

ORDER RESULTS FOR IMPLICIT RUNGE-KUTTA METHODS APPLIED TO DIFFERENTIAL/ALGEBRAIC SYSTEMS*

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Abstract. In this paper we study the order, stability and convergence properties of implicit Runge-Kutta methods applied to a relatively simple class of nonlinear differential/algebraic systems. These methods often do not attain the same order of accuracy for differential/algebraic systems as they do for purely differential systems. We derive a set of order conditions which the method coefficients should satisfy in addition to the usual order conditions to ensure a given order of accuracy, and we present results on the stability and convergence properties of these methods.

Key words. differential/algebraic equations, stiff equations, Runge-Kutta methods

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1. Introduction. In this paper we study the order, stability and convergence properties of implicit Runge-Kutta methods applied to systems of differential/algebraic equations (DAE) of the form

$$(1.1) \quad 0 = F(t, y, y')$$

where the initial values of y are given at $t=0$ and F is linear in y' . These methods often do not attain the same order of accuracy for differential/algebraic systems as they do for purely differential systems. We derive a set of order conditions which the method coefficients must satisfy in addition to the usual order conditions to ensure a given order of accuracy of the local truncation error. Also, we present results on the stability properties and order of convergence of the global error of these methods. Finally, we describe some numerical experiments which are in agreement with our results.

An M -stage implicit Runge-Kutta method for the solution of a system of ordinary differential equations (ODEs)

$$(1.2) \quad y' = f(t, y)$$

is given by

$$(1.3) \quad \begin{aligned} Y'_i &= f\left(t_n + c_i h, y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j\right), \quad i = 1, 2, \dots, M, \\ y_n &= y_{n-1} + h \sum_{i=1}^M b_i Y'_i, \end{aligned}$$

where $h = t_n - t_{n-1}$. The method is often written in the shorthand notation which displays

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the matrix of coefficients,

(1.4)

c_1 c_2 \vdots c_M

a_{11} a_{21} \vdots a_{M1}

a_{12} a_{22} \vdots a_{M2}

\cdots \cdots \ddots \cdots

a_{1m} a_{2M} \vdots a_{MM}

We can consider formally applying this method to DAE systems (1.1) by

(1.5)

$$F\left(t_{n-1} + c_i h, y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j, Y'_i\right) = 0, \quad i = 1, 2, \dots, M,$$

(1.6)

$$y_n = y_{n-1} + h \sum_{i=1}^M b_i Y'_i.$$

The intermediate Y_i 's are given by

(1.7)

$$Y_i = y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j,$$

and the method reduces to (1.3) if we happen to be solving a DAE which is also an ODE (that is, if $F(t, y, y') = y' - f(t, y) = 0$). In this paper we shall only consider methods where the matrix $\mathcal{A} = (a_{ij})$ in (1.4) is nonsingular.

The particular class of DAE systems that we will be concerned with is the systems whose *index* is equal to one. For a linear DAE system of the form

(1.8)

$$A(t)y'(t) + B(t)y(t) = g(t),$$

the index is one if there exist nonsingular time-dependent matrices $P(t)$, $Q(t)$ such that

(1.9)

$$P(t)A(t)Q(t) = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix},$$
$$P(t)B(t)Q(t) = \begin{pmatrix} C(t) & 0 \\ 0 & I \end{pmatrix}.$$

These transformations decouple the system into a “differential” part and an “algebraic” part. In the nonlinear case, we associate the matrices A and B with $\partial F/\partial y'$ and $\partial F/\partial y$, respectively.

The concept of index is discussed in much greater detail in [1]. Here we note that index one systems are in some sense the simplest nontrivial ($A(t)$ is singular) DAE systems, and that these types of systems arise frequently in practical applications [2]. For the special DAE systems which can be written in the form

(1.10)

$$y' = f(t, y, z), \quad 0 = g(t, y, z),$$

the index is one if $[\partial g/\partial z]^{-1}$ exists and is bounded. Practical means of deciding for a general DAE system whether the index is one are discussed in [1].

Several other authors have obtained results which are in some ways related to the results given in this paper. Gear and Petzold [1] show that backward differentiation formulas (BDF) converge with the expected order of accuracy for index one DAE systems. März [3] has studied general linear multistep methods applied to index one DAE systems, and showed that the method coefficients must satisfy an extra set of conditions (which happen to be satisfied for BDF) for the method to be convergent with the expected order of accuracy for DAE systems. Hence, it is not entirely surprising that implicit Runge-Kutta methods should suffer some order reduction when applied

to DAE systems. In the context of stiff differential systems, which are related to DAEs, Prothero and Robinson [4] observed some order reduction effects for certain Runge-Kutta methods in 1974. Recently, Frank, Schneid, and Ueberhuber [5] give order conditions for implicit Runge-Kutta methods applied to stiff systems. Some of the results in [5] appear similar to ours, but the order conditions are somewhat different due to the different types of systems that we are considering; we will comment on this in greater detail later.

The remainder of this paper is divided into three sections. In § 2 we consider linear constant-coefficient index one DAE systems. We give a set of conditions that are necessary and sufficient to ensure that the local truncation error of a method (1.5) attains a given order for these systems. We also give conditions on the coefficients which must be satisfied for the method to be stable and convergent to a given order of accuracy for linear constant-coefficient DAE systems. Stability for solving the DAE is related to the method's stability properties for linear stiff ODEs. Finally, we discuss the stability and order properties for differential/algebraic systems of a few methods which have recently appeared in the literature for stiff ODEs.

In § 3 we study nonlinear index one systems of the form (1.1). Because of "mixing" which can occur between the differential and algebraic parts of the solution, these systems are more troublesome to solve than linear constant-coefficient systems. We give a set of order conditions which are sufficient to ensure that a method is accurate to a given order for these systems. These conditions are more restrictive than the order conditions for linear constant-coefficient systems.

In the last section we present the results of some numerical experiments which confirm that the order reduction effects predicted in the earlier sections can occur in practice.

