\min(p_z, q^{(k)})+1}) \tag{1.8}$$

$$g(y_1^{(k)}, z_1^{(k)}) = \begin{cases} \mathcal{O}(h^{\zeta^{(k)}+1}) & \textit{if } b_i = a_{si}, \quad i = 1, \cdots, s \\ \mathcal{O}(h^{\min(p_z, q^{(k)})+1}) & \textit{elsewhere} \end{cases} \tag{1.9}$$

where

$$\begin{aligned} q^{(k)} &= q + k \\ \zeta^{(k)} &= \max(r + k, \min(p_y + 1, q + k)) \end{aligned} \qquad \textit{in the modified Newton case.}$$

$$\begin{aligned} q^{(k)} &= 2^k(r + 1) + q - r - 1 \\ \zeta^{(k)} &= \max(2^k(r + 1) - 1,\ 2(\min(p_y, q^{(k-1)})) + 1) \end{aligned} \qquad \textit{in the exact Newton case.}$$

$$\begin{aligned} q^{(k)} &= r + k \\ \zeta^{(k)} &= r + k \end{aligned} \qquad \textit{in the } \mathcal{O}(h) \textit{ perturbed case.}$$

□

Further we have

Theorem 1.2 *Under the assumptions of Theorem 1.1, the global errors are given by*

$$y_n^{(k)} - y(x_n) = \mathcal{O}(h^{\min(p_y, q^{(k)}+1)}), \qquad z_n^{(k)} - z(x_n) = \mathcal{O}(h^{\xi^{(k)}})$$

where

$$\xi^{(k)} = \begin{cases} \min(p_y, p_z + 1, q^{(k)} + 1) & \textit{if} \quad |R(\infty)| < 1 \\ \min(p_y - 1, p_z, q^{(k)}) & \textit{if} \quad R(\infty) = 1 \\ \min(p_y, p_z + 1, q^{(k)}) & \textit{if} \quad R(\infty) = -1 \end{cases}$$

□

The proof of this theorem is given in section 4. Section 5 is devoted to the presentation of a numerical example confirming our theoretical results.

Recently, a few papers concerning the order increase for Newton type iterations on Runge-Kutta methods have been committed. Our work is heavily based on the work of Jackson et.al. [5], where these algorithms applied to nonstiff ODEs are studied. Dorsselaer and Spijker [1] have given an analysis for stiff, dissipative ODEs. What concerns DAEs, a rough analysis of the $\mathcal{O}(h)$ perturbed case is given by Hairer et. al. [3] for index 1, 2 and 3 problems.

2 Preliminaries

The proof of Theorem 1.1 is heavily based on the theory of *DA-series*, which is the DAE extension of the concepts of B-series. In this section we will introduce some necessary notations and results, which will be used for the proof. For a more comprehensive introduction to the order tree theory for DAEs, see [3], [7] and [8].

2.1 DA-series

We will need the following definitions:

Definition 2.1 [Definition, [8].] *We denote by $DAT = DAT_y \cup DAT_z$ the sets of trees defined recursively by*

a) $\emptyset \in DAT_y \cap DAT_z, \qquad \tau \in DAT_y$

b) If $t_1, \cdots, t_{m_y} \in DAT_y$ *and* $u_1, \cdots, u_{m_z} \in DAT_z$ *then* $t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y \in DAT_y$.

c) If $t_1, \cdots, t_{m_y} \in DAT_y$ *and* $u_1, \cdots, u_{m_z} \in DAT_z$ *then* $u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z \in DAT_z$, *provided that* $(m_y, m_z) \neq (0, 1)$.

Here, $\tau = \bullet$, and $t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y$ is the tree obtained by connecting the roots of $t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}$ by $m_y + m_z$ arcs to a new *meagre* vertex ($\bullet$) which becomes the root of t, and $t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z$ is the tree obtained in the same manner, but with a new *fat* ($\circ$) root.

Let $LDAT = LDAT_y \cup LDAT_z$ be the set of *monotonically labelled trees*, see Definition 2.3 of [7]. The number of meagre vertices of a tree $t \in DAT_y$, $u \in DAT_z$ is called *the order* of the tree, denoted by $\rho(t)$, respectively $\rho(u)$.

For simplicity we will in the following use the notation

$$f_{m_y m_z}(y, z) = \frac{\partial^{m_y + m_z}}{\partial y^{m_y} \partial z^{m_z}} f(y, z)$$

and similar for g.

Definition 2.2 [Definition 1, [8].] *For every tree $t \in DAT_y$ we define a function $F(t)$, and for every tree $u \in DAT_z$ a function $G(u)$ recursively by:*

a) $F(\emptyset)(y, z) = y, \qquad G(\emptyset)(y, z) = z, \qquad F(\tau)(y, z) = f(y, z).$

b) $F(t)(y, z) = f_{m_y m_z}(F(t_1), \cdots, F(t_{m_y}), G(u_1), \cdots, G(u_{m_z}))$ *if* $t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y$.

c) $G(u)(y, z) = (-g_z)^{-1} g_{m_y m_z}(F(t_1), \cdots, F(t_{m_y}), G(u_1), \cdots, G(u_{m_z}))$ *if* $u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z$.

where the obvious arguments have been omitted in b) and c).

Roche extended the concept of B-series:

Definition 2.3 [Definition 3.1, [7].] *Let $a : DAT_y \to \mathbb{R}^l$ and $b : DAT_z \to \mathbb{R}^l$. The series*

$$\begin{aligned} DA_y(a, y, z) &= \sum_{t \in LDAT_y} a(t) F(t)(y, z) \frac{h^{\rho(t)}}{\rho(t)!} \\ DA_z(b, y, z) &= \sum_{u \in LDAT_z} b(t) G(u)(y, z) \frac{h^{\rho(u)}}{\rho(u)!} \end{aligned}$$

are called DA_y, respectively DA_z-series.

For our purpose, l is either 1 or s, the number of stages of the method. In particular, the solution of (1.1) can be written as DA-series

$$y(x_0+h) = DA_y(p_y, y_0, z_0), \qquad z(x_0+h) = DA_z(p_z, y_0, z_0)$$

where $p_y(t) = p_z(u) = 1$ for all $t \in DAT_y$ and $u \in DAT_z$.

If $u, v \in I\!R^l$, let uv be the element-by-element product of the two vectors. Similar, if $v_i \in I\!R^l$, $i = 1, \cdots, m$, let

$$\prod_{i=1}^m v_i = v_1 v_2 \cdots v_m \in I\!R^l$$

For $m < 1$ define $\prod_{i=1}^m u_i = \varepsilon_l$, and if $u_i = u$, $i = 1, \cdots, m$ we denote $\prod_{i=1}^m u_i = u^m$, with $u^0 = \varepsilon_l$. Further, if $\mathcal{A} \in I\!R^{l\times l}$, then let

$$\mathcal{A}\prod_{i=1}^m v_i = \mathcal{A}(\prod_{i=1}^m v_i)$$

Definition 2.4 *For $a : DAT_y \to I\!R^l$, $b : DAT_z \to I\!R^l$, $\rho(t) \geq 1$, $\rho(u) \geq 1$, the* derivatives *$a'(t)$, $b'(u)$ are defined as*

$$\begin{aligned}
a'(\tau) &= \varepsilon_l \\
a'(t) &= \rho(t)\prod_{i=1}^{m_y} a(t_i)\prod_{j=1}^{m_z} b(u_j), \quad \textit{if} \quad t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y \\
b'(u) &= \prod_{i=1}^{m_y} a(t_i)\prod_{j=1}^{m_z} b(u_j) - b(u), \quad \textit{if} \quad u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z
\end{aligned}$$

From Theorem 3 and 4 of [8] we have

Theorem 2.1 *Suppose $Y = DA_y(a, y, z)$ and $Z = DA_z(b, y, z)$ with $a(\emptyset) = b(\emptyset) = \varepsilon_l$. Then*

$$\begin{aligned}
hf(Y, Z) &= DA_y(a', y, z) \\
(-g_z)^{-1} g(Y, Z) &= DA_z(b', y, z)
\end{aligned}$$

with $a'(\emptyset) = b'(\emptyset) = 0$

□

Here and in the following, $(-g_z)^{-1}$ denotes $diag\{-g_z^{-1}(y,z), \cdots, -g_z^{-1}(y,z)\}$. The last theorem of this subsection is an extension of Theorem 2.2 in [6].

Theorem 2.2 *Let* $Y = DA_y(a, y, z)$, $Z = DA_z(b, y, z)$, $U = DA_y(\alpha, y, z)$ *and* $V = DA_z(\beta, y, z)$ *be* DA*-series with* $a(\emptyset) = b(\emptyset) = \varepsilon_l$ *and* $\alpha(\emptyset) = \beta(\emptyset) = 0$. *Then*

$$\begin{aligned} hf_y(Y,Z)U &= DA_y((a,b)\circ\alpha), y, z) \\ hf_z(Y,Z)V &= DA_y((a,b)\circ\beta), y, z) \end{aligned} \tag{2.1}$$

$$\begin{aligned} (-g_z)^{-1}g_y(Y,Z)U &= DA_z((a,b)\circ\alpha), y, z) \\ (-g_z)^{-1}g_z(Y,Z)V &= DA_z((a,b)\circ\beta), y, z) \end{aligned} \tag{2.2}$$

where

$$((a,b)\circ\alpha)(t) = \rho(t)\sum_{l=1}^{m_y}\left(\prod_{\substack{i=1\\ i\neq l}}^{m_y} a(t_i)\prod_{j=1}^{m_z} b(u_j)\right)\alpha(t_l)$$

$$((a,b)\circ\beta)(t) = \rho(t)\sum_{l=1}^{m_z}\left(\prod_{i=1}^{m_y} a(t_i)\prod_{\substack{j=1\\ j\neq l}}^{m_z} b(u_j)\right)\beta(u_l)$$

for $t=[t_1,\cdots,t_{m_y},u_1,\cdots,u_{m_z}]_y$, *and*

$$((a,b)\circ\alpha)(u) = \sum_{l=1}^{m_y}\left(\prod_{\substack{i=1\\ i\neq l}}^{m_y} a(t_i)\prod_{j=1}^{m_z} b(u_j)\right)\alpha(t_l)$$

$$((a,b)\circ\beta)(u) = \sum_{l=1}^{m_z}\left(\prod_{i=1}^{m_y} a(t_i)\prod_{\substack{j=1\\ j\neq l}}^{m_z} b(u_j)\right)\beta(u_l)-\beta(u)$$

for $u=[t_1,\cdots,t_{m_y},u_1,\cdots,u_{m_z}]_z$. *Further are* $((a,b)\circ\alpha)(\emptyset)=((a,b)\circ\beta)(\emptyset)=((a,b)\circ\alpha)(\tau)=((a,b)\circ\beta)(\tau)=0$.

