Implications of Order Reduction for Implicit Runge-Kutta Methods

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Abstract

Stability analysis of Runge-Kutta (RK) formulas was originally limited to linear ordinary differential equations (ODEs). More recently such analysis has been extended to include the behaviour of solutions to non-linear problems. This extension led to additional stability requirements for RK methods. Although the class of problems has been widened, the analysis is still restricted to a fixed stepsize. In the case of differential algebraic equations (DAEs), additional order conditions must be satisfied [6] to achieve full classical ODE order and avoid possible 'order reduction'. In this case too, a fixed stepsize analysis is employed. Such analysis may be of only limited use in quantifying the effectiveness of adaptive methods on stiff problems.

In this paper we examine the phenomenon of 'order reduction' and its implications on variable-step algorithms. We introduce a global measure of order referred to here as the 'observed order' which is based on the average stepsize over the region of integration. This measure may be better suited to the study of stiff systems, where the stepsize selection algorithm will vary the stepsize considerably over the interval of integration. Observed order gives a better indication of the relationship between accuracy and cost. Using this measure, the 'observed order reduction' will be seen to be less severe than that predicted by fixed stepsize order analysis.

1 Introduction

1.1 Background

The problem that we are concerned with is,

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \tag{1}$$

$$\mathbf{y}(t_0) = \mathbf{y}_0, \tag{2}$$

$$t \geq t_0 \in \mathbb{R},\ \mathbf{y} \in \mathbb{R}^M, \qquad \mathbf{f} : \mathbb{R} \times \mathbb{R}^M \rightarrow \mathbb{R}^M.$$

We will assume that $\mathbf{f}(t, \mathbf{y})$ has as many derivatives as needed, and that approximate solutions $\mathbf{y}_n$ are to be generated on a mesh t_n, $n = 0, 1, \ldots, N$. The **global error** $\mathbf{GE}_n$ of IVP (1), (2) at the point t_n is $\mathbf{y}(t_n) - \mathbf{y}_n$. The **local error** $\mathbf{LE}_n$ at t_n is $\bar{\mathbf{y}}_n(t_n) - \mathbf{y}_n$, where $\bar{\mathbf{y}}_n(t)$ is the solution of (1) but with initial condition $\bar{\mathbf{y}}_n(t_{n-1}) = \mathbf{y}_{n-1}$.

RK formulas determine a discrete approximation to (1), (2) using,

$$\mathbf{Y}_i = \mathbf{y}_{n-1} + h \sum_{j=1}^{s} a_{ij} \mathbf{f}(t_{n-1} + c_j h, \mathbf{Y}_j), \quad i = 1, \ldots, s, \tag{3}$$

$$\mathbf{y}_n = \mathbf{y}_{n-1} + h \sum_{j=1}^{s} b_j \, \mathbf{f}(t_{n-1} + c_j h, \mathbf{Y}_j). \tag{4}$$

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A standard way of representing an RK formula is to use a Butcher tableau to display the coefficients,

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^t. \end{array}$$

To reduce the cost of integration, higher order formulas and computationally more efficient formulas have been investigated. Traditionally, order has been analysed by considering a uniform mesh and bounding the local error. This constant stepsize analysis may be inappropriate for a large class of problems, as we will see in the next section.

1.2 Stability and Stiffness

Stiff ODE's are a class of problems where some components, called transients or fast components, have a vastly different rate of decay than other components, and the transients become insignificant after a time period of very short duration, called the transient region. Transients do not always have to is significant at the initial point. However our discussion of stability and stiffness is simplified if we assume that the transient is significant the initial point.

In the transient region the stepsize will inevitablely be determined by the accuracy of the transient component. If the region of integration does not extend much beyond the transient region then the cost of integrating over the remaining 'smooth' region may not be significant even for standard methods.