2. Linear constant-coefficient index one systems. In this section we consider linear constant-coefficient index one systems. We derive conditions that are necessary and sufficient to ensure that the local truncation error of an implicit Runge-Kutta method attains a given order. We give conditions on the coefficients for the method to be stable, and we discuss the stability and order properties for DAEs of a few methods which have recently appeared in the stiff ODE literature.

Consider again the DAE system

$$(2.1) \quad F(t, y, y') = 0,$$

and an implicit M -stage Runge-Kutta method applied to this system,

$$(2.2) \quad \begin{aligned} F\left(t_{n-1} + c_i h, y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j, Y'_i\right) &= 0, \quad i = 1, 2, \dots, M, \\ y_n &= y_{n-1} + h \sum_{i=1}^M b_i Y'_i, \end{aligned}$$

where we will always assume that the matrix $\mathcal{A} = (a_{ij})$ is nonsingular. Another way to write the Runge-Kutta method is given by

$$(2.3) \quad y_n = y_{n-1} + h\Psi(y_{n-1}, t_{n-1}, h).$$

Before we can get started, we need a few definitions.

DEFINITION 2.1. The *local error* d_n is given by

$$(2.4) \quad y(t_n) = y(t_{n-1}) + h\Psi(y(t_{n-1}), t_{n-1}, h) - d_n.$$

DEFINITION 2.2. The Runge-Kutta method (2.2) is *strictly stable* for the DAE (2.1) if the difference between a perturbed Runge-Kutta step,

$$(2.5) \quad \begin{aligned} F\left(t_{n-1} + c_i h, z_{n-1} + h \sum_{j=1}^M a_{ij} Z'_j + \delta_n^{(i)}, Z'_i\right) &= 0, \quad i = 1, 2, \dots, M, \\ z_n &= z_{n-1} + h \sum_{i=1}^M b_i Z'_i + \delta_n^{(M+1)}, \end{aligned}$$

where $z_0 = y_0 + \delta_0^{(M+1)}$, and $\|\delta_n^{(i)}\| \leq \Delta$, $i = 1, 2, \dots, M+1$, and an unperturbed Runge-Kutta step (2.2), satisfies $\|z_n - y_n\| \leq K_0 \Delta$, where $0 < h \leq h_0$, and K_0 , h_0 are constants depending only on the method and the DAE.

Consider the constant-coefficient DAE

$$(2.6) \quad Ay' + By = g(t).$$

Since the index is assumed to be one, there exist nonsingular transformation matrices P and Q such that

$$(2.7) \quad PAQ = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \quad PBQ = \begin{pmatrix} C & 0 \\ 0 & I \end{pmatrix}.$$

Applying the implicit Runge-Kutta method to (2.6), we have

$$(2.8) \quad \begin{aligned} AY'_i + B\left(y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j\right) &= g(t_{n-1} + c_i h), \quad i = 1, 2, \dots, M, \\ y_n &= y_{n-1} + h \sum_{i=1}^M b_i Y'_i. \end{aligned}$$

Letting $\tilde{y}_n = Q^{-1}y_n$, $\tilde{Y}'_i = Q^{-1}Y'_i$, $\tilde{g}(t) = Pg(t)$, and premultiplying by P , we can rewrite (2.8)

$$(2.9) \quad \begin{aligned} (PAQ)\tilde{Y}'_i + (PBQ)\left(\tilde{y}_{n-1} + h \sum_{j=1}^M a_{ij}\tilde{Y}'_j\right) &= \tilde{g}(t_{n-1} + c_i h), \\ \tilde{y}_n &= \tilde{y}_{n-1} + h \sum_{i=1}^M b_i \tilde{Y}'_i. \end{aligned}$$

In this form, the differential and algebraic parts of the systems are completely decoupled from each other. Thus, it is sufficient to study the differential and algebraic parts separately to get an understanding of the general linear constant-coefficient DAE. Since we have assumed the index is one, the system (2.6) decouples into a system of differential equations, and a set of algebraic equations of the form

$$(2.10) \quad y = g(t),$$

where for the remainder of this section y and g represent the second parts of \tilde{y} and \tilde{g} in (2.9), where the partitioning is given in (2.7).

We now study the Runge-Kutta method (2.2) applied to these algebraic equations in detail. Applying the implicit Runge-Kutta method (2.2) to (2.10) gives

$$(2.11a) \quad y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j = g(t_{n-1} + c_i h), \quad i = 1, 2, \dots, M,$$

$$(2.11b) \quad y_n = y_{n-1} + h \sum_{i=1}^M b_i Y'_i.$$

From (2.11) it is easy to see why we should assume the matrix $\mathcal{A} = (a_{ij})$ is nonsingular, for then $Y' = (Y'_1, \dots, Y'_M)^T$ is determined uniquely by (2.11a).

To find the local error, let $y_{n-1} = g(t_{n-1})$. Solving for Y' in (2.11a), we have

$$(2.12a) \quad Y' = \mathcal{A}^{-1}G,$$

where

$$(2.12b) \quad G = \begin{pmatrix} (g(t_{n-1} + c_1 h) - g(t_{n-1}))/h \\ (g(t_{n-1} + c_2 h) - g(t_{n-1}))/h \\ \vdots \\ (g(t_{n-1} + c_M h) - g(t_{n-1}))/h \end{pmatrix}.$$

Then from (2.11b), we have

$$(2.13) \quad y_n = g(t_{n-1}) + h b^T \mathcal{A}^{-1} G,$$

where $b = (b_1, b_2, \dots, b_M)^T$. Thus, the local error is given by

$$(2.14) \quad d_n = g(t_{n-1}) + h b^T \mathcal{A}^{-1} G - g(t_n).$$

Expanding the terms in (2.14) in a Taylor series around t_{n-1} , we have

$$(2.15) \quad d_n = - \left(h g' + \frac{h^2}{2} g'' + \frac{h^3}{6} g''' + \frac{h^4}{24} g^{iv} + \dots \right) + b^T \mathcal{A}^{-1} \begin{pmatrix} c_1 h g' + \frac{c_1^2 h^2}{2} g'' + \frac{c_1^3 h^3}{6} g''' + \dots \\ c_2 h g' + \frac{c_2^2 h^2}{2} g'' + \frac{c_2^3 h^3}{6} g''' + \dots \\ \vdots \\ c_M h g' + \frac{c_M^2 h^2}{2} g'' + \frac{c_M^3 h^3}{6} g''' + \dots \end{pmatrix}.$$

Equating like powers of h , $d_n = O(h^{k+1})$ iff $b^T \mathcal{A}^{-1} c^j = 1$, $j = 1, \dots, k$ where $c^j = (c_1^j, \dots, c_M^j)^T$.