Proof: Let $c(t)=a(t)+\delta\alpha(t)$, and $d(u)=b(u)+\delta\beta(u)$. Since $\alpha(\emptyset)=\beta(\emptyset)=0$ then $c(\emptyset)=d(\emptyset)=\varepsilon_l$ for all $\delta\in\mathbb{R}$. Thus Theorem 2.1 can be applied to DA-series with coefficients $c(t)$ or $d(u)$. Let us first prove the first statement of (2.1). We have

$$hf(Y+\delta U,Z)-hf(Y,Z)=DA_y(c',y,z)-DA_y(a',y,z)=DA_y(c'-a',y,z)$$

where for $t=[t_1,\cdots,t_{m_y},u_1,\cdots,u_{m_z}]_y$

$$\begin{aligned} c'(t)-a'(t) &= \rho(t)\prod_{i=1}^{m_y}(a+\delta\alpha)(t_i)\prod_{j=1}^{m_z} b(u_j)-\rho(t)\prod_{i=1}^{m_y} a(t_i)\prod_{j=1}^{m_z} b(u_j)\\ &= \left\{\rho(t)\sum_{l=1}^{m_y}\left(\prod_{\substack{i=1\\ i\neq l}}^{m_y} a(t_i)\prod_{j=1}^{m_z} b(u_j)\right)\alpha(t_l)\right\}\delta+\mathcal{O}(\delta^2)\end{aligned}$$

Thus

$$hf(Y+\delta U,Z)-hf(Y,Z)=\left\{\sum_{t\in LDAT_y}((a,b)\circ\alpha)(t)F(t)(y,z)\frac{h^{\rho(t)}}{\rho(t)!}\right\}\delta+\mathcal{O}(\delta^2)$$

By the definition of direction derivative the statement follows. The second statement of (2.1) is found in a similar way. To prove (2.2) we first have

$$(-g_z)^{-1} g(Y + \delta U, Z) - (-g_z)^{-1} g(Y, Z) = DA_z(d' - b', y, z)$$

where for $u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z$

$$\begin{aligned}
d'(u) - b'(u) &= \prod_{i=1}^{m_y} (a + \delta\alpha)(t_i) \prod_{j=1}^{m_z} b(u_j) - b(u) - \prod_{i=1}^{m_y} a(t_i) \prod_{j=1}^{m_z} b(u_j) + b(u) \\
&= \left\{ \sum_{l=1}^{m_y} \left(\prod_{\substack{i=1 \\ i \neq l}}^{m_y} a(t_i) \prod_{j=1}^{m_z} b(u_j) \right) a(t_l) \right\} \delta + \mathcal{O}(\delta^2)
\end{aligned}$$

Similar

$$(-g_z)^{-1} g(Y, Z + \delta V) - (-g_z)^{-1} g(Y, Z) = DA_z(d' - b', y, z)$$

where now

$$\begin{aligned}
d'(u) - b'(u) &= \prod_{i=1}^{m_y} a(t_i) \prod_{j=1}^{m_z} (b + \delta\beta)(u_j) - (b + \delta\beta)(u) - \prod_{i=1}^{m_y} a(t_i) \prod_{j=1}^{m_z} b(u_j) + b(u) \\
&= \left\{ \sum_{l=1}^{m_z} \left(\prod_{i=1}^{m_y} a(t_i) \prod_{\substack{j=1 \\ j \neq l}}^{m_z} b(u_j) \right) \beta(u_l) - \beta(u) \right\} \delta + \mathcal{O}(\delta^2)
\end{aligned}$$

which completes the proof of (2.2).

□

2.2 Order conditions

Now, consider the Runge-Kutta scheme (1.2), (1.3). Y, Z, y_1 and z_1 can all be written as DA-series.

Theorem 2.3 *Let the initial values (y_0, z_0) be consistent, that is $g(y_0, z_0) = 0$. Then we have*

$$Y = DA_y(\phi_y, y_0, z_0), \qquad Z = DA_z(\phi_z, y_0, z_0)$$

$$y_1 = DA_y(\psi_y, y_0, z_0), \qquad z_1 = DA_z(\psi_z, y_0, z_0)$$

with coefficients

$$\begin{aligned}
\phi_y(\emptyset) &= \phi_z(\emptyset) = \varepsilon_s \\
\phi_y(\tau) &= c \\
\phi_y(t) &= \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y(t_i)\prod_{j=1}^{m_z}\phi_z(u_j) \quad \mathit{for} \quad t = [t_1,\cdots,t_{m_y},u_1,\cdots,u_{m_z}]_y \\
\phi_z(u) &= \prod_{i=1}^{m_y}\phi_y(t_i)\prod_{j=1}^{m_z}\phi_z(u_j) \quad \mathit{for} \quad u = [t_1,\cdots,t_{m_y},u_1,\cdots,u_{m_z}]_z
\end{aligned}$$

$$\begin{aligned}
\psi_y(\emptyset) &= 1, & \psi_z(\emptyset) &= 1 \\
\psi_y(t) &= b^T\mathcal{A}^{-1}\phi_y(t), & \psi_z(u) &= b^T\mathcal{A}^{-1}\phi_z(u)
\end{aligned} \tag{2.3}$$

Proof: The proof is a consequence of Theorem 5 in [8].

□

From this it follows that the method is of *local order* (p_y+1, p_z+1) if and only if

$$\begin{aligned}
\psi_y(t) &= 1, & \forall t \in DAT_y,\ \ \rho(t) \le p_y \\
\psi_z(u) &= 1, & \forall u \in DAT_z,\ \ \rho(u) \le p_z
\end{aligned} \tag{2.4}$$

Further we have that $p_y \ge p_z$, and if $b_i = a_{si}$, then $p_y = p_z$, see [8].

2.3 Φ-sets

The Φ-sets are the sets of all order weights of a certain order. Thus

$$\Phi_{y,p} = \{\phi_y(t) \mid \forall t \in DAT_y,\ \rho(t) = p\}, \qquad \Phi_{z,p} = \{\phi_z(u) \mid \forall u \in DAT_z,\ \rho(u) = p\}$$

and $\Phi_p = \Phi_{y,p} \cup \Phi_{z,p}$. We will also need the sets

$$\begin{aligned}
\Omega_{y,p} &= \{\phi_1 + \sum_{i=1}^{\mu}\kappa_i(\phi_{i1}-\phi_{i2}) \mid \phi_1,\phi_{i1},\phi_{i2} \in \Phi_{y,p},\ \kappa_i \in \mathbb{R},\ i = 1,2,\cdots\mu\} \\
\Omega_{z,p} &= \{\phi_1 + \sum_{i=1}^{\mu}\kappa_i(\phi_{i1}-\phi_{i2}) \mid \phi_1,\phi_{i1},\phi_{i2} \in \Phi_{z,p},\ \kappa_i \in \mathbb{R},\ i = 1,2,\cdots,\mu\}
\end{aligned}$$

and $\Omega_p = \Omega_{y,p} \cup \Omega_{z,p}$. It follows immediately from the definitions that $\Phi_{y,p} \subset \Omega_{y,p}$, $\Phi_{z,p} \subset \Omega_{z,p}$ and $\Phi_p \subset \Omega_p$. We have the following result

Lemma 2.1

a) If $\phi_{y,1}, \phi_{y,l,1}, \phi_{y,l,2} \in \Omega_{y,p}$, *and* $\phi_{z,1}, \phi_{z,l,1}, \phi_{z,l,2} \in \Omega_{z,p}$, $\eta_l \in I\!R$, $l = 1 \cdots, \nu$ *then*

$$\phi_{y,1} + \sum_{l=1}^{\nu} \eta_l(\phi_{y,l,1} - \phi_{y,l,2}) \in \Omega_{y,p}, \quad \phi_{z,1} + \sum_{l=1}^{\nu} \eta_l(\phi_{z,l,1} - \phi_{z,l,2}) \in \Omega_{z,p}$$

b) If $\phi_1 \in \Phi_{p_1}, \cdots, \phi_m \in \Phi_{p_m}$, *and* $p = \sum_{i=1}^{m} p_i + 1$ *then*

$$p\mathcal{A} \prod_{i=1}^{m} \phi_i \in \Phi_{y,p}, \quad \prod_{i=1}^{m} \phi_i \in \Phi_{z,p-1}$$

c) Similar, if $\phi_1 \in \Omega_{p_1}, \cdots, \phi_m \in \Omega_{p_m}$ *then*

$$p\mathcal{A} \prod_{i=1}^{m} \phi_i \in \Omega_{y,p}, \quad \prod_{i=1}^{m} \phi_i \in \Omega_{z,p-1}$$

d) If the method is of local order $(p_y + 1, p_z + 1)$ *then*

$$\phi_y \in \Omega_{y,r_y} \quad \Rightarrow \quad b^T \mathcal{A}^{-1} \phi_y = 1, \;\; r_y \le p_y$$

$$\phi_z \in \Omega_{z,r_z} \quad \Rightarrow \quad b^T \mathcal{A}^{-1} \phi_z = 1, \;\; r_z \le p_z$$

Proof: The proof of *a)* is straightforward. Result *b)* follows from Theorem 2.3 and the fact that $\rho(t = [t_1, \cdots, t_m]_y) = \sum_{i=1}^{m} \rho(t_i) + 1$ and $\rho(t = [t_1, \cdots, t_m]_z) = \sum_{i=1}^{m} \rho(t_i)$. *c)* is proved in a similar way as the proof of Lemma 2.5 of [5]. *d)* follows from the fact that if $\phi_y \in \Omega_{y,r_y}$, $r_y \le p_y$ then

$$b^T \mathcal{A}^{-1} \phi_y = b^T \mathcal{A}^{-1} \phi_{y,1} + \sum_{l=1} \kappa_l (b^T \mathcal{A}^{-1} \phi_{y,l,1} - b^T \mathcal{A}^{-1} \phi_{y,l,2}) = 1 - \sum_{l=1} \kappa_l (1 - 1) = 1$$

where each of the elements in the sum is equal to 1 because of (2.4). Similar if $\phi_z \in \Omega_{z,r_z}$, $r_z \le p_z$.