In classical analysis and the recent analysis of the order of formulas for special classes of problems, the stepsize h is assumed to be constant over the interval of integration. As is evident from the above discusion this assumption is inappropriate when considering the behaviour of methods for stiff systems. The stepsize can vary considerably over the interval $[a, b]$ when the problem is stiff. Over the transient region small steps will be taken to accurately integrate the transient. In the smooth region the stepsize should increase as long as the transient component is stable and continues to be damped and remain insignificant. An analysis relating average stepsize to achieved accuracy could be more relevant than classical order which, when it is extended to variable stepsize relates the maximum stepsize to the achieved accuracy.

Nonlinear stiffness has been examined, by considering singular perturbation problems of the form,

$$\begin{aligned} \mathbf{y}' &= \mathbf{f}(\mathbf{y}, \mathbf{z}, t), & (5) \\ \epsilon \mathbf{z}' &= \mathbf{g}(\mathbf{y}, \mathbf{z}, t), & (6) \end{aligned}$$

which are parameterized by $\epsilon > 0$. If $\partial \mathbf{g}/\partial \mathbf{z}$ has all eigenvalues in the left half plane, then as ϵ approaches zero this system will become progressively stiffer. In the limiting case where ϵ is allowed to go to zero, (6) can be written as,

$$0 = \mathbf{g}(\mathbf{y}, \mathbf{z}, t), \tag{7}$$

and we have an algebraic system (7) and a differential system (5) to solve. If (5), (7) can be further uncoupled as,

$$\begin{aligned} \mathbf{y}' &= \hat{\mathbf{f}}(\mathbf{y}, \mathbf{z}, t), & (8) \\ 0 &= \hat{\mathbf{g}}(\mathbf{z}, t), & (9) \end{aligned}$$

and $\partial \hat{\mathbf{g}}/\partial \mathbf{z}$ is nonsingular then the two components $\mathbf{y}$ and $\mathbf{z}$ can be determined independently and the stepsize required to integrate (8) will not be determined by the 'transient' component $\mathbf{z}$ which is now just an algebraic component (9). In particular, a nonlinear solver can be used to obtain a discrete solution to the algebraic component at each required abscissa and this solution can used to determine $\mathbf{y}'$ from (8).

To analyse the stability of a RK formula applied to $y' = \lambda y$, a rational function of $z = h\lambda$ (see for example [8], pages 240–270) of the form,

$$\begin{aligned} R(z) &= 1 + z\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e}, \quad \mathbf{e} = (1, 1, \ldots, 1)^t & (10) \\ &= \frac{P(z)}{Q(z)}, \end{aligned}$$

is introduced. Such formulas can have unbounded stability regions and they are considered suitable for stiff problems if the degree of $P(z) \leq$ degree $Q(z)$ and $\lim_{|z| \to \infty} \frac{P(z)}{Q(z)} <= 1$. A-stable formulas of this kind have been extensively investigated. A formula is **L-stable** if in addition to being A-stable it also satisfies

$\lim_{|z|\to\infty} R(z) = 0$. L-stability is a stronger requirement than A-stability since the degree of $P(z)$ must be strictly less than $Q(z)$ in (10).

Butcher ([8] page 238) suggests that L-stability may be too strong a requirement and a weaker form of L-stability where $\lim_{|z|\to\infty} |R(z)| < 1$ may be easier to satisfy and still provide sufficient damping to allow the stepsize to increase more rapidly when integrating in the smooth region.

Differential algebraic equations (DAEs) are a class of problems that can impose stronger stability requirements than those associated with standard ODEs. The system (5), and (7) is a special case of a DAE. For an extensive introduction to DAEs in general see [3] or [6]. In particular for a detailed survey of the RK method applied to different classes of DAEs see [3].There have been recent attempts to find classes of DAEs where effects of stiffness can be quantified. Brenan and Petzold [6] examined the application of fixed stepsize RK formulas to a subclass of DAEs called constant coefficient linear index one DAEs of the form,