DEFINITION 2.3. The *algebraic order* of an implicit Runge-Kutta method (2.12) is equal to k_a if $d_n = O(h^{k_a+1})$ for all equations (2.10) with $g(t)$ sufficiently smooth. Then we have just shown,

THEOREM 2.1. The algebraic order of an implicit Runge-Kutta method (2.2) is equal to k_a iff the method coefficients satisfy

$$(2.16) \quad b^T \mathcal{A}^{-1} c^j = 1, \quad j = 1, \dots, k_a$$

where

$$c^j = (c_1^j, \dots, c_M^j)^T.$$

We now turn to the question of stability for linear constant-coefficient systems. Solving (2.10) by the perturbed Runge-Kutta method (2.5), we have

$$(2.17) \quad z_{n-1} + h \sum_{j=1}^M a_{ij} Z'_j + \delta_n^{(i)} = g(t_{n-1} + c_i h), \quad i = 1, 2, \dots, M,$$

$$z_n = z_{n-1} + h \sum_{i=1}^M b_i Z'_i + \delta_n^{(M+1)}.$$

Subtracting (2.17) from the corresponding expressions for the unperturbed solution (2.11), and letting $e_n = y_n - z_n$, $E'_i = Y'_i - Z'_i$, we obtain

$$(2.18) \quad \begin{aligned} e_{n-1} + h \sum_{j=1}^M a_{ij} E'_j - \delta_n^{(i)} &= 0, \quad i = 1, 2, \dots, M, \\ e_n &= e_{n-1} + h \sum_{i=1}^M b_i E'_i - \delta_n^{(M+1)}. \end{aligned}$$

Rewriting,

$$(2.19) \quad e_n = e_{n-1} + b^T \mathcal{A}^{-1} (\delta_n - \varepsilon_M e_{n-1}) - \delta_n^{(M+1)},$$

where $\varepsilon_M = (1, 1, \dots, 1)^T$ and $\delta_n = (\delta_n^{(1)}, \delta_n^{(2)}, \dots, \delta_n^{(M)})^T$. Collecting terms,

$$(2.20) \quad e_n = (1 - b^T \mathcal{A}^{-1} \varepsilon_M) e_{n-1} + (b^T \mathcal{A}^{-1} \delta_n - \delta_n^{(M+1)}).$$

Thus we have shown,

THEOREM 2.2. *An implicit Runge-Kutta method (2.2) is strictly stable for linear constant-coefficient index one DAEs iff the method coefficients satisfy*

$$(2.21) \quad |1 - b^T \mathcal{A}^{-1} \varepsilon_M| < 1.$$

We note that the inequality in (2.21) must be a strict inequality; for an example see März [6].

Since DAEs can be regarded as “infinitely stiff” ODEs, it is natural to ask what is the relationship between the above criterion for stability, and the stability criterion for the same methods applied to the stiff model problem $y' = \lambda y$. From Hall and Watt [7], an implicit Runge-Kutta method (1.3) is stable for $z = h\lambda$ iff $|R(z)| \leq 1$, where

$$(2.22) \quad R(z) = 1 + zb^T(I - z\mathcal{A})^{-1}\varepsilon_M.$$

It follows from (2.22) that

$$(2.23) \quad \lim_{|z| \rightarrow \infty} R(z) = 1 - b^T \mathcal{A}^{-1} \varepsilon_M.$$

Thus, a method is stable for constant-coefficient index one DAEs iff

$$(2.24) \quad r = \lim_{|z| \rightarrow \infty} |R(z)| < 1.$$

Now that we have an understanding of the local truncation error and stability properties of a method, we can estimate the size of the global error. Clearly, if $r = 0$ in (2.24) then the local error is equal to the global error, for the “algebraic part” of the system. For $r < 1$, we have from (2.20),

$$(2.25) \quad \|e_n\| \leq r \|e_{n-1}\| + M\Delta,$$

where M is some positive constant, so that

$$(2.26) \quad \|e_n\| \leq r^n \|e_0\| + \left(\frac{1 - r^n}{1 - r} \right) M\Delta.$$

Since r is independent of h and $\lim_{n \rightarrow \infty} ((1 - r^n)/(1 - r)) = 1/(1 - r)$ we have in this case that the order of the local error is the same as the order of the global error, for the “algebraic part” of the system. Combining these results, we have

DEFINITION 2.4. The *constant-coefficient order* of an implicit Runge-Kutta method (2.2) is equal to k_c if the method converges with global error $O(h^{k_c})$ for all linear constant-coefficient index one systems (2.6) with $g(t)$ sufficiently smooth.

THEOREM 2.3. *The constant-coefficient order k_c of the global error of an implicit Runge-Kutta method which satisfies*

(1) *the matrix \mathcal{A} of method coefficients is nonsingular,*

(2) *the method coefficients satisfy the stability condition (2.21),*

is given by

$$(2.27) \quad k_c = \min(k_a + 1, k_d),$$

where k_d is the order of the method for purely differential (nonstiff) systems, and k_a is the algebraic order.

We see there is a reduction of order when $k_a + 1 < k_d$. This order reduction effect actually does occur for some of the implicit Runge-Kutta methods in the stiff ODE literature. Here we give examples of some implicit Runge-Kutta methods, along with their properties for constant-coefficient index one DAE systems.

METHOD 1 (Hall and Watt [7]). Semi-explicit third order Runge-Kutta.

$$\begin{array}{c|cc} \frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} & 0 \\ \frac{3-\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$$r = \frac{1+\sqrt{3}}{2+\sqrt{3}},$$

$$k_d = 3,$$

$$k_a = 1,$$

$$k_c = 2.$$

METHOD 2 (Burrage [8]). Singly implicit first order Runge-Kutta with error estimate.