□

2.4 Functions on trees and minimal order trees.

Jackson et.al. [5] define the *q-lifted number of ramifications* $R(t, q)$ and *the* (r, q)*-lifted Newton doubling index* $D(t, r, q)$ on the set of classical order trees. We will adopt these functions for the order trees given for DAE-problems.

$$\begin{aligned}
R(t, q) &= 0, && \forall t \in DAT, \;\; \rho(t) \le q \\
R(t, q) &= 1, && \forall t \in DAT, \;\; \rho(t) = q + 1 \\
R(t = [t_1, \cdots, t_m]_\bullet, q) &= \begin{cases} R(t_1, q) & \text{if} \quad m = 1 \\ 1 + \max\limits_{i=1,\cdots,m} R(t_i, q) & \text{if} \quad m \ge 2 \end{cases}, && \forall t \in DAT, \;\; \rho(t) \ge q + 2
\end{aligned}$$

where $\bullet$ is either y or z. Let $q \ge r \ge 0$. $D(t, r, q)$ is defined by

$$
\begin{aligned}
&D(t,r,q) = 0, \quad \forall t \in DAT,\ \ \rho(t) \le q \\
&D(t,r,q) = 1, \quad \forall t \in DAT,\ \ \rho(t) = q+1
\end{aligned}
$$

For $\rho(t) \ge q+2$, let $t = [t_1, \cdots, t_m]_\bullet$,
If $m = 1$ then
    $D(t,r,q) = D(t_1,r,q)$
else
    let $\gamma_q = \max\limits_{i=1,\cdots,m} D(t_i,r,q)$
        choose t_R such that $D(t_R,r,q) = \gamma_q$ and
        let $\gamma_r = \max\limits_{\substack{i=1,\cdots,m \\ i\neq R}} D(t_i,r,r)$
    if $\gamma_q \le \gamma_r$ then
        $D(t,r,q) = \gamma_q + 1$
    else
        $D(t,r,q) = \gamma_q$
    end if
end if

The relations between the order of the trees and these functions are

Lemma 2.2 *For all $t \in DAT_y$, $u \in DAT_z$ and $k \ge 1$ we have*

$$
\begin{aligned}
R(t,q) = 1 \quad &\Rightarrow \quad \rho(t) \ge q+1 \\
R(u,q) = 1 \quad &\Rightarrow \quad \rho(u) \ge q+1 \\
R(t,q) = k \quad &\Rightarrow \quad \rho(t) \ge q+k+1 \\
R(u,q) = k \quad &\Rightarrow \quad \rho(u) \ge q+k
\end{aligned}
$$

$$
\begin{aligned}
D(t,r,q) = 1 \quad &\Rightarrow \quad \rho(t) \ge q+1 \\
D(u,r,q) = 1 \quad &\Rightarrow \quad \rho(u) \ge q+1 \\
D(t,r,q) = k \quad &\Rightarrow \quad \rho(t) \ge 2^{k-1}(r+1) + (q-r) + 1 \\
D(u,r,q) = k \quad &\Rightarrow \quad \rho(u) \ge 2^{k-1}(r+1) + (q-r)
\end{aligned}
$$

Proof: Let $t_{R,k}, t_{D,r,k}, t_{D,q,k} \in DAT_y$ be (the general nonunique) trees of minimal order satisfying respectively $R(t_{R,k}, r) = k$, $D(t_{D,r,k}, r, r) = k$ and $D(t_{D,q,k}, r, q) = k$, and let $u_{R,k}, u_{D,r,k}, u_{D,q,k} \in DAT_z$ be defined similarly. Further, let $t_q, t_r \in DAT$ be any trees of order $q+1$ respectively $r+1$. Obviously $t_{R,1} = t_q$, $t_{D,q,1} = t_q$ and $t_{D,r,1} = t_r$ are possible choices if $t_q, t_r \in DAT_y$, and $u_{R,1} = t_q$, $u_{D,q,1} = t_q$, $t_{D,r,1} = t_r$ if $t_q, t_r \in DAT_z$, proving the lemma for $k = 1$. Further for $k = 2$ we have

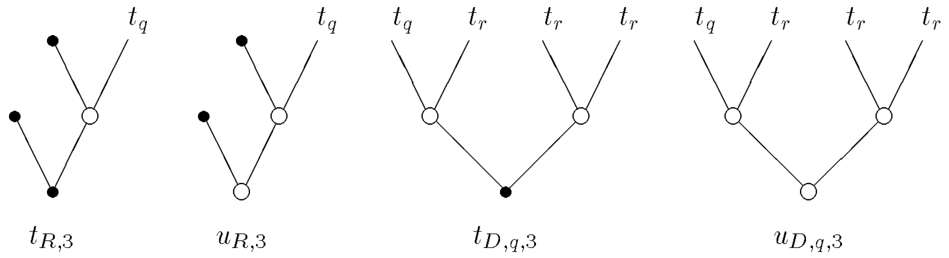

Figure 2.1: Some "minimal order trees".

$$
\begin{aligned}
t_{R,2} = [\tau, t_q]_y &\quad\Rightarrow\quad \rho(t_{R,2}) = \rho(t_q) + 2 = q + 3 \\
u_{R,2} = [\tau, t_q]_z &\quad\Rightarrow\quad \rho(u_{R,2}) = \rho(t_q) + 1 = q + 2 \\
t_{D,q,2} = [t_r, t_q]_y &\quad\Rightarrow\quad \rho(t_{D,q,2}) = \rho(t_r) + \rho(t_q) + 1 = q + r + 3 \\
u_{D,q,2} = [t_r, t_q]_z &\quad\Rightarrow\quad \rho(u_{D,q,2}) = \rho(t_r) + \rho(t_q) = q + r + 2 \\
t_{D,r,2} = [t_r, t_r]_y &\quad\Rightarrow\quad \rho(t_{D,r,2}) = 2\rho(t_r) + 1 = 2r + 3 \\
u_{D,r,2} = [t_r, t_r]_z &\quad\Rightarrow\quad \rho(u_{D,r,2}) = 2\rho(t_r) = 2r + 2
\end{aligned}
$$

It is now easy to show by induction on k that

$$
\begin{aligned}
t_{R,k} = [\tau, u_{R,k-1}]_y &\quad\Rightarrow\quad \rho(t_{R,k}) = \rho(u_{R,k-1}) + 2 = (q + k - 1) + 2 = q + k + 1 \\
u_{R,k} = [\tau, u_{R,k-1}]_z &\quad\Rightarrow\quad \rho(u_{R,k}) = \rho(u_{R,k-1}) + 1 = q + k \\
t_{D,q,k} = [u_{D,r,k-1}, u_{D,q,k-1}]_y &\quad\Rightarrow\quad \rho(t_{D,q,k}) = \rho(u_{D,r,k-1}) + \rho(u_{D,q,k-1}) + 1 \\
&\quad\quad = 2^{(k-1)}(r+1) + (q-r) + 1 \\
u_{D,q,k} = [u_{D,r,k-1}, u_{D,q,k-1}]_z &\quad\Rightarrow\quad \rho(u_{D,q,k}) = \rho(u_{D,r,k-1}) + \rho(u_{D,q,k-1}) \\
&\quad\quad = 2^{(k-1)}(r+1) + (q-r) \\
t_{D,r,k} = [u_{D,r,k-1}, u_{D,r,k-1}]_y &\quad\Rightarrow\quad \rho(t_{D,r,k}) = 2\rho(u_{D,r,k-1}) + 1 = 2^{(k-1)}(r+1) + 1 \\
u_{D,r,k} = [u_{D,r,k-1}, u_{D,r,k-1}]_z &\quad\Rightarrow\quad \rho(u_{D,r,k}) = 2\rho(u_{D,r,k-1}) = 2^{(k-1)}(r+1)
\end{aligned}
$$

□

See Figure 2.1 for examples of "minimal order trees ". As a consequence of the lemma we have

Corollary 2.1 *For all $t \in DAT_y$, $u \in DAT_z$ and $k \geq 1$ we have*

$$\begin{array}{lllllll} \rho(t) & \leq & q+k+1 & \Rightarrow & R(t,q) & \leq & k \\ \rho(u) & \leq & q+k & \Rightarrow & R(t,q) & \leq & k \\ \rho(t) & \leq & 2^k(r+1)+q-r & \Rightarrow & D(t,q) & \leq & k \\ \rho(t) & \leq & 2^k(r+1)+q-r-1 & \Rightarrow & D(t,q) & \leq & k \end{array}$$

□

3 Proof of Theorem 1.1 and related results.

The iteration scheme (1.4) can, by rearranging the terms and multiplying the last equation by $(-g_z)_0^{-1} = diag\{(-g_z^{-1}(y_0,z_0),\cdots,-g_z^{-1}(y_0,z_0)\}$ be written as:

$$Y^{(k+1)} = y_0\varepsilon_s + h\mathcal{A}f(Y^{(k)},Z^{(k)}) + h\mathcal{A}J_{11}(Y^{(k+1)}-Y^{(k)}) + h\mathcal{A}J_{12}(Z^{(k+1)}-Z^{(k)}) \tag{3.1}$$

$$0 = (-g_z)_0^{-1}g(Y^{(k)},Z^{(k)}) + (-g_z)_0^{-1}J_{21}(Y^{(k+1)}-Y^{(k)}) + (-g_z)_0^{-1}J_{22}(Z^{(k+1)}-Z^{(k)}) \tag{3.2}$$

Using the DA-series notations, we have:

$$Y^{(k)} = DA_y(\phi_y^{(k)},y_0,z_0), \qquad Z^{(k)} = DA_z(\phi_z^{(k)},y_0,z_0)$$

$$y_1^{(k)} = DA_y(\psi_y^{(k)},y_0,z_0), \qquad z_1^{(k)} = DA_z(\psi_z^{(k)},y_0,z_0)$$

$$(-g_z)_0^{-1}g(Y^{(k)},Z^{(k)}) = DA_z(\phi_z'^{(k)},y_0,z_0)$$

$$(-g_z)_0^{-1}g(y_1^{(k)},z_1^{(k)}) = DA_z(\psi_z'^{(k)},y_0,z_0)$$

where $\psi_y^{(k)}(t)$, $\psi_z^{(k)}(u)$ are given by (2.3), and $\phi_z'^{(k)}(t)$, $\psi_z'^{(k)}(u)$ by Definition 2.4.

Using the results from Section 2, Theorem 1.1 can be rewritten as:

Theorem 1.1, version 2. *Assume that:*

$$\psi_y(t) = 1,\ \forall t \in DAT_y,\ \rho(t) \leq p_y,\ \text{and}\ \psi_z(u) = 1,\ \forall u \in DAT_z,\ \rho(u) \leq p_z \tag{3.3}$$

$$\phi_y^{(0)}(t) = c^{\rho(t)} \in \Phi_{\rho(t)},\ \phi_z^{(0)}(u) = c^{\rho(u)} \in \Phi_{\rho(u)},\ \forall t,u \in DAT,\ \rho(t),\rho(u) \leq q \tag{3.4}$$

$$\phi_y^{(0)}(t) = \phi_y(t),\ \phi_z^{(0)} = \phi_z(u),\ \forall t,u \in DAT,\ \rho(t),\rho(u) \leq r = \min(q,\eta) \tag{3.5}$$

Then

$$\begin{aligned} \phi_y^{(k)}(t) &= \phi_y(t), \qquad \forall t \in DAT_y,\ \rho(t) \leq r^{(k)}+1 \\ \phi_z^{(k)}(u) &= \phi_z(u), \qquad \forall u \in DAT_z,\ \rho(u) \leq r^{(k)} \end{aligned} \tag{3.6}$$

$$
\begin{aligned}
&\phi_y^{(k)}(t) \in \Omega_{y,\rho(t)}, \qquad \forall t \in DAT_y,\ \rho(t) \le q^{(k)} + 1 \\
&\phi_z^{(k)}(u) \in \Omega_{z,\rho(u)}, \qquad \forall u \in DAT_z,\ \rho(u) \le q^{(k)}
\end{aligned}
\tag{3.7}
$$

For methods satisfying $b_i = a_{si}$, $i = 1, \cdots, s$ we have

$$
\psi_z'^{(k)}(u) = 0,\ \forall u \in DAT_z,\ \rho(u) \le \begin{cases} \max(r^{(k)}, \min(p_y + 1, q^{(k)})) & \textit{(modified Newton)} \\ \max(r^{(k)}, 2\min(p_y, q^{(k-1)}) + 1) & \textit{(exact Newton)} \end{cases}
\tag{3.8}
$$

The assumption (3.3) corresponds to (1.5) by (2.4). The second assumptions (1.6) and (3.4) correspond to each other because

$$
\begin{aligned}
Y_i^{(0)} &= y(x_0 + c_i h) + \mathcal{O}(h^{q+1}) = \sum_{\substack{p=0 \\ p \le q}} y^{(p)}(x_0)\frac{(c_i h)^p}{p!} + \mathcal{O}(h^{q+1}) \\
&= \sum_{\substack{t \in LDAT_y \\ \rho(t) \le q}} c_i^{\rho(t)} F(t)(y_0, z_0)\frac{h^{\rho(t)}}{\rho(t)!} + \mathcal{O}(h^{q+1})
\end{aligned}
$$

similar for Z_i. The simplifying assumption $C(\eta)$ implies that $\Omega_{\rho(t)} = \Phi_{\rho(t)} = \{c^{\rho(t)}\}$, for all $t \in DAT$, $\rho(t) \le \eta$, giving (3.5).