$$\mathbf{B}\mathbf{y}' + \mathbf{C}\mathbf{y} = \mathbf{g}(t), \tag{11}$$

where $\mathbf{B}$ and $\mathbf{C}$ are matrices, with $\mathbf{B}$ not of full rank. They show that there are additional order requirements which are sufficient for a RK formula to achieve its classical fixed stepsize, ODE order. The **Algebraic Order** of an implicit RK formula is equal to k_α if the local error for (11) is $O(h^{k_\alpha+1})$ for sufficiently differentiable $g(t)$. They show that this definition is equivalent to the formula satisfying the additional order requirements $\mathbf{b}^t\mathbf{A}^{-1}\mathbf{c}^j = 1,\ j = 1,\ldots,k_\alpha$ where $\mathbf{c}^j = (c_1^j,\ldots,c_s^j)^t$. Stability for this class of problems also imposes a stronger requirement than A-stability. An implicit RK formula is stable for linear constant coefficient index one DAEs iff $|1 - \mathbf{b}^t\mathbf{A}^{-1}\mathbf{e}| = r < 1$. This is seen to be equivalent to the weaker version of L-stability as $r = \lim_{z\to\infty} |R(z)|$. Brenan and Petzold define the **Constant coefficient order** of an implicit RK formula to be equal to k_c if the method converges with global error $O(h^{k_c})$ for all linear constant coefficient index one systems with $\mathbf{g}(t)$ sufficiently smooth. They then show that the **Constant coefficient order** k_c of an implicit RK formula with $|1-\mathbf{b}^t\mathbf{A}^{-1}\mathbf{e}| = r < 1$ is given as $k_c = min(k_\alpha+1, k_d)$ where k_d is the standard differential order.

Formulas whose classical differential order is not achieved when applied to some problems are said to exhibit **order reduction**. Just as we have seen that the DAE (5), (7) can be viewed as the limiting case of the stiff problem (5), (6) as the 'stiffness' becomes more and more severe one can view (11), as the limiting case of a standard ODE (with B nonsingular) as the stiffness becomes more severe (as B becomes singular). With this interpretation we should not be surprised that the difficulty of 'order reduction' which is associated with the limiting case may also cause difficulties for standard IVPs whose stiffness is severe.

Order reduction has also been associated with the solution of some nonlinear stiff systems of IVPs. Gear [10] considered a formula's behaviour when applied to,

$$\begin{aligned} y' &= \lambda(y - g(t)) + g'(t), \quad y(0) = g(0) + c, & (12)\\ y(t) &= e^{\lambda t}c + g(t). & (13) \end{aligned}$$

By letting $g(t) \equiv 0$ we see this as a generalization of the A-stable scalar test problem. The stability of a formula applied to (12) depends on the initial condition and on the 'smooth' solution $g(t)$.

In using some A-stable formulas to solve stiff nonlinear systems related to (12), Prothero and Robinson [15] found that the discrete solution did not always behave as expected. The accuracy of solutions often appeared inconsistent with the fixed stepsize order of the formula, and the solution was sometimes unstable.

Prothero and Robinson suggested that in the smooth region the original ODE (1) with solution $\mathbf{y} = \mathbf{g}(t)$ can be approximated locally by,

$$\begin{aligned} \mathbf{y}' &\approx \mathbf{f}(t, \mathbf{g}(t)) + \mathbf{J}(t)(\mathbf{y} - \mathbf{g}(t)), & (14)\\ & where\ \mathbf{J}(t) = \frac{\partial \mathbf{f}}{\partial \mathbf{y}}|_{\mathbf{y}=\mathbf{g}(t)}, \end{aligned}$$

in a neighbourhood of the solution.

By looking at a subset of eigenvalues $\lambda(t)$ of $\mathbf{J}(t)$ such that $Re(\lambda(t)) \ll 0$ they observed that the discrete numerical solution to (12) will behave like the corresponding transient component of (14). This problem led them to define a formula to be S-stable iff for all sufficiently differentiable functions $g(t)$ and for all λ in the left half plane, $\exists\ h_0 > 0$ so that the numerical solution y_n associated with (12) satisfies $|\frac{y_{n+1}-g(t_{n+1})}{y_n-g(t_n)}| \leq 1$ for

$y_n \neq g(t_n)$, and for all $0 < h < h_0$. They also defined a formula to be **strongly S-stable** iff it is **S-stable** and $|\frac{y_{n+1}-g(t_{n+1})}{y_n-g(t_n)}| \rightarrow 0$ as $Re(\lambda) \rightarrow \infty$. Since the accuracy of formulas that are not S-stable can be sensitive to the 'stiffness parameter' λ, Prothero and Robinson also defined the stiff order for sufficiently smooth $g(t)$ to be (s,t) iff $\epsilon_n = O(h^{s+1}\lambda^{-t})$ as $Re(-h\lambda) \rightarrow \infty$ and $h \rightarrow 0$ where $\epsilon_n = y_n - g(t_n)$.