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$$

$$r = 0,$$

$$k_d = 1,$$

$$k_a = \infty,$$

$$k_c = 1.$$

Error-estimating method,

$$\begin{array}{c|cc} 1 & 1 & 0 \\ 0 & -1 & 1 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$$r = \frac{1}{2},$$

$$k_d = 2,$$

$$k_a = \infty,$$

$$k_c = 2.$$

METHOD 3 (Burrage [8]). Singly implicit second order Runge-Kutta with error estimate.

$\lambda(2-\sqrt{2})$	$\lambda(4-\sqrt{2})/4$	$\lambda(4-3\sqrt{2})/4$
$\lambda(2+\sqrt{2})$	$\lambda(4+3\sqrt{2})/4$	$\lambda(4+\sqrt{2})/4$
	$(4\lambda(1+\sqrt{2})-\sqrt{2})/(8\lambda)$	$(4\lambda(1-\sqrt{2})+\sqrt{2})/(8\lambda)$

$$\lambda = (2 \pm \sqrt{2})/2,$$

$$r = 0,$$

$$k_d = 2,$$

$$k_a = \infty,$$

$$k_c = 2.$$

Error-estimating method,

$\lambda(2-\sqrt{2})$	$\lambda(4-\sqrt{2})/4$	$\lambda(4-3\sqrt{2})/4$	0
$\lambda(2+\sqrt{2})$	$\lambda(4+3\sqrt{2})/4$	$\lambda(4+\sqrt{2})/4$	0
$1-\lambda$	$(-\lambda^2(11\sqrt{2}+8)$	$(\lambda^2(11\sqrt{2}-8)$	λ
	$+4\lambda(1+2\sqrt{2})-\sqrt{2})/(8\lambda)$	$+4\lambda(1-2\sqrt{2})+\sqrt{2})/(8\lambda)$	
	b_1	b_2	b_3

$$b_1 = (6\lambda^2(2+\sqrt{2})-3\lambda(3+\sqrt{2})+1)/(12\lambda(\lambda(3\sqrt{2}-2)-\sqrt{2})),$$

$$b_2 = (6\lambda^2(\sqrt{2}-2)+3\lambda(3-\sqrt{2})-1)/(12\lambda(\lambda(3\sqrt{2}+2)-\sqrt{2})),$$

$$b_3 = (6\lambda^2-6\lambda+1)/3(7\lambda^2-6\lambda+1),$$

$$r = .276,$$

$$k_d = 3,$$

$$k_a = 2,$$

$$k_c = 3.$$

3. Nonlinear index one systems. In this section we study nonlinear index one systems of the form (1.1). The Runge-Kutta methods are, in general, even less accurate for nonlinear systems than for linear constant-coefficient systems. The additional loss of accuracy comes about because of mixing which can occur between the differential and algebraic parts of the solution. We give a set of order conditions which are sufficient to ensure that a method is accurate to a given order for these systems.

To state our results, we need some notation. First, we must define the internal local truncation errors, which are defined similarly in [5]

$$\delta_i^{(n)} = y(t_{n-1}).$$

DEFINITION 3.1. The i th internal local truncation error $\delta_i^{(n)}$ at t_n of an M -stage implicit Runge-Kutta method (1.5) is given by

$$(3.1) \quad \begin{aligned} \delta_i^{(n)} &= y(t_{n-1}) + h \sum_{j=1}^M a_{ij} y'(t_{n-1} + c_j h) - y(t_{n-1} + c_i h), \quad i = 1, \dots, M, \\ \delta_{M+1}^{(n)} &= y(t_{n-1}) + h \sum_{i=1}^M b_i y'(t_{n-1} + c_i h) - y(t_n). \end{aligned}$$

DEFINITION 3.2. The internal order k_I of an M -stage implicit Runge-Kutta method (1.5) is given by

$$k_I = \min(k_1, \dots, k_M, k_{M+1})$$

where

$$\delta_i = O(h^{k_i+1}), \quad i = 1, \dots, (M+1).$$

It is simple to find the internal order of an implicit Runge-Kutta method in terms of its coefficients by expanding (3.1) in Taylor series around t_{n-1} , as in [5], leading to

THEOREM 3.1. The internal order of an M -stage implicit Runge-Kutta method is equal to k_I iff the method coefficients satisfy

$$\sum_{j=1}^M a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \quad i = 1, \dots, M,$$

$$\sum_{j=1}^M b_j c_j^{k-1} = \frac{1}{k}$$

for $k = 1, \dots, k_I$.

Following [1], we will say that a nonlinear system (1.1) is *uniform index one* if the index of the constant-coefficient problem

$$Ay'(t) + By(t) = g(t)$$

where $A = \partial F / \partial y'$, $B = \partial F / \partial y$ is one in a neighborhood of the solution $y(t)$, and if the matrices P , Q which transform (A, B) to the canonical form (1.8) satisfy:

- (1) $Q(t, y(t))$ and $Q^{-1}(t, y(t))$ exist and are bounded for all $(t, y(t))$ solving (1.1),
- (2) $Q^{-1}(t_1, ty(t_1))Q(t_2, y(t_2)) = I + O(t_2 - t_1)$,
- (3) $C(t_1, y(t_1)) = C(t_2, y(t_2)) + O(t_2 - t_1)$.

These conditions are satisfied if in a neighborhood of the solution A and B are sufficiently smooth, the index is one, and the rank of A is constant.

Suppose the dimension of the “differential part” of the system is n_1 and the dimension of the “algebraic part” is n_2 . Then we can state the following result.

THEOREM 3.2. Suppose

- (1) System (1.1) is uniform index one.
- (2) F is linear in y' .
- (3) The Runge-Kutta method (1.5) satisfies the strict stability condition (2.21) with $0 \leq r < 1$.
- (4) The initial conditions satisfy $\|y_0 - y(t_0)\| = O(h^{k_G})$, where $k_G = \min(k_d, k_I + 1)$.
- (5) If $k_G = 1$, then $r = 0$.

Then the global error of the Runge-Kutta method (1.5) is $O(h^{k_G})$.