(3.7) implies (1.8), which is proved by Lemma 2.1, Theorem 2.3 and (2.4). By Theorem 2.1, (3.3) together with (3.7) give $\psi_z'^{(k)}(u) = 0$ for all $u \in DAT_z$ and $\rho(u) \le \min(p_z, q^{(k)})$ which, together with (3.8) implies (1.9).

Thus, the proof of Theorem 1.1 is reduced to prove that the assumptions (3.4) and (3.5) implies (3.7) and (3.6), in addition to (3.8). In the next subsections we will prove this theorem, and find the expressions for $r^{(k)}$, $q^{(k)}$ for modified and exact Newton iterations. In subsection 3.3 we are concerned about how a $\mathcal{O}(h^\beta)$-perturbation of the Jacobian will affect the value of $r^{(k)}$ and $q^{(k)}$.

3.1 Modified Newton iteration

In the modified Newton case, the Jacobian is updated every step so that $J_{11}^{(k)} = f_y(y_0\varepsilon_s, z_0\varepsilon_s)$, denoted by $f_{y,0}$, $J_{12}^{(k)} = f_z(y_0\varepsilon_s, z_0\varepsilon_s)$, denoted by $f_{z,0}$, etc. Hence the iteration schemes (3.1) and (3.2) can be written as

$$
Y^{(k+1)} = y_0\varepsilon_s + h\mathcal{A}f(Y^{(k)}, Z^{(k)}) + h\mathcal{A}f_{y,0}(Y^{(k+1)} - Y^{(k)}) + h\mathcal{A}f_{z,0}(Z^{(k+1)} - Z^{(k)}) \tag{3.9}
$$

$$
Z^{(k+1)} = Z^{(k)} + (-g_z)_0^{-1} g(Y^{(k)}, Z^{(k)}) + (-g_z)_0^{-1} g_{y,0}(Y^{(k+1)} - Y^{(k)}) \tag{3.10}
$$

Then we have the following:

Lemma 3.1 *$\phi_y^{(k)}$ and $\phi_z^{(k)}$ satisfy the following recursion:*

$$\phi_y^{(k+1)}(\emptyset) = \varepsilon_s \tag{3.11}$$

If $\phi_y^{(k)}(\emptyset) = \phi_z^{(k)}(\emptyset) = \varepsilon_s$, then

$$\phi_z^{(k+1)}(\emptyset) = \varepsilon_s, \quad \phi_y^{(k+1)}(\tau) = c \tag{3.12}$$

$$\phi_y^{(k+1)}(t) = \begin{cases} \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) & \text{if} \quad t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y, \ m_y + m_z \geq 2 \\ \rho(t)\mathcal{A}\phi_y^{(k+1)}(t_1) & \text{if} \quad t = [t_1]_y \\ \rho(t)\mathcal{A}\phi_z^{(k+1)}(u_1) & \text{if} \quad t = [u_1]_y \end{cases} \tag{3.13}$$

$$\phi_z^{(k+1)}(u) = \begin{cases} \prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) & \text{if} \quad u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z, \quad m_y + m_z \geq 2 \\ \phi_y^{(k+1)}(t_1) & \text{if} \quad u = [t_1]_z \end{cases} \tag{3.14}$$

Proof: The result $\phi_y^{(k+1)}(\emptyset) = \varepsilon_s$ is given immediately by comparing the $\mathcal{O}(1)$ terms of (3.9). To prove the rest of the lemma, let (3.9) and (3.10) be written as DA-series and let the assumptions $\phi_y^{(k)}(\emptyset) = \phi_z^{(k)}(\emptyset) = \varepsilon_s$ be satisfied. Theorem 2.1 can therefore be applied to the terms $hf(Y^{(k)}, Z^{(k)})$ and $(-g_z)_0^{-1}g(Y^{(k)}, Z^{(k)})$, hence (3.9) and (3.10) are given by:

$$\begin{aligned} \sum_{t\in LDAT_y}\phi_y^{(k+1)}(t)F(t)(y_0,z_0)\frac{h^{\rho(t)}}{\rho(t)!} &= y_0\varepsilon_s + \mathcal{A}\sum_{t\in LDAT_y}\phi_y'^{(k)}(t)F(t)(y,z)\frac{h^{\rho(t)}}{\rho(t)!} \\ &+\rho(t)\mathcal{A}\sum_{\substack{t_1\in LDAT_y\\ t=[t_1]_y}}(\phi_y^{(k+1)}(t_1) - \phi_y^{(k)}(t_1))F(t)(y_0,z_0)\frac{h^{\rho(t)}}{\rho(t)!} \\ &+\rho(t)\mathcal{A}\sum_{\substack{u_1\in LDAT_z\\ t=[u_1]_y}}(\phi_z^{(k+1)}(u_1) - \phi_z^{(k)}(u_1))F(t)(y_0,z_0)\frac{h^{\rho(t)}}{\rho(t)!} \end{aligned} \tag{3.15}$$

$$\begin{aligned} \sum_{u\in LDAT_z}\phi_z^{(k+1)}(u)G(u)(y_0,z_0)\frac{h^{\rho(u)}}{\rho(u)!} &= \sum_{u\in LDAT_z}\phi_z^{(k)}(u)G(u)(y_0,z_0)\frac{h^{\rho(u)}}{\rho(u)!} \\ &+ \sum_{u\in LDAT_z}\phi_z'^{(k)}(u)G(u)(y_0,z_0)\frac{h^{\rho(u)}}{\rho(u)!} \\ &+ \sum_{\substack{t_1\in LDAT_y\\ u=[t_1]_z}}(\phi_y^{(k+1)}(t_1) - \phi_y^{(k)}(t_1))G(u)(y_0,z_0)\frac{h^{\rho(u)}}{\rho(u)!} \end{aligned} \tag{3.16}$$

where $\phi_y'^{(k)}(\emptyset) = \phi_z'^{(k)}(\emptyset) = 0$. The last two terms of (3.15) and the last term of (3.16) have been obtained by the use of Theorem 3.5 of [7], which says that

$$f_{y,0}F(t_1) = F([t_1]_y), \quad f_{z,0}G(u_1) = F([u_1]_y), \quad (-g_z)_0^{-1} g_{y,0}F(t_1) = G([t_1]_z).$$

$\phi_z^{(k+1)}(\emptyset) = \phi_z^{(k)}(\emptyset) = \varepsilon_s$ is now given by comparing $\mathcal{O}(1)$ terms of (3.15), (3.16). To find (3.13), compare corresponding trees on both sides of (3.15). In particular, for $t = \tau = [\emptyset]_y$, the last two terms of (3.15) are both equal to 0, and $\phi_y^{(k+1)}(\tau) = \mathcal{A}\phi_y'^{(k)}(\tau) = c$. If $m_y + m_z \geq 2$ the last two terms of (3.15) give no contributions, and

$$\phi_y^{(k+1)}(t) = \mathcal{A}\phi_y'^{(k)}(t) = \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j), \quad t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y$$

For $t = [t_1]_y$ we have

$$\phi_y^{(k+1)}(t) = \mathcal{A}\phi_y'^{(k)}(t) + \rho(t)\mathcal{A}(\phi_y^{(k+1)}(t_1) - \phi_y^{(k)}(t_1)) = \rho(t)\mathcal{A}\phi_y^{(k+1)}(t_1)$$

and similar for $t = [u_1]_y$, proving (3.13). Similarly, (3.14) is found by comparing corresponding trees of (3.16).

□

Lemma 3.2 *For $\nu \geq q \geq r \geq 0$ and $k \geq 0$ we have:*
If

$$\phi_y^{(k)}(t) = \phi_y(t),\ \forall t \in DAT_y, R(t,r) \leq k,\ \ \textit{and}\ \ \phi_z^{(k)}(u) = \phi_z(u),\ \forall u \in DAT_z, R(u,r) \leq k$$

$$\phi_y^{(k)}(t) \in \Phi_{\rho(t)},\ \forall t \in DAT_y, R(t,q) \leq k,\ \ \textit{and}\ \ \phi_z^{(k)}(u) \in \Phi_{\rho(u)},\ \forall u \in DAT_z, R(u,q) \leq k$$

$$\phi_y^{(k)}(t) \in \Omega_{\rho(t)},\ \forall t \in DAT_y, R(t,\nu) \leq k,\ \ \textit{and}\ \ \phi_z^{(k)}(u) \in \Omega_{\rho(u)},\ \forall u \in DAT_z, R(u,\nu) \leq k$$

then

$$\phi_y^{(k+1)}(t) = \phi_y(t),\ \forall t \in DAT_y, R(t,r) \leq k+1,\ \ \textit{and}\ \ \phi_z^{(k+1)}(u) = \phi_z(u),\ \forall u \in DAT_z, R(u,r) \leq k+1$$

$$\phi_y^{(k+1)}(t) \in \Phi_{y,\rho(t)},\ \forall t \in DAT_y, R(t,q) \leq k+1,\ \ \textit{and}\ \ \phi_z^{(k+1)}(u) \in \Phi_{z,\rho(u)},\ \forall u \in DAT_z, R(u,q) \leq k+1$$

$$\phi_y^{(k+1)}(t) \in \Omega_{y,\rho(t)},\ \forall t \in DAT_y, R(t,q) \leq k+1,\ \ \textit{and}\ \ \phi_z^{(k+1)}(u) \in \Omega_{z,\rho(u)},\ \forall u \in DAT_z, R(u,q) \leq k+1$$

Proof: The results follow directly from the definition of R, Theorem 2.3, Lemma 2.1 and Lemma 3.1, see [5] for details.

□

Using this together with Corollary 2.1 we have the following result.