By letting $g \equiv 0$ we see that S-stability implies A-stability. Alexander [5] showed that the requirement of S-stability reduced the maximum obtainable order of 2 stage diagonally implicit Runge-Kutta formulas (DIRK) from 3 to 2, and that there are only two such formulas. In general, he observes, S-stability seems to be so restrictive a property that formulas will be of less than optimum order. For this reason, he investigates DIRKs that have less computational cost than fully implicit RK formulas.

In the next section the relationship between stiff order and algebraic order will be discussed.

2 The Stiff Order of Three A-stable Formulas

The two stage diagonally implicit RK formula (DIRK), and the Gauss(2) and Gauss(3) formulas are A-stable. It is known that this DIRK is the only diagonally implicit two stage formula that is A-stable and of order three (see for instance [5]). The two stage Radau IA and Radau IIA are S-stable.

Applying the general RK formula (3), and (4) to the S-stable test problem, we obtain the following expression for the associated stages,

$$\mathbf{Y} = (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e}y_{n-1} - (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{A}(z\hat{\mathbf{g}} - h\hat{\mathbf{g}}'), \tag{15}$$

where $\mathbf{e} = (1, 1, \ldots, 1)^t$ and $\hat{\mathbf{g}}$ and $\hat{\mathbf{g}}'$ are vectors with components $[\hat{\mathbf{g}}]_i = g(t_{n-1} + hc_i)$ and $[\hat{\mathbf{g}}']_i = g'(t_{n-1} + hc_i)$. The discrete solution at the next mesh point is then,

$$\begin{aligned} y_n &= (1 + z\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e})y_{n-1} - \mathbf{b}^t(\mathbf{I} + z(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{A})(z\hat{\mathbf{g}} - h\hat{\mathbf{g}}'), & (16) \\ &= (1 + z\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e})\epsilon_{n-1} + (1 + z\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e})g(t_{n-1}) - \mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}(z\hat{\mathbf{g}} - h\hat{\mathbf{g}}'), & (17) \end{aligned}$$

where $\epsilon_{n-1} = y_{n-1} - g(t_{n-1})$, the distance of the discrete solution from the smooth solution. The local solution is seen to satisfy,

$$\bar{y}_{n-1}(t_n) = \epsilon_{n-1}e^z + g(t_n). \tag{18}$$

Subtracting (17) from (18), the expression for local error is,

$$\begin{aligned} LE_n &= \bar{y}_{n-1}(t_n) - y_n \\ &= (e^z - (1 + z\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e})\ )\,\epsilon_{n-1} \\ &\quad -(1 + z\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e})g(t_{n-1}) \\ &\quad +\mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}(z\hat{\mathbf{g}} - h\hat{\mathbf{g}}') + g(t_n) & (19) \\ &\equiv (e^z - R(z))\epsilon_{n-1} + \beta(z, h, g) & (20) \end{aligned}$$

If we assume that we are in the smooth region then $|\epsilon_{n-1}|$, the distance of the approximate solution from the smooth solution at t_{n-1} is negligible. The form (20) is only meaningful in the smooth region. The sensitivity of the local error to h will then be determined primarily by the term $\beta(z, h, g)$ in equation (20) and $\beta(z, h, g)$ is $O(h^{\bar{k}})$ for some $\bar{k} \leq k_d + 1$ where k_d is the classical order. In the transient region $|z| = |h\lambda|$ will be small due to the accuracy requirement while in the smooth region $|h\lambda|$ should be large if stability is not restricting the stepsize.