Proof. Consider the Runge-Kutta method (1.5). The numerical solution satisfies

$$(3.2a) \quad F\left(t_{n-1} + c_i h, y_{n-1} + h \sum_{j=1}^M a_{ij} Y'_j, Y'_i\right) = 0, \quad i = 1, 2, \dots, M,$$

$$(3.2b) \quad y_n = y_{n-1} + h \sum_{i=1}^M b_i Y'_i.$$

The true solution satisfies

$$(3.3a) \quad F\left(t_{n-1} + c_i h, y(t_{n-1}) + h \sum_{j=1}^M a_{ij} y'(t_{n-1} + c_j h) - \delta_i, y'(t_{n-1} + c_i h)\right) = 0,$$

$$i = 1, 2, \dots, M,$$

$$(3.3b) \quad y(t_n) = y(t_{n-1}) + h \sum_{i=1}^M b_i y'(t_{n-1} + c_i h) - \delta_{M+1}.$$

Let $E'_i = Y'_i - y'(t_{n-1} + c_i h)$, $E_i = Y_i - y(t_{n-1} + c_i h)$, and $e_n = y_n - y(t_n)$. Subtracting (3.3) from (3.2), we obtain

$$(3.4a) \quad A_i E'_i + B_i \left(e_{n-1} + h \sum_{j=1}^M a_{ij} E'_j + \delta_i \right) = \eta_i, \quad i = 1, 2, \dots, M,$$

$$(3.4b) \quad e_n = e_{n-1} + h \sum_{i=1}^M b_i E'_i + \delta_{M+1},$$

where $A_i = \partial F / \partial y'$ and $B_i = \partial F / \partial y$ are evaluated at $(t_{n-1} + c_i h, y(t_{n-1} + c_i h))$ and η_i is the sum of residuals from the Newton iteration and higher order terms in e_{n-1} and E'_i .

We can rewrite (3.4a) in the form

$$(3.5) \quad \begin{pmatrix} A_1 + a_{11} h B_1 & a_{12} h B_1 & \cdots & a_{1M} h B_1 \\ a_{21} h B_2 & A_2 + a_{22} h B_2 & \cdots & a_{2M} h B_2 \\ \vdots & \vdots & \ddots & \vdots \\ a_{M1} h B_M & a_{M2} h B_M & \cdots & A_M + a_{MM} h B_M \end{pmatrix} \begin{pmatrix} E'_1 \\ E'_2 \\ \vdots \\ E'_M \end{pmatrix} = - \begin{pmatrix} B_1(e_{n-1} + \delta_1) \\ B_2(e_{n-1} + \delta_2) \\ \vdots \\ B_M(e_{n-1} + \delta_M) \end{pmatrix} + \begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_M \end{pmatrix}.$$

For notational convenience, we will henceforth assume that all matrices without subscripts or superscripts are evaluated at $(t_n, y(t_n))$. Let $A = \partial F / \partial y'$ and $B = \partial F / \partial y$ be evaluated at $(t_n, y(t_n))$, and let P and Q be the transformation matrices which bring A and B to the canonical form (1.8). Let $\tilde{e}_{n-1} = Q^{-1} e_{n-1}$, $\tilde{E}'_i = Q^{-1} E'_i$, $\tilde{\delta}_i = Q^{-1} \delta_i$, and $\tilde{\eta}_i = P_i \eta_i$. Then we can rewrite (3.5),

$$(3.6) \quad \begin{pmatrix} X_1 + a_{11} h W_1 & a_{12} h W_1 & \cdots & a_{1M} h W_1 \\ a_{21} h W_2 & X_2 + a_{22} h W_2 & \cdots & a_{2M} h W_2 \\ \vdots & \vdots & \ddots & \vdots \\ a_{M1} h W_M & a_{M2} h W_M & \cdots & X_M + a_{MM} h W_M \end{pmatrix} \begin{pmatrix} \tilde{E}'_1 \\ \tilde{E}'_2 \\ \vdots \\ \tilde{E}'_M \end{pmatrix} = - \begin{pmatrix} W_1(\tilde{e}_{n-1} + \tilde{\delta}_1) \\ W_2(\tilde{e}_{n-1} + \tilde{\delta}_2) \\ \vdots \\ W_M(\tilde{e}_{n-1} + \tilde{\delta}_M) \end{pmatrix} + \begin{pmatrix} \tilde{\eta}_1 \\ \tilde{\eta}_2 \\ \vdots \\ \tilde{\eta}_M \end{pmatrix},$$

where $W_i = P_i B_i Q_i (Q_i^{-1} Q)$ and $X_i = P_i A_i Q_i (Q_i^{-1} Q)$.

By the definition of P , Q and the assumption on Q that $Q_i^{-1} Q = I + O(h)$ (we will use the order symbol to denote a matrix whose elements are all $O(h)$), we have

$$(3.7) \quad \begin{aligned} W_i &= \begin{pmatrix} C_i & 0 \\ 0 & I_2 \end{pmatrix} (I + O(h)), \\ X_i &= \begin{pmatrix} I_1 & 0 \\ 0 & 0 \end{pmatrix} (I + O(h)). \end{aligned}$$

The matrices I_1 and I_2 are identity matrices of order n_1 and n_2 , respectively.

Partition $\tilde{E}'_i = (\tilde{E}'^{(1)}_i, \tilde{E}'^{(2)}_i)^T$, where $\tilde{E}'^{(1)}_i$ has dimension n_1 and $\tilde{E}'^{(2)}_i$ has dimension n_2 . By partitioning $\tilde{\delta}_i$, \tilde{e}_{n-i} and $\tilde{\eta}_i$ in the same way, using (3.7) and rearranging the variables and equations in (3.6), we can write

$$(3.8) \quad \begin{pmatrix} T_1 & h^2 T_2 \\ h^2 T_3 & h T_4 \end{pmatrix} \begin{pmatrix} \tilde{E}'^{(1)} \\ \tilde{E}'^{(2)} \end{pmatrix} = - \begin{pmatrix} S_1 & h S_2 \\ h S_3 & S_4 \end{pmatrix} \begin{pmatrix} \tilde{e}_{n-1}^{(1)} + \tilde{\delta}^{(1)} \\ \tilde{e}_{n-1}^{(2)} + \tilde{\delta}^{(2)} \end{pmatrix} + \begin{pmatrix} \tilde{\eta}^{(1)} \\ \tilde{\eta}^{(2)} \end{pmatrix}$$