Corollary 3.1 *For $q \geq 0$ and $k \geq 1$ we have:*
If

$$\phi_y^{(0)}(t) = \phi_y(t), \quad \phi_z^{(0)}(u) = \phi_z(u), \quad \forall t, u \in DAT, \quad \rho(t), \rho(u) \leq r$$
$$\phi_y^{(0)}(t) \in \Phi_{\rho(t)}, \quad \phi_z^{(0)}(u) \in \Phi_{\rho(u)}, \quad \forall t, u \in DAT, \quad \rho(t), \rho(u) \leq q$$

then

$$\begin{aligned}
\phi_y^{(k)}(t) &= \phi_y(t), && \forall t \in DAT_y, \quad \rho(t) \leq r + k + 1 \\
\phi_z^{(k)}(u) &= \phi_z(u), && \forall u \in DAT_z, \quad \rho(u) \leq r + k \\
\phi_y^{(k)}(t) &\in \Phi_{y,\rho(t)}, && \forall t \in DAT_y, \quad \rho(t) \leq q + k + 1 \\
\phi_z^{(k)}(u) &\in \Phi_{z,\rho(u)}, && \forall u \in DAT_z, \quad \rho(u) \leq q + k
\end{aligned}$$

□

Thus, the first part of Theorem 1.1 is proved, with $q^{(k)} = q + k$ and $r^{(k)} = r + k$. (3.8) is proved by the fact that if $b_i = a_{si}$, then $\psi_y^{(k)}(t) = \{\phi_y^{(k)}(t)\}_s$, similar for u. Thus,

$$\psi_y^{(k+1)}(t) = \psi_y^{(k)}(t) = \psi_y(t), \; \psi_z^{(k+1)}(u) = \psi_z^{(k)}(u) = \psi_z(u), \; \forall t, u \in DAT, \; \rho(t), \rho(u) \leq \mu^{(k)} \tag{3.17}$$

where $\mu^{(k)} = \max(r^{(k)}, \min(q^{(k)}, p_y))$, using that $p_y = p_z$ for such methods. Now, assume $\rho(t_i), \rho(u_j) \leq \mu^{(k)}$, $i = 1 \cdots, m_y$, $j = 1, \cdots, m_z$, and let $\bar{t} \in DAT_y$ be any tree whatever. Then

$$\begin{aligned}
\psi_z^{(k+1)}(u) &= \prod_{i=1}^{m_y} \psi_y(t_i) \prod_{j=1}^{m_z} \psi_z(u_j) && \text{for } u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z \\
\psi_z^{(k+1)}(u) &= \psi_y^{(k+1)}(\bar{t}) && \text{for } u = [\bar{t}]_z
\end{aligned}$$

Using this we have

$$\psi_z'^{(k+1)}(u) = \prod_{i=1}^{m_y} \psi_y^{(k+1)}(t_i) \prod_{j=1}^{m_z} \psi_z^{(k+1)}(u_j) - \psi_z^{(k+1)}(u) = 0, \qquad \forall u \in DAT_z, \; R(t, \mu^{(k)}) \leq 1$$

which by Corollary 2.1 proves (3.8).

□

3.2 Exact Newton iterations

We will now consider the case where the Jacobian is updated every iteration, thus $J_{11}^{(k)} = f_y(Y^{(k)}, Z^{(k)})$ etc. The iteration scheme is given by

$$\begin{aligned}
Y^{(k+1)} &= y_0 \varepsilon_s + h\mathcal{A} f(Y^{(k)}, Z^{(k)}) && (3.18) \\
&+ h\mathcal{A} f_y(Y^{(k)}, Z^{(k)})(Y^{(k+1)} - Y^{(k)}) + h\mathcal{A} f_z(Y^{(k)}, Z^{(k)})(Z^{(k+1)} - Z^{(k)}) \\
0 &= (-g_z)_0^{-1} g(Y^{(k)}, Z^{(k)}) && (3.19) \\
&+ (-g_z)_0^{-1} g_y(Y^{(k)}, Z^{(k)})(Y^{(k+1)} - Y^{(k)}) + (-g_z)_0^{-1} g_z(Y^{(k)}, Z^{(k)})(Z^{(k+1)} - Z^{(k)})
\end{aligned}$$

The iterated stage weights are given by

Lemma 3.3

$$\phi_y^{(k+1)}(\emptyset) = \varepsilon_s \tag{3.20}$$

If $\phi_y^{(k)}(\emptyset) = \phi_z^{(k)}(\emptyset) = \varepsilon_s$ *then*

$$\begin{aligned}
\phi_z^{(k+1)}(\emptyset) &= \varepsilon_s, \quad \phi_y^{(k+1)}(\tau) = c & (3.21)\\
\phi_y^{(k+1)}(t) &= \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) & (3.22)\\
&+ \rho(t)\mathcal{A}\sum_{l=1}^{m_y}\left(\prod_{\substack{i=1\\ i\neq l}}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)\right)(\phi_y^{(k+1)}(t_l)-\phi_y^{(k)}(t_l))\\
&+ \rho(t)\mathcal{A}\sum_{l=1}^{m_z}\left(\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{\substack{j=1\\ j\neq l}}^{m_z}\phi_z^{(k)}(u_j)\right)(\phi_z^{(k+1)}(u_l)-\phi_z^{(k)}(u_l))\\
\phi_z^{(k+1)}(u) &= \prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) & (3.23)\\
&+ \sum_{l=1}^{m_y}\left(\prod_{\substack{i=1\\ i\neq l}}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)\right)(\phi_y^{(k+1)}(t_l)-\phi_y^{(k)}(t_l))\\
&+ \sum_{l=1}^{m_z}\left(\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{\substack{j=1\\ i\neq l}}^{m_z}\phi_z^{(k)}(u_j)\right)(\phi_z^{(k+1)}(u_l)-\phi_z^{(k)}(u_l))
\end{aligned}$$

for $t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y$ *and* $u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z$.

Proof: Once again we will write (3.18) and (3.19) by their DA-series notation. (3.20) is obvious. In the following let us assume that $\phi_y^{(k)}(\emptyset) = \phi_z^{(k)}(\emptyset) = \varepsilon_s$. Under these assumptions, the $\mathcal{O}(1)$ term of the terms $(-g_z)_0^{-1}g(Y^{(k)}, Z^{(k)})$ and $(-g_z)_0^{-1}g_y(Y^{(k)}, Z^{(k)})(Y^{(k+1)} - Y^{(k)})$ are both equal to 0 by Theorem 2.1 and 2.2 respectively. Thus, the $\mathcal{O}(1)$ term of the last term of (3.19) is 0, giving $\phi_z^{(k+1)}(\emptyset) = \phi_z^{(k)}(\emptyset) = \varepsilon_s$. Now, all the assumptions of Theorem 2.1 and 2.2 are satisfied, therefore we can write (3.18) and (3.19) as

$$\begin{aligned} DA_y(\phi_y^{(k+1)}, y_0, z_0) &= y_0\varepsilon_s + \mathcal{A}\cdot DA_y(\phi_y'^{(k)}, y_0, z_0) \\ &+ \mathcal{A}\cdot DA_y((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_y^{(k+1)} - \phi_y^{(k)}), y_0, z_0) \\ &+ \mathcal{A}\cdot DA_y((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_z^{(k+1)} - \phi_z^{(k)}), y_0, z_0) \\ 0 &= DA_z(\phi_z'^{(k)}, y_0, z_0) \\ &+ DA_z((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_y^{(k+1)} - \phi_y^{(k)}), y_0, z_0) \\ &+ DA_z((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_z^{(k+1)} - \phi_z^{(k)}), y_0, z_0) \end{aligned}$$

By comparing terms of equal trees we get

$$\phi_y^{(k+1)}(t) = \mathcal{A}(\phi_y'^{(k)}(t) + ((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_y^{(k+1)} - \phi_y^{(k)}))(t) + ((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_z^{(k+1)} - \phi_z^{(k)}))(t))$$

which gives $\phi^{(k+1)}(\tau) = \mathcal{A}\varepsilon_s = c$ and (3.22). Further

$$0 = \phi_z'^{(k)}(u) + ((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_y^{(k+1)} - \phi_y^{(k)}))(u) + ((\phi_y^{(k)}, \phi_z^{(k)}) \circ (\phi_z^{(k+1)} - \phi_z^{(k)}))(u)$$

giving (3.23).

$\square$

Lemma 3.4 *Let $\nu \geq r \geq 0$ and $k \geq 0$. If*

$$\phi_y^{(k)}(t) = \phi_y(t),\ \ \forall t \in DAT_y, D(t,r,r) \leq k \ \text{ and } \phi_z^{(k)}(u) = \phi_z(u),\ \ \forall u \in DAT_z, D(u,r,r) \leq k$$

$$\phi_y^{(k)}(t) \in \Omega_{\rho(t)},\ \ \forall t \in DAT_y, D(t,r,\nu) \leq k \ \text{ and } \phi_z^{(k)}(u) \in \Omega_{\rho(u)},\ \ \forall u \in DAT_z, D(u,r,\nu) \leq k$$

then

$$\begin{aligned} \phi_y^{(k+1)}(t) &= \phi_y(t),\ \ \forall t \in DAT_y, D(t,r,r) \leq k+1 \\ \phi_z^{(k+1)}(u) &= \phi_z(u),\ \ \forall u \in DAT_z, D(u,r,r) \leq k+1 \end{aligned} \tag{3.24}$$

$$\begin{aligned} \phi_y^{(k+1)}(t) &\in \Omega_{y,\rho(t)},\ \ \forall t \in DAT_y, D(t,r,\nu) \leq k+1, \\ \phi_z^{(k+1)}(u) &\in \Omega_{z,\rho(u)},\ \ \forall u \in DAT_z, D(u,r,\nu) \leq k+1 \end{aligned} \tag{3.25}$$

Remark: As the following proof will show, the assumption $\phi_y^{(k)}(t) \in \Phi_{\rho(t)}$, $\phi_z^{(k)}(u) \in \Phi_{\rho(u)}$, for all t, u so that $D(t,r,q) \leq k$ and $D(u,r,q) \leq k$ does not guarantee that $\phi_y^{(k+1)}(t) \in \Phi_{y,\rho(t)}$ and similar for $\phi_z^{(k+1)}(u)$ for all trees $D(t,r,q) \leq k+1$ and $D(u,r,k) \leq k+1$.

Proof: Let us first prove the lemma for all trees $t \in DAT_y \cup DAT_z$, with $\rho(t) \leq \nu$, that is $D(t,r,\nu) = 0$. It is obviously true for $\nu = r = 0$. Let the assumptions of the lemma be satisfied for $\nu \geq r \geq 0$. Then, by (3.21) $\phi_y^{(k+1)}(\tau) = \phi_y(\tau)$, and by (3.23)

$$\phi_z^{(k+1)}([\tau]_z) = \phi_y^{(k)}(\tau) + (\phi_y^{(k+1)}(\tau) - \phi_y^{(k)}(\tau)) = \phi_z([\tau]_z)$$

since $\phi_y(\tau) = \phi_z([\tau]_z)$, proving the lemma for trees of order 1 if $\nu = r = 1$. Now, assume the lemma to be true for all trees of order less than or equal to $\bar{r} < r$. Let $t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}$ be trees of order less than or equal to $\bar{r}$, so that $\rho(t) = \bar{r}+1$ for $t = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y$. By Lemma 3.3 and Theorem 2.3 we have

$$\phi_y^{(k+1)}(t) = \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) = \phi_y(t) \tag{3.26}$$

since the last two terms of (3.22) is 0 by assumptions. Thus, the lemma is true for all $t \in DAT_y$, $\rho(t) = \bar{r}+1$. Similar, let $u = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z$ with $\rho(u) = \bar{r}+1$. Then by (3.23)

$$\phi_z^{(k+1)}(u) = \prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) = \phi_z(u)$$

By (3.23), (3.26) we also have that $\phi_z^{(k+1)}([t]_z) = \phi_y^{(k+1)}(t) = \phi_z([t]_z)$ for all $t \in DAT_y$, $\rho(t) = \bar{r}+1$. Thus, (3.24) is proved for all trees of order less than or equal to $\bar{r}+1 \leq r$, and then for all trees of order less than or equal to r. For trees of order less than or equal to ν, (3.25) is proved similarly. The only difference is that each of the terms on the right hand side of (3.22), (3.23) now belongs to $\Omega_{y,\rho(t)}$, resp. $\Omega_{z,\rho(u)}$, so do the whole sum, by Lemma 2.1, item c) and a).