If $g(t) \equiv 0$ then $\beta(z, h, g)$ in (20) is zero leaving only the first term which is known to be $O(h^{k_d+1})$. The Taylor expansion of $\beta(z, h, g)$ leads to a set of equations for determining $\bar{k}$,

$$\begin{aligned} LE_n &= (e^z - R(z))\epsilon_{n-1} + \\ &\quad \sum_{k=1}^{\infty} \frac{1}{k!}(1 + \mathbf{b}^t(\mathbf{I} - z\mathbf{A})^{-1}(z\mathbf{c}^{(k)} - k\mathbf{c}^{(k-1)}))g^{(k)}(t_{n-1})h^k, & (21) \end{aligned}$$

where $\mathbf{c}^{(k)} = (c_1^k, c_2^k, \ldots, c_s^k)^t$. Now $\bar{k}$ is seen to be the largest positive integer such that,

$$1+\mathbf{b}^t(\mathbf{I}-z\mathbf{A})^{-1}(z\mathbf{c}^{(k)}-k\mathbf{c}^{(k-1)}) \quad = \quad 0, \tag{22}$$

is satisfied for $0 \le k < \bar{k}$. The limit of these order conditions as $Re(z) \to \infty$ is $1-\mathbf{b}^t\mathbf{A}^{-1}\mathbf{c}^k = 0$ and is equivalent to the algebraic order conditions of DAEs referred to in the last section. S-stable order is then a generalization of algebraic order.

We have derived the stiff orders of the five specific RK formulas identified at the beginning of this section by substituting the appropriate formula coefficients into (21) with the assistance of MAPLE [17]. For example, the local error for Gauss(2) is,

$$\begin{aligned}
LE_n \quad = \quad & (e^z - \frac{12+6z+z^2}{12-6z+z^2})\epsilon_{n-1} + \\
& \frac{1}{36}\frac{z^2}{12-6z+z^2}g^{(3)}(t_{n-1})h^3 + \\
& \frac{1}{72}\frac{-z+z^2}{12-6z+z^2}g^{(4)}(t_{n-1})h^4 + \\
& \frac{1}{4320}\frac{12-30z+17z^2}{12-6z+z^2}g^{(5)}(t_{n-1})h^5 + O(h^6)
\end{aligned} \tag{23}$$

This expansion explicitly reveals the nature of reduced order. The coefficients of all powers of h are rational functions of z bounded for z in the left half plane. The polynomial degree of the denominator and numerator of these rational functions is bounded by the number of stages. The local error depends partly on which derivatives of $g(t)$ are non zero. In the worst case, the first non-zero term in the expansion of β determines the dominent term in the local error. If $h \to 0$ and $z \to 0$ then full order is achieved. If as $h \to 0$, z remains large the worst case fixed stepsize order is realized. In this case, if the local error is $O(h^q)$ for $q \le k_d + 1$ then the global error is also $O(h^q)$. This follows since in the smooth region, $\epsilon_{n-1}e^z$ is very small and the discrete solution, the actual solution and the smooth solution are close to each other. There is no error amplification since from the definition of LE and (18) we have,

$$\begin{aligned}
LE_n \quad &= \quad e^z\underbrace{(y_{n-1}-g(t_{n-1}))}_{O(h^q)} - \underbrace{(y_n-g(t_n))}_{O(h^q)} \\
&= \quad e^z\epsilon_{n-1} - \epsilon_n
\end{aligned} \tag{24}$$

and the first term is being strongly damped out independently of the formula and therefore LE, GE and ϵ must be of the same order q, where q is the reduced order. The global error is then,

$$\begin{aligned}
GE_n \quad &= \quad y(t_n) - y_n, \\
&= \quad \underbrace{(y(t_n)-g(t_n))}_{<\tau} - \underbrace{(y_n-g(t_n))}_{O(h^q)}, \\
&= \quad \epsilon_0 e^{\lambda t} - \quad \epsilon_n.
\end{aligned} \tag{25}$$