where

$$\tilde{E}'^{(i)} = (\tilde{E}'^{(i)}_1, \tilde{E}'^{(i)}_2, \dots, \tilde{E}'^{(i)}_M)^T,$$

$$\tilde{\delta}^{(i)} = (\tilde{\delta}^{(i)}_1, \tilde{\delta}^{(i)}_2, \dots, \tilde{\delta}^{(i)}_M)^T,$$

$$\tilde{\eta}^{(i)} = (\tilde{\eta}^{(i)}_1, \tilde{\eta}^{(i)}_2, \dots, \tilde{\eta}^{(i)}_M)^T,$$

$$\tilde{e}_{n-1}^{(i)} = (\tilde{e}_{n-1}^{(i)}_1, \tilde{e}_{n-1}^{(i)}_2, \dots, \tilde{e}_{n-1}^{(i)}_{n-1})^T$$

for $i = 1, 2$, and

$$T_1 = \hat{T}_1 + O(h),$$

$$T_4 = \hat{T}_4 + O(h),$$

$$S_1 = \hat{S}_1 + O(h),$$

$$S_4 = I + O(h)$$

where $\hat{T}_1 = I + h\mathcal{A} \otimes C$, $\hat{T}_4 = \mathcal{A} \otimes I$, $S_1 = I \otimes C$, and T_2, T_3, S_2, S_3 are matrices whose elements are $O(1)$.

Let T_n denote the left-hand matrix in (3.8). T_n can be written as

$$(3.9) \quad T_n = \begin{pmatrix} I & 0 \\ 0 & hI \end{pmatrix} \begin{pmatrix} \hat{T}_1 + O(h) & h^2 T_2 \\ h T_3 & \hat{T}_4 + O(h) \end{pmatrix}.$$

\hat{T}_4 is invertible because the matrix \mathcal{A} of coefficients of the Runge-Kutta method is invertible. By inverting the right-hand side of (3.9) the inverse of T_n is given by

$$(3.10) \quad T_n^{-1} = \begin{pmatrix} \hat{T}_1^{-1} + O(h) & O(h) \\ O(h) & \hat{T}_4^{-1}/h + O(1) \end{pmatrix}.$$

Using (3.10) to solve (3.8) for $(\tilde{E}'^{(1)}, \tilde{E}'^{(2)})^T$, we have

$$(3.11) \quad \begin{pmatrix} \tilde{E}'^{(1)} \\ \tilde{E}'^{(2)} \end{pmatrix} = - \begin{pmatrix} \hat{T}_1^{-1} \hat{S}_1 + O(h) & O(h) \\ O(1) & \hat{T}_4^{-1}/h + O(1) \end{pmatrix} \cdot \begin{pmatrix} \tilde{e}_{n-1}^{(1)} + \tilde{\delta}^{(1)} \\ \tilde{e}_{n-1}^{(2)} + \tilde{\delta}^{(2)} \end{pmatrix} + T_n^{-1} \begin{pmatrix} \tilde{\eta}^{(1)} \\ \tilde{\eta}^{(2)} \end{pmatrix}.$$

Multiplying (3.4b) by Q^{-1} , which we now denote by Q_n^{-1} to show its dependence upon $(t_n, y(t_n))$ we obtain

$$(3.12) \quad Q_n^{-1} e_n = \tilde{e}_{n-1} + h \sum_{i=1}^M b_i \tilde{E}'_i + \tilde{\delta}_{M+1}.$$

Inserting (3.11) into (3.12), we have

$$(3.13) \quad Q_n^{-1} e_n = S_n Q_n^{-1} e_{n-1} - h U_n \tilde{\delta}^{(n)} + \tilde{\delta}_{M+1}^{(n)} + h B T_n^{-1} \tilde{\eta}^{(n)}$$

where

$$\begin{aligned}
 S_n &= \left(I - h \begin{pmatrix} b_1^T \hat{T}_1^{-1} \hat{S}_1 + O(h) & O(h) \\ O(1) & b_2^T \hat{T}_4^{-1}/h + O(1) \end{pmatrix} \begin{pmatrix} Z_1 & 0 \\ 0 & Z_2 \end{pmatrix} \right), \\
 U_n &= \begin{pmatrix} b_1^T \hat{T}_1^{-1} \hat{S}_1 + O(h) & O(h) \\ O(1) & b_2^T \hat{T}_4^{-1}/h + O(1) \end{pmatrix}, \\
 Z_1 &= \varepsilon_M \otimes I_1, \\
 Z_2 &= \varepsilon_M \otimes I_2, \\
 b_1^T &= b^T \otimes I_1, \\
 b_2^T &= b^T \otimes I_2, \\
 B &= \begin{pmatrix} b^T I_1 & 0 \\ 0 & b^T I_2 \end{pmatrix}, \\
 \tilde{\delta}^{(n)} &= (\tilde{\delta}^{(1)}, \tilde{\delta}^{(2)})^T, \\
 \tilde{\eta}^{(n)} &= (\tilde{\eta}^{(1)}, \tilde{\eta}^{(2)})^T
 \end{aligned}$$

where $\varepsilon_M = (1, 1, \dots, 1)^T$. By the definition of \hat{T}_4 , we have

$$b_2^T \hat{T}_4^{-1} Z_2 = (1 - r) I_2,$$

where r is defined in (2.24), and $0 \leq r < 1$ by the assumption that the method is stable for constant-coefficient systems. Thus, S_n has the form

$$(3.14) \quad S_n = K + O(h),$$

where

$$K = \begin{pmatrix} I_1 & 0 \\ 0 & r I_2 \end{pmatrix}.$$

Solving for e_n in (3.13), we obtain

$$\begin{aligned}
 (3.15) \quad e_n &= \prod_{j=1}^{n-1} Q_{n-j} S_{n-j} Q_{j-j}^{-1} e_0 + \sum_{i=1}^{n-1} \left[\left(\prod_{j=0}^{i-1} Q_{n-j} S_{n-j} Q_{n-j}^{-1} \right) \right. \\
 &\quad \cdot \left. (h Q_{n-i} U_{n-i} \tilde{\delta}^{(n-i)} + Q_{n-i} \tilde{\delta}_{M+1}^{(n-i)} + h Q_{n-i} B T_{n-i}^{-1} \tilde{\eta}^{(n-i)}) \right].
 \end{aligned}$$