Let us now assume the lemma to be true for all trees with $D(t,r,r) \leq \bar{k} \leq k$. We have already proved it to be true for $\bar{k} = 0$. Let $t_1, \cdots, t_{m_y}$, $u_1, \cdots u_{m_z}$ satisfy $D(t_i,r,r) \leq \bar{k}$, $i = 1, \cdots, m_y$ and $D(u_j,r,r) \leq \bar{k}$ for $j = 1 \cdots, m_y$. Further we assume that $\bar{t} = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_y$ satisfies $D(\bar{t},r,r) = \bar{k}+1$ and $\bar{u} = [t_1, \cdots, t_{m_y}, u_1, \cdots, u_{m_z}]_z$, $D(\bar{u},r,r) \leq \bar{k}+1$, thus $m_y+m_z \geq 2$. By Lemma 3.3 we have

$$\phi_y^{(k+1)}(\bar{t}) = \rho(\bar{t})\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) = \phi_y(\bar{t}) \tag{3.27}$$

$$\phi_z^{(k+1)}(\bar{u}) = \prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j) = \phi_z(\bar{u}) \tag{3.28}$$

since the last two terms of (3.22) and (3.23) is 0 by assumptions. Now, let $t = [t_1, \cdots, t_{m_y}, \bar{t}, u_1, \cdots, u_{m_z}]_y$ and $u = [t_1, \cdots, t_{m_y}, \bar{t}, u_1, \cdots, u_{m_z}]_z$. Thus, by the definition of D, $D(t,r,r) = D(u,r,r) = \bar{k}+1$. By Lemma 3.3 we have

$$\phi_y^{(k+1)}(t) = \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\phi_y^{(k)}(\bar{t})\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)$$

$$
\begin{aligned}
&+ \quad \rho(t)\mathcal{A}\left(\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)\right)(\phi_y^{(k+1)}(\bar t)-\phi_y^{(k)}(\bar t)) \\
&= \quad \rho(t)\mathcal{A}\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)\phi_y^{(k+1)}(\bar t)
\end{aligned}
$$

$$
\begin{aligned}
\phi_z^{(k+1)}(\bar u) &= \prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\phi_y^{(k)}(\bar t)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)+\left(\prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)\right)(\phi_y^{(k+1)}(\bar t)-\phi_y^{(k)}(\bar t)) \\
&= \prod_{i=1}^{m_y}\phi_y^{(k)}(t_i)\prod_{j=1}^{m_z}\phi_z^{(k)}(u_j)\phi_y^{(k+1)}(\bar t)
\end{aligned}
$$

thus by Theorem 2.3 and the assumptions we have

$$
\phi_y^{(k+1)}(t) = \phi_y(t) \tag{3.29}
$$

$$
\phi_z^{(k+1)}(u) = \phi_z(u) \tag{3.30}
$$

Obviously, (3.29) and (3.30) would be valid if $\bar t$ was replaced by $\bar u$. In fact, $\bar t$ could have been replaced with one of all the trees $\bar t \in DAT_y \cup DAT_z$ satisfying $\phi_\bullet^{(k+1)}(\bar t) = \phi_\bullet(\bar t)$. But then these equations are true for all trees satisfying $D(t,r,r) \le \bar k + 1$, and for all $\bar k \le k$. (3.24) is then proved. By replacing $\bar t$ with a tree satisfying $\phi^{(k+1)}(\bar t) \in \Omega_{\rho(\bar t)}$ we can use Lemma 2.1 to prove

$$
\begin{aligned}
\phi_y^{(k+1)}(t) &\in \Omega_{y,\rho(t)} \\
\phi_z^{(k+1)}(u) &\in \Omega_{z,\rho(u)}
\end{aligned}
$$

for all trees satisfying $D(t,r,\nu) \le \bar k + 1$. Since it is true for $\bar k = 0$, it is true for all $\bar k \le k$, thus (3.25) is proved.

□

Again, by using Corollary 2.1 we have

Corollary 3.2 *Let $q \ge r \ge 0$ and $k \ge 1$.*
If

$$
\begin{aligned}
&\phi_y^{(0)}(t) = \phi_y(t), \quad \phi_z^{(0)}(u) = \phi_z(u), \quad \forall t,u \in DAT, \quad \rho(t),\rho(u) \le r \\
&\phi_y^{(0)}(t) \in \Phi_{\rho(t)}, \quad \phi_z^{(0)}(u) \in \Phi_{\rho(u)}, \quad \forall t,u \in DAT, \quad \rho(t),\rho(u) \le q
\end{aligned}
$$

then

$$
\begin{aligned}
&\phi_y^{(k)}(t) = \phi_y(t), && \forall t \in DAT_y, \quad \rho(t) \le 2^k(r+1) \\
&\phi_z^{(k)}(u) = \phi_z(u), && \forall u \in DAT_z, \quad \rho(u) \le 2^k(r+1)-1 \\
&\phi_y^{(k)}(t) \in \Omega_{y,\rho(t)}, && \forall t \in DAT_y, \quad \rho(t) \le 2^k(r+1)+q-r \\
&\phi_z^{(k)}(u) \in \Omega_{z,\rho(u)}, && \forall u \in DAT_z, \quad \rho(u) \le 2^k(r+1)+q-r-1
\end{aligned}
$$

proving the first part of Theorem 1.1 in the exact Newton case, with $q^{(k)} = 2^k(r+1)+q-r-1$ and $r^{(k)} = 2^k(r+1)-1$. To prove (3.8), we again assume that (3.17) to be satisfied. Consider a tree $u = [t_1, \cdots, t_{m_z}, \bar{t}, u_1, \cdots, u_{m_z}]_z$, where the trees t_i, u_j satisfy $\rho(t_i), \rho(u_j) \le \mu^{(k)}$, and $\bar{t}$ can be any tree whatsoever, but for simplicity, we assume $\bar{t} \in DAT_y$. From the proof of Theorem 3.4 it is easy to show that

$$\psi_z^{(k+1)}(u) = \prod_{i=1}^{m_y} \psi_y(t_i) \prod_{j=1}^{m_z} \psi_z(u_j) \psi_y^{(k+1)}(\bar{t})$$

and

$$\psi_z'^{(k+1)}(u) = \prod_{i=1}^{m_y} \psi_y^{(k+1)}(t_i) \prod_{j=1}^{m_z} \psi_z^{(k+1)}(u_j) \psi_y^{(k+1)}(\bar{t}) - \psi_z^{(k+1)}(u) = 0, \ \forall u \in DAT_z, \ D(u, \mu^{(k)}, \mu^{(k)}) \le 1$$

which by Corollary 2.1 proves (3.8).

□

3.3 Perturbed Jacobians.

In this section we consider the case where the Jacobian is perturbed by a term $\mathcal{O}(h^\beta)$, thus

$$\begin{bmatrix} \hat{J}_{11}^{(k)} & \hat{J}_{12}^{(k)} \\ \hat{J}_{21}^{(k)} & \hat{J}_{22}^{(k)} \end{bmatrix} = \begin{bmatrix} J_{11}^{(k)} & J_{12}^{(k)} \\ J_{21}^{(k)} & J_{22}^{(k)} \end{bmatrix} + h^\beta \begin{bmatrix} \Theta_{11}^{(k)} & \Theta_{12}^{(k)} \\ \Theta_{21}^{(k)} & \Theta_{22}^{(k)} \end{bmatrix}$$

where $J_{11}^{(k)} = f_y(y_0\varepsilon_s, y_0\varepsilon_s)$ in the modified Newton case, and $J_{11}^{(k)} = f_y(Y^{(k)}, Z^{(k)})$ in the exact Newton case, etc. $\Theta_{ij}^{(k)}$ are some real, bounded matrices. The iteration scheme can now be written as:

$$\begin{bmatrix} Y^{(k+1)} \\ 0 \end{bmatrix} = \begin{bmatrix} y_0\varepsilon_s + h\mathcal{A}f(Y^{(k)}, Z^{(k)}) \\ (-g_z)_0^{-1} g(Y^{(k)}, Z^{(k)}) \end{bmatrix} + \begin{bmatrix} h\mathcal{A}J_{11}^{(k)} & h\mathcal{A}J_{12}^{(k)} \\ (-g_z)_0^{-1} J_{21}^{(k)} & (-g_z)_0^{-1} J_{22}^{(k)} \end{bmatrix} \begin{bmatrix} Y^{(k+1)} - Y^{(k)} \\ Z^{(k+1)} - Z^{(k)} \end{bmatrix}$$

$$+ \ h^\beta \begin{bmatrix} h\mathcal{A}\Theta_{11}^{(k)} & h\mathcal{A}\Theta_{12}^{(k)} \\ (-g_z)_0^{-1}\Theta_{21}^{(k)} & (-g_z)_0^{(k)}\Theta_{22}^{(k)} \end{bmatrix} \begin{bmatrix} Y^{(k+1)} - Y^{(k)} \\ Z^{(k+1)} - Z^{(k)} \end{bmatrix} \tag{3.31}$$

The first two terms on the right hand side equal the unperturbed scheme, thus we can use results from the previous subsections to write (3.31) as

$$\begin{bmatrix} DA_y(\phi_y^{(k+1)}, y_0, z_0) \\ DA_z(\phi_z^{(k+1)}, y_0, z_0) \end{bmatrix} = \begin{bmatrix} DA_y(\bar{\phi}_y^{(k+1}), y_0, z_0) \\ DA_z(\bar{\phi}_z^{(k+1)}, y_0, z_0) \end{bmatrix} \tag{3.32}$$

$$+ \ h^\beta \begin{bmatrix} h\mathcal{A}\Theta_{11}^{(k)} & h\mathcal{A}\Theta_{12}^{(k)} \\ (-g_z)_0^{-1}\Theta_{21}^{(k)} & (-g_z)_0^{(k)}\Theta_{22}^{(k)} \end{bmatrix} \begin{bmatrix} DA_y(\phi_y^{(k+1)} - \phi_y^{(k)}, y_0, z_0) \\ DA_z(\phi_z^{(k+1)} - \phi_z^{(k)}, y_0, z_0) \end{bmatrix}$$

where $\bar{\phi}_y^{(k+1)}(t)$, $\bar{\phi}_z^{(k+1)}(t)$ are given by Lemma 3.1 or 3.3, with $\phi_\bullet^{(k+1)}$ replaced by $\bar{\phi}_\bullet^{(k+1)}$.