The order q is determined most easily as the order of ϵ_n which can be derived directly by equating (21) and (24) and solving the recurence relation,

$$\epsilon_n \quad = \quad R(z)\epsilon_{n-1} - \beta_{n-1}(z,h,g).$$

In the worst case if $R(z) \approx 1$ then for a fixed stepsize $\epsilon_n = O(h^{\bar{k}-1})$ where from (22) $\bar{k}$ is defined by $|\beta_{n-1}| = O(h^{\bar{k}})$. As $z \to -\infty$ this is true for the Gauss(2) formula and the order is $q = \bar{k}-1 = 2$. The Gauss(3) formula will gain accuracy from $R(z) < 0$, which causes the error to oscillate in sign, so we do not expect to lose one power of h empirically. The DIRK's stability polynomial $R(z) \to -.73205$ as $z \to -\infty$

damping β_n strongly and also should not lose a power of h. The Radau IA is S-stable and Radau IIA is strongly S-stable.

To damp out the error coming from the β_n expansion a method called smoothing can be implemented [18]. This method uses one step of a related symmetric method every n steps to damp out the error that has accumulated from the β term. The optimal choice for n is of current interest but is beyond the scope of this paper.

Frank, Schneid and Ueberhuber [16], considered problems of the form,

$$y' = \lambda y + e^{-t}, \quad where\ y(0) = -(1+\lambda)^{-1}. \tag{26}$$

They suggested that problems of this form, gain one power of λ^{-1} in the stiff order result. This can be seen by rearranging this equation as,

$$\begin{aligned} y' &= \lambda(y - (-\frac{e^{-t}}{1+\lambda})) + \frac{e^{-t}}{1+\lambda}, & (27)\\ &= \lambda(y - g(t;\lambda)) + g'(t;\lambda). & (28)\end{aligned}$$

The $g(t)$ in this case depends on λ, and the derivatives of $g(t)$ contain the factor $\frac{1}{1+\lambda}$. This results in higher accuracy than expected for large λ as the local error is $O(h^q\lambda^{-t})$ (see [2]).

Table 2 summarizes the resulting orders and stability of the example formulas introduced. In the table a '-' indicates that the relevant property does not hold.

Formula	k_d k_α k_c	$R(z)$	$\bar{k}$ TERM	(q,t)	S-*stable*
DIRK	3 1 2	$\frac{6-2\sqrt{3}z-(1+\sqrt{3})z^2}{6-(6+2\sqrt{3})z+(2+\sqrt{3})z^2}$	$\frac{1}{12}\frac{(3+2\sqrt{3})z^2}{6-(6+2\sqrt{3})z+(2+\sqrt{3})z^2}g''(t_{n-1})h^2$	(2,0)	-
Gauss(2)	4 2 3	$\frac{12+6z+z^2}{12-6z+z^2}$	$\frac{1}{36}\frac{z^2}{12-6z+z^2}g^{(3)}(t_{n-1})h^3$	(3,0)	-
Gauss(3)	6 3 4	$\frac{120+60z+12z^2+z^3}{120-60z+12z^2-z^3}$	$\frac{1}{480}\frac{-z^3}{120-60z+12z^2-z^3}g^{(4)}(t_{n-1})h^4$	(4,0)	-
Radau IA	3 1 2	$\frac{6+2z}{6-4z+z^2}$	$\frac{z^2}{36-24z+6z^2}g^{(2)}(t_{n-1})h^2$	(2,0)	$\checkmark$
Radau IIA	3 ∞ 3	$\frac{6+2z}{6-4z+z^2}$	$\frac{z}{54-36z+9z^2}g^{(3)}(t_{n-1})h^3$	(3,1)	$\checkmark$

3 Observed Order and the Implications of Order Reduction

We are interested in quantifying the relationship between accuracy and cost. Cost can be related directly to the number of steps. This will be seen to be sufficient for our purposes, although it will not reflect the lower cost per step of DIRKs relative to the other fully implicit formulas. The order and stability analysis discussed in the last two sections relates accuracy to cost by means of a fixed stepsize. As we have noted, this limits the relevance of the results to variable stepsize codes applied to stiff problems.

If the problem is stiff then average, maximum and minimum stepsizes can vary over several orders of magnitude and are not determined only by accuracy. Using the maximum stepsize may not be an appropriate measure of the cost of integration.