Now,

$$\begin{aligned}
 \prod_{j=0}^{n-1} Q_{n-j} S_{n-j} Q_{n-j}^{-1} &= Q_n \left(\prod_{j=0}^{n-2} S_{n-j} Q_{n-j}^{-1} Q_{n-j-1} \right) S_1 Q_1^{-1} \\
 &= Q_n (K^n + O(h)) Q_1^{-1}
 \end{aligned}$$

and

$$\prod_{j=0}^{i-1} Q_{n-j} S_{n-j} Q_{n-j}^{-1} = Q_n (K^i + O(h)) Q_{n-i+1}^{-1}.$$

We can rewrite (3.15),

$$(3.16) \quad Q_n^{-1}e_n = (K^n + O(h))(Q_0^{-1}e_0) + \sum_{i=1}^{n-1} (K^i + O(h))(hU_{n-i}\tilde{\delta}^{(n-i)} + \tilde{\delta}_{M+1}^{(n-i)} + h\bar{B}T_{n-i}^{-1}\tilde{\eta}^{(n-i)}).$$

Thus we find

$$(3.17) \quad \tilde{e}_n = (K^n + O(h))\tilde{e}_0 + \sum_{i=1}^{n-1} (K^i + O(h))hU_{n-i}\tilde{\delta}^{(n-i)} + \sum_{i=1}^{n-1} (K^i + O(h))\tilde{\delta}_{M+1}^{(n-i)} + \sum_{i=1}^{n-1} (K^i + O(h))h\bar{B}T_{n-i}^{-1}\tilde{\eta}^{(n-i)}.$$

Let

$$\hat{U}_n = \begin{pmatrix} b_1^T \hat{T}_1 \hat{S}_1 & 0 \\ 0 & b_2^T \hat{T}_4^{-1}/h \end{pmatrix}.$$

Rewriting (3.17) and noting that $\|\tilde{\delta}_i\| = O(h^{k_i+1})$, we have

$$(3.18) \quad \tilde{e}_n = (K^n + O(h))\tilde{e}_0 + \sum_{i=1}^{n-1} K^i (h\hat{U}_{n-i}\tilde{\delta}^{(n-i)} + \tilde{\delta}_{M+1}^{(n-i)}) + \sum_{i=1}^{n-1} (K^i + O(h))(h\bar{B}T_{n-i}^{-1}\tilde{\eta}^{(n-i)}) + O(h^{k_r+1}).$$

Observe that

$$(3.19) \quad h\hat{U}_{n-i}\tilde{\delta}^{(n-i)} + \tilde{\delta}_{M+1}^{(n-i)} = (O(h^{k_d+1}), O(h^{k_a+1}))^T.$$

We can see this by noting that the local error for the constant-coefficient problem $A_n z'(t) + B_n z(t) = g(t)$ is given by

$$h\hat{U}_{n-i}\tilde{\delta}^{(n-i)} + \tilde{\delta}_{M+1}^{(n-i)},$$

where $\tilde{\delta}_i = Q_n^{-1}\delta_i$, and we know from §2 that this local error is $O(h^{k_d+1})$ in the differential part and $O(h^{k_a+1})$ in the algebraic part. Although the solution to our problem and the solution to the constant-coefficient problem are different, the cancellation of various derivatives of the solution in the local error does not in general depend on the solution. Also note that because $\tilde{\delta}_i = O(h^{k_i+1})$, $h\hat{U}_{n-i}\tilde{\delta}^{(n-i)} + \tilde{\delta}_{M+1}^{(n-i)} = (O(h^{k_r+1}), O(h^{k_i+1}))^T$. Thus $k_a \geq k_r$ and $k_d \geq k_r$.

Suppose that $\|\tilde{\eta}^{(i)}\| \leq \Delta_i$, $\|\tilde{e}_0^{(i)}\| = O(\xi_i)$, $i = 1, 2$. Expanding the terms in (3.18) and noting that $\sum_{i=1}^{\infty} r^i = O(1)$ and making use of (3.19), we find that

$$(3.20) \quad \begin{aligned} \tilde{e}_n^{(1)} &= O(\xi_1) + O(h\xi_2) + O(h^{k_d}) + O(h^{k_r+1}) + O(\Delta_1) + O(\Delta_2), \\ \tilde{e}_n^{(2)} &= O(h\xi_1) + O(r^n\xi_2) + O(h\xi_2) + O(h^{k_r+1}) + O(h\Delta_1) + O(\Delta_2). \end{aligned}$$

For linear systems, $\Delta_1 = \Delta_2 = 0$ and we can conclude that $\|e_n\| = O(h^{k_G})$, where $k_G = \min(k_d, k_r + 1)$. For nonlinear systems, we sketch the proof. The higher order term $\tilde{\eta}$ is composed of terms of the form

$$(3.21) \quad \begin{aligned} &\frac{\partial^2 F}{\partial y^2} \left(e_{n-1} + h \sum_{j=1}^M a_{ij} E'_j + \delta_i \right) \left(e_{n-1} + h \sum_{j=1}^M a_{ij} E'_j + \delta_i \right), \\ &\frac{\partial^2 F}{\partial y \partial y'} \left(e_{n-1} + h \sum_{j=1}^M a_{ij} E'_j + \delta_i \right) E'_i. \end{aligned}$$

Thus we find that $\|\tilde{\eta}\|$ is proportional to $(\|\tilde{e}_{n-1}\| + h^{k_G})^2/h$. Substituting this relation for $\tilde{\eta}$ into (3.18), we obtain a nonlinear recurrence for \tilde{e}_n . The solutions to this recurrence can then be shown by induction to be of $O(h^{k_G})$. We make use of assumption (5) of the theorem to bound the solutions to the recurrence.