For simplicity we will in the following use R and D to distinguish the modified from the exact Newton case. Thus $RD(t,r,\nu)$ means $R(t,\nu)$ when talking of modified Newton iterations, while it means $D(t,r,\nu)$ for the exact Newton case. Using (3.32), we can state the following:

Lemma 3.5 *Let $\nu \geq q \geq r \geq 0$, $\beta \geq 0$ and $k > 0$.*
If

$$\begin{array}{llll} \phi_y^{(k)}(t) = \phi(t), & \phi_z^{(k)}(u) = \phi_z(u), & \forall t,u \in DAT, & \rho(t),\rho(u) \leq r \\ \phi_y^{(k)}(t) \in \Phi_{\rho(t)}, & \phi_z^{(k)}(u) \in \Phi_{\rho(u)}, & \forall t,u \in DAT, & \rho(t),\rho(u) \leq q \\ \phi_y^{(k)}(t) \in \Omega_{\rho(t)}, & \phi_z^{(k)}(u) \in \Omega_{\rho(u)}, & \forall t,u \in DAT, & \rho(t),\rho(u) \leq \nu \end{array}$$

then

$$\begin{array}{llll} \phi_y^{(k+1)}(t) = \phi_y(t), & \forall t \in DAT_y, & RD(t,r,r) \leq 1, & \rho(t) \leq r+\beta+1 \\ \phi_z^{(k+1)}(u) = \phi_z(u), & \forall u \in DAT_z, & RD(u,r,r) \leq 1, & \rho(u) \leq r+\beta \\ \phi_y^{(k+1)}(t) \in \Phi_{y,\rho(t)}, & \forall t \in DAT_y, & R(t,q) \leq 1, & \rho(t) \leq r+\beta+1 \\ \phi_z^{(k+1)}(u) \in \Phi_{z,\rho(u)}, & \forall u \in DAT_z, & R(u,q) \leq 1, & \rho(u) \leq r+\beta \\ \phi_y^{(k+1)}(t) \in \Omega_{y,\rho(t)}, & \forall t \in DAT_y, & RD(t,r,\nu) \leq 1, & \rho(t) \leq r+\beta+1 \\ \phi_z^{(k+1)}(u) \in \Omega_{z,\rho(u)}, & \forall u \in DAT_z, & RD(u,r,\nu) \leq 1, & \rho(u) \leq r+\beta \end{array}$$

Proof: The last term of (3.32) gives contributions only to the iterated stage weights of trees of order greater than $\beta+r+1$ in the y-component, and of order greater than $\beta+r$ in the z-component. Thus $\phi_y^{(k+1)}(t) = \bar{\phi}_y^{(k+1)}(t)$ for all t with $\rho(t) \leq r+\beta+1$, and $\phi_z^{(k+1)}(u) = \bar{\phi}_z^{(k+1)}(u)$ for all u with $\rho(u) \leq r+\beta$. This together with the results from subsection 3.1 and 3.2 prove the lemma.

□

The main result of this subsection is:

Theorem 3.1 *Let $\nu \geq q \geq r \geq 0$, $\beta \geq 0$ and $k \geq 1$.*
If

$$\begin{array}{llll} \phi_y^{(0)}(t) = \phi_y(t), & \phi_z^{(0)}(u) = \phi_z(u), & \forall t,u \in DAT, & \rho(t),\rho(u) \leq r \\ \phi_y^{(0)}(t) \in \Phi_{\rho(t)}, & \phi_z^{(0)}(u) \in \Phi_{\rho(u)}, & \forall t,u \in DAT, & \rho(t),\rho(u) \leq q \\ \phi_y^{(0)}(t) \in \Omega_{\rho(t)}, & \phi_z^{(0)}(u) \in \Omega_{\rho(u)}, & \forall t,u \in DAT, & \rho(t),\rho(u) \leq \nu \end{array}$$

then

$$\begin{array}{lll}
\phi_y^{(k)}(t) = \phi_y(t), & \forall t \in DAT_y, & \rho(t) \le r_k^{RD} + 1 \\
\phi_z^{(k)}(u) = \phi_z(u), & \forall u \in DAT_z, & \rho(u) \le r_k^{RD} \\
\phi_y^{(k)}(t) \in \Phi_{y,\rho(t)}, & \forall t \in DAT_y, & \rho(t) \le q_k^{R} + 1 \\
\phi_z^{(k)}(u) \in \Phi_{z,\rho(u)}, & \forall u \in DAT_z, & \rho(u) \le q_k^{R} \\
\phi_y^{(k)}(t) \in \Omega_{y,\rho(t)}, & \forall t \in DAT_y, & \rho(t) \le \nu_k^{RD} + 1 \\
\phi_z^{(k)}(u) \in \Omega_{z,\rho(u)}, & \forall u \in DAT_z, & \rho(u) \le \nu_k^{RD}
\end{array}$$

where

$$r_k^R = q_k^R = \nu_k^R = r \qquad \text{for } \beta = 0 \tag{3.33}$$

$$r_k^R = r + k, \ q_k^R = \min(q, r+\beta) + k, \ \nu_k^R = \min(\nu, r+\beta) + k \quad \text{for } \beta \ge 1 \tag{3.34}$$

$$r_k^D = \begin{cases} 2^k(r+1) - 1, & \text{for } k \le k_m \\ 2^{k_m}(r+1) + \beta(k - k_m) - 1, & \text{for } k > k_m \end{cases} \tag{3.35}$$

$$\nu_k^D = \begin{cases} 2^k(r+1) + \nu - r - 1, & \text{for } k \le k_n \\ 2^{k-1}(r+1) + \beta - 1, & \text{for } k_n < k \le k_m \\ 2^{k_m}(r+1) + \beta(k - k_m) - 1, & \text{for } k > k_m \end{cases} \tag{3.36}$$

and

$$k_n = \begin{cases} \left[\log_2\left(\frac{\beta - \nu + r}{r+1}\right)\right] + 1, & \nu + 1 < \beta \\ 0 & \text{otherwise} \end{cases}$$

$$k_m = \begin{cases} \left[\log_2\left(\frac{\beta}{r+1}\right)\right] + 1, & r + 1 < \beta \\ 0 & \text{otherwise} \end{cases}$$

where $[\bullet]$ *denotes the integer part of* $\bullet$*.*

Proof: From Corollary 2.1 we have

$$\begin{array}{lll}
\rho(u) \le r + 1 & \Rightarrow & R(t, r) \le 1 \\
\rho(u) \le 2r + 1 & \Rightarrow & D(t, r, r) \le 1 \\
\rho(u) \le r + \nu + 1 & \Rightarrow & D(t, r, \nu) \le 1
\end{array}$$

which together with Lemma 3.5 give the following recursions:

$$\begin{aligned}
r^R_{k+1} &= \min(r^R_k + 1, r^R_k + \beta) \\
q^R_{k+1} &= \min(q^R_k + 1, r^R_k + \beta) \\
\nu^R_{k+1} &= \min(\nu^R_k + 1, r^R_k + \beta) \\
r^D_{k+1} &= \min(2r^D_k + 1, r^D_k + \beta) \\
\nu^D_{k+1} &= \min(r^D_k + \nu^D_k + 1, r^D_k + \beta)
\end{aligned}$$

with $r^{RD}_0 = r$, $q^R_0 = q$ and $\nu^{RD}_0 = \nu$. (3.33) and (3.34) are now given directly.

The exact Newton case is somewhat more complicated. As long as $2r^D_{k-1} + 1 \leq r^D_{k-1} + \beta$, the convergence is quadratic, and by Corollary 2.1 $r^D_k = 2^k(r+1) - 1$. This is the case as long as

$$2(2^{k-1}(r+1) - 1) + 1 \leq 2^{k-1}(r+1) - 1 + \beta$$

or

$$k \leq \log_2\left(\frac{\beta}{r+1}\right) + 1$$

giving k_m and the first equation of (3.35). For $k > k_m$, $r^D_{k+1} = r^D_k + \beta$, with $r^D_{k_m} = 2^{k_m}(r+1) - 1$, which proves the second equation of (3.35). For $r + 1 \geq \beta$ the r^D_k will be given by the last term of the recursion, thus $r^D_k = r + \beta k$, proving the case for which $k_m = 0$.

(3.36) is found similarly.

□

4 Convergence results.

This section is devoted to the proof of Theorem 1.2.

The exact Runge-Kutta method is given by (1.2) and (1.3). From (1.2) it is clear that the stage values Y and Z are independent of the starting value z_n, thus $Y = Y(y_n; h)$ and $Z = Z(y_n; h)$. The method can then be written as

$$y_{n+1} = y_n + h\mathcal{F}(y_n; h), \qquad z_{n+1} = R(\infty)z_n + \mathcal{G}(y_n; h)$$

where $\mathcal{F} = b^T f(Y, Z)$ and $\mathcal{G} = b^T \mathcal{A}^{-1} Z$. The exact solution of the problem satisfies

$$y(x_n + h) = y(x_n) + h\mathcal{F}(y(x_n); h) + d_{y,n+1} \tag{4.1}$$

$$z(x_n + h) = R(\infty)z(x_n) + \mathcal{G}(y(x_n); h) + d_{z,n+1} \tag{4.2}$$

$d_{y,n+1}$ and $d_{z,n+1}$ are the local error terms of the exact method. These terms can be written as

$$d_{y,n+1} = d_{y,p_y+1}(x_n)h^{p_y+1} + \mathcal{O}(h^{p_y+2}), \qquad d_{z,n+1} = d_{z,p_z+1}(x_n)h^{p_z+1} + \mathcal{O}(h^{p_z+2})$$

The iterated method satisfy

$$y_{n+1}^{(k)} = y_n^{(k)} + h\mathcal{F}(y_n^{(k)}; h) + \mathcal{O}(h^{\nu_y^{(k)}+1}) \quad (4.3)$$

$$z_{n+1}^{(k)} = R(\infty)z_n^{(k)} + \mathcal{G}(y_n^{(k)}; h) + \mathcal{O}(h^{\nu_z^{(k)}+1}) \quad (4.4)$$

where $\nu_y^{(k)} = \max(r^{(k)}+1, \min(p_y, q^{(k)}+1))$ and $\nu_z^{(k)} = \max(r^{(k)}, \min(p_z, q^{(k)}))$. Subtracting (4.1) from (4.3) gives

$$y_{n+1}^{(k)} - y(x_n+h) = y_n^{(k)} - y(x_n) + h\frac{\partial \mathcal{F}}{\partial y}(\xi; h)(y_n^{(k)} - y(x_n)) + \mathcal{O}(h^{\min(p_y, q^{(k)}+1)+1})$$

and well known theory, f.inst. [4], Theorem 3.4, can be used to prove

$$y_n^{(k)} - y(x_n) = \mathcal{O}(h^{\min(p_y, q^{(k)}+1)})$$

If $q^{(k)}+1 > p_y$ then

$$y(x_n+h) = y(x_n) + h\mathcal{F}(y(x_n); h) + d_{y,p_y+1}^{(k)}(x_n)h^{p_y+1} + \mathcal{O}(h^{p_y+2})$$

where $d_{y,p_y+1}^{(k)} = d_{y,p_y+1}$ if $r^{(k)} \geq p_y+1$. By [4], Theorem 8.1 we have

$$y_n^{(k)} - y(x_n) = e_{y,p_y}^{(k)}(x_n)h^{p_y} + \mathcal{O}(h^{p_y+1}) \quad (4.5)$$

where $e_{y,p_y}^{(k)}(x)$ is differentiable.