If we are to introduce a more meaningful definition of order $\bar{p}$, then it must more directly quantify the relationship between cost and accuracy. Rather than use the maximum h we will use the average h, but we first need to introduce notation for the global error associated with integration over the interval $[a,b]$ given the required tolerance τ.

Let

$$\overline{GE}_\tau = \max_{i=1,\ldots,N_\tau} |y(t_i) - y_i|,$$

where N_τ is the number of steps required by the method to integrate from $t_0 = a$ to $t_{N_\tau} = b$. If the stepsize selection scheme, the error estimate and the problem are sufficiently smooth, it is reasonable to fit the observed global error to the model,

$$\overline{GE}_\tau \;=\; c\,\bar{h}_\tau^{\bar{p}} + O(\bar{h}_\tau^{\bar{p}+1}), \tag{29}$$

where $\bar{h}_\tau = \frac{b-a}{N_\tau}$. When this is done we can consider $\bar{p}$ to be the **observed order** while c may depend on the problem and the underlying formula but not on N_τ. In order to estimate this observed order we solve a problem with two different values of the tolerance, determine $\overline{GE}_{\tau_1}$ and $\overline{GE}_{\tau_2}$ (either analytically or numerically), and using (29) and the assumption that $\bar{h}_{\tau_1}$ and $\bar{h}_{\tau_2}$ are sufficiently small, we can approximate $\bar{p}$ by,

$$\bar{p} \approx \hat{p} \;\equiv\; -(\log(\frac{\overline{GE}_{\tau_1}}{\overline{GE}_{\tau_2}}))/(\log(\frac{\bar{h}_{\tau_1}}{\bar{h}_{\tau_2}})). \tag{30}$$

4 Numerical Testing

In testing, as h becomes small it is necessary to know when the round-off error (RO) dominates the local error. One indication of this dominance is when the global error begins to oscillate or becomes larger with stricter tolerances. We will ignore the resulting observed order in this case.

We have used Newton's method to solve the non-linear system to evaluate the stages of both the implicit and semi-explicit formulas, and a standard step size control based on bounding the error per unit step,

$$\hat{h} \;=\; .9\left(\frac{\tau h}{\|\mathbf{est}_{n-1}\|}\right)^{1/k_d} h. \tag{31}$$

To avoid large increases in h when est_{n-1} is anomalously small, we do not allow h to more than double at each step.

The problems used in testing were chosen from a variety of sources. Each problem had a parameter to vary the stiffness, and was originally proposed to reveal the effects of order reduction. The two scalar problems reported here are instances of the S-stable test problem [16].

Problem 1.

$$\begin{aligned} y' &= \lambda(y+1) + e^{-t}, \\ y(0) &= -(1+\lambda)^{-1} + 1, \\ & t \in [0,5] \end{aligned}$$

with true solution,

$$y(t) = -\frac{e^{-t}}{1+\lambda} - 1 + 2e^{t\,\lambda},$$

which decays to -1 as $t \longrightarrow +\infty$. The smooth solution $-\frac{e^{-t}}{1+\lambda} - 1$ depends on λ.

Problem 2.

$$\begin{aligned} y' &= \lambda(y - sin(\frac{\pi}{4}+t)) + cos(\frac{\pi}{4}+t), \\ y(0) &= \frac{\sqrt{2}}{2} + 1, \\ & t \in [0,5] \end{aligned}$$

with true solution,

$$y(t) \;=\; sin(\frac{\pi}{4}+t) + e^{t\,\lambda}.$$

The smooth solution $sin(\frac{\pi}{4}+t)$ is independent of λ.