4. Numerical experiments. In this section we present the results of some numerical experiments which confirm that the order reduction effects predicted in § 3 can occur in practice.

The test problem we use was constructed to illustrate the effects of coupling between the differential and algebraic parts of the system. The problem is given by

$$(4.1) \quad \begin{pmatrix} 1 & -t \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{Y}'_1 \\ \tilde{Y}'_2 \end{pmatrix} + \begin{pmatrix} 1 & -(1+t) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{Y}_1 \\ \tilde{Y}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ \sin(t) \end{pmatrix}$$

with the initial values given by

$$\begin{pmatrix} \tilde{Y}_1(0) \\ \tilde{Y}_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} \tilde{Y}'_1(0) \\ \tilde{Y}'_2(0) \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}.$$

This problem has true solution

$$(4.2) \quad \begin{pmatrix} \tilde{Y}_1(t) \\ \tilde{Y}_2(t) \end{pmatrix} = \begin{pmatrix} \exp(-t) + t \sin(t) \\ \sin(t) \end{pmatrix}.$$

The problem was obtained from the constant-coefficient index one DAE

$$(4.3) \quad \begin{aligned} Y'_1 &= -Y_1, \\ Y'_2 &= \sin(t) \end{aligned}$$

by introducing a change of variables

$$(4.4) \quad \begin{pmatrix} \tilde{Y}_1 \\ \tilde{Y}_2 \end{pmatrix} = \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}.$$

The test problem is uniform index one for all t , and because of the mixing introduced by the time-dependent transformation in (4.4), we would expect it to exhibit many of the order reduction effects described in § 3.

In the experiments to determine the global error, we solved the problem with a sequence of fixed stepsizes over the interval $[0, 1]$. The reported observed order of the global error reflects the behaviour of the global error at the end of the interval as the stepsize is decreased by successive factors of two. To compute the observed local error, we solved (4.1) with the various Runge-Kutta methods with one step. The reported observed local error reflects the behaviour of the error after one step as the stepsize is decreased by successive factors of two.

We experimented with several Runge-Kutte methods which might appear to be likely candidates for solving stiff or differential/algebraic systems. A description of the methods follows:

- (1) 5-Stage '4th order' Strongly S -stable Diagonally Implicit method (Cash [9])
- (2) 2-Stage '2nd order' Strongly S -Stable Diagonally Implicit method (Alexander [10]) with $\alpha = 1 - \sqrt{2}/2$
- (3) 3-Stage '2nd order' L -Stable Semi-Implicit method (Houbak and Thomsen [11])

- (4) 7-Stage '3rd order' Extrapolation method based on fully implicit backward Euler and polynomial extrapolation, written as a semi-implicit Runge-Kutta method
- (5) 3-Stage '4th order' Lobatto III_C method (Chipman [12])
- (6) 2-Stage '2nd order' Singly-Implicit method (Burrage [8], described in § 2)

Table 4.1 gives the results of the experiments. In Table 4.1, k_g is the order of the observed global error and k_G is the lower bound which is predicted by the theory, based on k_d and k_r .

TABLE 4.1
Numerical results.

Method	k_d	k_a	$k_l + 1$	k_G	k_g
1	4	∞	2	2	2
2	2	∞	2	2	2
3	2	1	2	2	2
4	3	∞	2	2	3
5	4	∞	3	3	4
6	2	∞	2	2	2

Based on the results in Table 4.1, we can make a few observations. It is reassuring that in no case was the lower bound for the order predicted by the theory higher than the order which was actually observed, and in many cases these two orders coincided. The observed orders for the extrapolation method and for the Lobatto III_C formula were higher than would be expected based on the theory. We do not know whether all of the different order extrapolation methods based on backward Euler would have this property, or even whether there might exist problems for which the observed order is given by the lower bound.

Since k_r for a semi-implicit Runge-Kutta method is limited to one (because the first stage is necessarily a backward Euler step), we would expect the order of the global errors for these methods to be limited to two. This appears to be the case, with the exception again being the extrapolation method, which can be written as a semi-implicit Runge-Kutta method. Orders higher than two appear to be easily achieved by going to a fully implicit formula such as the Lobatto III_C method where the stage orders are higher. At least, in this case higher orders are predicted by the results in § 3. We have yet to achieve a complete understanding of the order reduction phenomenon, as evidenced by the better than predicted behaviour of the extrapolation method reported in Table 4.1; however it is clear that many of the order reduction effects predicted in the earlier sections actually do occur.

The orders that we predict and observe for the DAE systems tend to be somewhat higher than those predicted by Prothero and Robinson [4] and Frank, Schneid, and Ueberhuber [5] for related classes of stiff systems. For example, the theory of Frank, Schneid, and Ueberhuber [5] predicts an order of one for the global error of all semi-implicit Runge-Kutta methods for stiff systems, while we predict and observe an order of two for those methods applied to index one DAEs. Neither set of results is wrong. The differences are due mainly to considering different classes of problems. For example, Prothero and Robinson [4] consider the model problem

$$(4.5) \quad y' = \lambda(y - g(t)) + g'(t)$$

for $\operatorname{Re}(-\lambda) \rightarrow \infty$ and say that a method has order (p, q) if the error behaves as $h^{p+1}\lambda^q$ as $\operatorname{Re}(-h\lambda) \rightarrow \infty$ and $h \rightarrow 0$.

For methods where $q = -1$, the error behaves as h^{p+1} , but in addition it tends to zero for any h as $\operatorname{Re}(-\lambda) \rightarrow \infty$. In [4], [5] these methods with $q = -1$ are said to have order p , whereas for DAEs the order is infinite because these methods are exact for the algebraic equation

$$(4.6) \quad y = g(t)$$

which is the limit of (4.5) as $\operatorname{Re}(-\lambda) \rightarrow \infty$. By looking at DAEs, we see everything in the limit as $|\lambda| \rightarrow \infty$. On the other hand, for stiff equations where $|\lambda|$ is very large, it may be that the errors are already so small that the behaviour as h is reduced is not important. There is no question, however, that even after neglecting order reduction effects which disappear as $|\lambda| \rightarrow \infty$, order reduction can occur.

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