To find the global error of the z-component, we subtract (4.2) from (4.4).

$$z_{n+1}^{(k)} - z(x_n+h) = R(\infty)(z_n^{(k)} - z(x_n)) + \delta_{z,n+1}$$

where $\delta_{z,n+1} = \mathcal{O}(h^{\min(p_y, p_z+1, q^{(k)}+1)})$. Thus

$$z_n^{(k)} - z(x_n) = \sum_{i=1}^{n} R(\infty)^{n-i}\delta_{z,i}$$

proving the result for the z-component of Theorem 1.2 for $R(\infty) \neq -1$, and for $R(\infty) = -1$ and $q^{(k)}+1 \leq \min(p_y, p_z+1)$. For the case $R(\infty) = -1$ and $q^{(k)}+1 > \min(p_y, p_z+1)$ we have to study the term $\delta_{z,i}$ in more detail. The term is given by

$$\delta_{z,i} = \frac{\partial \mathcal{G}}{\partial y}(y(x_i); 0)e_{y,p_y}^{(k)}(x_i) + \mathcal{O}(h^{p_y+1}) + d_{z,p_z+1}^{(k)}(x_i)h^{p_z+1} + \mathcal{O}(h^{p_z+2})$$

Thus, for $R(\infty) = -1$, $z_n^{(k)} - z(x_n)$ is a sum of differences

$$\delta_{z,i+1} - \delta_{z,i} = \mathcal{O}(h^{\min(p_y+1, p_z+2)})$$

proving the statement of the theorem for this situation as well.

□

Remark: The result for $R(\infty) = -1$, the global error result is based on the assumption that the the local truncation error of the exact method is a smooth function. However, the iteration error term consists of the $\mathcal{O}(h^q)$ term of the predictor. We have made no assumption on the smoothness on these terms. If the predictor satisfy

$$Y_i^{(0)} - y(x_n + c_i h) = d_{y,i}^{(0)}(x_n)(c_i h)^{q+1} + \mathcal{O}(h^{q+2})$$

and similar for z, then similar arguments as above can be used, and the global order for the z-component is $\min(p_y, p_z + 1, q^{(k)} + 1)$.

$k=1$	$q^{(k)}=1$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-1.469	-2.494	-1.632	1.63	1.13	1.81
$6.25 \cdot 10^{-2}$	-2.017	-2.983	-2.209	1.82	1.62	1.92
$3.125 \cdot 10^{-2}$	-2.593	-3.534	-2.800	1.91	1.83	1.96
$1.5625 \cdot 10^{-2}$	-3.182	-4.112	-3.397	1.96	1.92	1.98

$k=2$	$q^{(k)}=2$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-3.406	-2.911	-2.434	3.63	3.34	3.29
$6.25 \cdot 10^{-2}$	-4.556	-3.862	-3.368	3.82	3.16	3.10
$3.125 \cdot 10^{-2}$	-5.735	-4.790	-4.284	3.92	3.08	3.04
$1.5625 \cdot 10^{-2}$	-6.928	-5.706	-5.193	3.96	3.04	3.02

$k=3$	$q^{(k)}=3$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-5.599	-3.849	-3.325	5.75	4.13	4.15
$6.25 \cdot 10^{-2}$	-7.459	-5.083	-4.562	6.18	4.10	4.11
$3.125 \cdot 10^{-2}$	-9.672	-6.304	-5.783	7.35	4.06	4.06
$1.5625 \cdot 10^{-2}$	-11.066	-7.517	-6.996	4.63	4.03	4.03
$7.8125 \cdot 10^{-3}$	-12.285	-8.725	-8.204	4.05	4.03	4.01

Table 5.1: Global error and order when modified Newton and the trivial predictor are used.

5 Numerical experiments

The theoretical results have been confirmed by several numerical tests. We will here only describe one example. Consider the problem

$$\begin{aligned} y' &= \frac{yz}{x} \\ 0 &= y - e^z \end{aligned} \tag{5.1}$$

with the exact solution $y(x) = e^x$, $z(x) = x$. The 3-stage, 5'th order RadauIIA method was used as corrector. Two different predictors were chosen, the trivial predictor $Y_i^{(0)} = y_n$, $Z^{(0)} = z_n$ giving $q = 0$, and the collocation polynomial which satisfies $q = 3$. For each step, the algebraic equations were solved by a constant number of iterations. However, when the collocation polynomial was used, the first step was solved by more iterations, to ensure sufficiently high order of the first step. The problem was integrated between $x = 0.2$ and $x = 1.2$, using constant stepsize h. The order was found by comparing the errors at the endpoint for different values of h. The results are given in Table 1-4. Here k is the number of iterations, and $q^{(k)}$ is given by Theorem 1.1. The global errors are given by

$$e_y^{(k)} = |y_n^{(k)} - y(1.2)| = \mathcal{O}(h^{p_y^{(k)}}), \quad e_z^{(k)} = |z_n^{(k)} - z(1.2)| = \mathcal{O}(h^{p_z^{(k)}}), \quad g^{(k)} = |y_n^{(k)} - e^{z_n^{(k)}}| = \mathcal{O}(h^{p_g^{(k)}})$$

$k=1$	$q^{(k)}=1$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-1.469	-2.494	-1.632	1.63	1.13	1.81
$6.25 \cdot 10^{-2}$	-2.017	-2.983	-2.209	1.82	1.62	1.92
$3.125 \cdot 10^{-2}$	-2.593	-3.534	-2.800	1.91	1.83	1.96
$1.5625 \cdot 10^{-2}$	-3.182	-4.112	-3.397	1.96	1.92	1.98

$k=2$	$q^{(k)}=3$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-4.078	-4.254	-3.993	3.71	3.85	3.96
$6.25 \cdot 10^{-2}$	-5.239	-5.437	-5.197	3.85	3.93	4.00
$3.125 \cdot 10^{-2}$	-6.422	-6.632	-6.401	3.93	3.97	4.00
$1.5625 \cdot 10^{-2}$	-7.616	-7.831	-7.606	3.97	3.98	4.00

$k=3$	$q^{(k)}=7$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-6.050	-6.57	-8.789	5.04	5.06	8.01
$6.25 \cdot 10^{-2}$	-7.570	-8.091	-11.206	5.05	5.05	8.03
$3.125 \cdot 10^{-2}$	-9.086	-9.607	-13.612	5.04	5.04	7.99
$1.5625 \cdot 10^{-2}$	-10.597	-11.119	–	5.02	5.02	–

Table 5.2: Global error and order when exact Newton and the trivial predictor are used.

where $n = 1.0/h$.

In no cases the observed order is lower than the predicted for h sufficiently small. In one case, Table 1 with $k = 2$, the observed order of y is one more than predicted. The order is restricted only because $\psi^{(k)} = \psi$ are not satisfied for the minimal order trees, thus only for one or a very few trees of a given order. If the problem does not contain the elementary differentials corresponding to the minimal order trees, or the given predictor-corrector scheme is such constructed that $\psi^{(k)} = \psi$ for these trees, then the order will be higher than predicted by Theorem 1.1 and 1.2.

6 Discussion

We have in the preceding sections given a complete characterization of the local error when Newton type methods are used to solve the implicit equations which appears when a Runge-Kutta method is applied to a semi-explicit DAE of index 1. By this theory, we know the exact number of iterations which is necessary to preserve the order of the exact method.

Compared with the results given by Jackson et.al., [5] for nonstiff ODEs, the number of iterations needed is approximately twice as many for the DAE problem as for the nonstiff ODE. In the nonstiff case rather arbitrary starting values ($q = -1$) for the iterations are

$k = 1$	$q^{(k)} = 4$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-5.304	-3.567	-3.048	3.78	1.99	1.97
$6.25 \cdot 10^{-2}$	-6.632	-4.847	-4.328	4.41	4.25	4.25
$3.125 \cdot 10^{-2}$	-8.033	-8.046	-7.686	4.65	10.62	11.15
$1.5625 \cdot 10^{-2}$	-9.480	-9.710	-9.499	4.81	5.53	6.03
$7.8125 \cdot 10^{-3}$	-10.956	-11.231	-11.076	4.90	5.05	5.24
$3.90625 \cdot 10^{-3}$	-12.441	-12.739	-12.014	4.94	5.01	5.11

$k = 2$	$q^{(k)} = 5$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-6.060	-6.256	-6.014	5.02	5.60	5.98
$6.25 \cdot 10^{-2}$	-7.575	-7.896	-7.809	5.03	5.45	5.96
$3.125 \cdot 10^{-2}$	-9.088	-9.497	-9.619	5.03	5.32	6.01
$1.5625 \cdot 10^{-2}$	-10.598	-11.060	-11.431	5.02	5.19	6.02

$k = 3$	$q^{(k)} = 6$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-6.050	-6.657	-6.798	5.04	3.22	7.83
$6.25 \cdot 10^{-2}$	-7.570	-8.109	-8.974	5.05	4.83	7.23
$3.125 \cdot 10^{-2}$	-9.086	-9.611	-11.111	5.04	4.99	7.10
$1.5625 \cdot 10^{-2}$	-10.597	-11.120	-13.235	5.02	5.01	7.06

Table 5.3: Global error and order when modified Newton and the collocation polynomial predictor are used.

allowed. If such starting values are used for DAE-problems, the iterations might still converge to the correct solution, but for each iteration the global error will be $e^{(k)} = \mathcal{O}(1)$ in the z-component. Further, $\mathcal{O}(1)$ perturbation of the Jacobian will usually give no convergence at all. As a conclusion we might say that the numerical solution of DAE-problems needs more iterations, more accurate starting values for the iterations, and a better approximation to the Jacobian than what is the case for nonstiff ODEs. Hairer et. al. [2] shows that the order of a method applied to some stiff problems is determined by the methods behaviour when solving DAEs. It is thus reasonable to believe that the conclusions given here for DAEs are valid for such stiff ODEs as well.

References

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$k=1$	$q^{(k)}=7$					
h	$log_{10}(e_y^{(k)})$	$\log_{10}(e_z^{(k)})$	$\log_{10}(g^{(k)})$	$p_y^{(k)}$	$p_z^{(k)}$	$p_g^{(k)}$
$1.25 \cdot 10^{-1}$	-6.050	-6.570	-9.217	5.05	5.05	8.14
$6.25 \cdot 10^{-2}$	-7.570	-8.091	-11.645	5.05	5.05	8.06
$3.125 \cdot 10^{-2}$	-9.086	-9.607	-14.074	5.04	5.04	8.07
$1.5625 \cdot 10^{-2}$	-10.597	-11.119	–	5.02	5.02	–

Table 5.4: Global error and order when exact Newton and the collocation polynomial predictor are used.

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