Tests were also performed on two vector problems and results are reported in [1]. In all our tests the initial stepsize was set to $-log(\tau)/\lambda$ so that the transient region of the linearized problem could be crossed in

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.72E-06	76		0.37E-05	12		102	
0.1E-03	0.73E-07	164	2.99	0.34E-05	16	0.26	210	0.10
0.1E-04	0.73E-08	353	3.01	0.60E-06	27	3.33	446	2.31
0.1E-05	0.73E-09	762	2.99	0.81E-07	65	2.28	970	2.58
0.1E-06	0.72E-10	1642	3.00	0.81E-08	256	1.68	2208	2.80
0.1E-07	0.72E-11	3539	3.00	0.42E-09	1159	1.95	5366	3.32
0.1E-08	0.72E-12	7626	3.00	0.86E-11	4031	3.13	13096	4.37
0.1E-09	0.11E-12	16954	2.40	0.24E-12	11083	3.56	31136	4.16

Table 1: problem 1 , using DIRK $t \in [0, 5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.73E-09	762		0.33E-08	9		957	
0.1E-03	0.72E-10	1643	3.00	0.31E-08	9	∞	2042	0.09
0.1E-04	0.72E-11	3539	3.00	0.37E-08	9	∞	4380	-0.23
0.1E-05	0.72E-12	7626	3.00	0.33E-08	9	∞	9417	0.15
0.1E-06	0.11E-12	16941	2.39	0.37E-08	9	∞	20781	-0.16

Table 2: problem 1 , using DIRK $t \in [0, 5]$, $\lambda = -10^6$

a small number of steps . This choice of the initial stepsize resulted in a few more rejected steps at the start of the integration, when tolerances were stringent but the number of rejected steps was always negligible compared to the number of successful steps.

The tables of detailed results present the observed order over the transient region and over the smooth region, as well as the global result over the whole interval $[0, xend]$ where $xend$ is the end of the integration interval. The transient region that we have selected is $[0, T]$ where $T = -5/\lambda$. The transient region of the linearized problem is actually $[0, -log(\tau)/\lambda]$ but this has been averaged to compare results over varying tolerances. The smooth region occurs after the discrete solution is within tolerance of the smooth solution. This region begins after T. It has been set to be $[.01, xend]$.

The results reported for each region include *error* - maximum true error, N - the number of steps taken to integrate over the region and *order* - the observed order. For the global result in all of our tests the maximum error was always equal to the smooth region error and has therefore been omitted from the tables. The number of steps is a count of successful steps, and ignores rejected steps. After the method has taken a few steps, it generally rejects a very small number of steps.

The program terminated after trying the tolerance beyond the last shown in a table to a minimum of $\tau = 10^{-15}$. The reason for premature termination was either because h was too small in the transient ($h < \mu$ where μ is unit round-off error), or too many steps were taken ($N > 10^7$).

For problem 1 the error coefficient in the smooth region contains the factor $1/(1 + \lambda)$ and so we expect high accuracy as λ increases in magnitude (over the smooth region). The DIRK produces full order in the transient as expected (see table 1-2). As λ increases in magnitude, a higher percentage of the work is associated with the transient and eventually the smooth region is integrated with only 9 steps. Achieved accuracy doesn't improve beyond 10^{-8}. For this reason the observed order results outside the transient region are not meaningful. This is also true of the Radau formulas (see table 5-8). Both Radau formulas have comparable cost to achieved accuracy to DIRK. In the transient regions the Radau formulas have almost identical results because they have the same stability polynomial. The Radau IA exhibits an observed order of 2.85 for $\lambda = -10^3$ and $\tau = 10^{-6}$ which is better than the worst case of order 2.

The discrete solution using the Gauss formula on the whole region achieves full order for $|\lambda| \leq 10^3$ and has no observable order for $\lambda = -10^6$ (see table 3-4). The program terminates successfully for Gauss(3) and it stops when $h < \mu$ for DIRK.

For problem 2 the number of steps taken over the transient region generally increases as λ increases in

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.86E-06	4		0.86E-06	10		15	
0.1E-03	0.53E-07	5	12.4	0.84E-07	10	∞	18	12.7
0.1E-04	0.37E-08	7	7.94	0.86E-07	11	-0.19	22	-0.09
0.1E-05	0.40E-09	11	4.93	0.63E-07	13	1.86	28	1.29
0.1E-06	0.43E-10	15	7.18	0.22E-07	15	7.35	37	3.77
0.1E-07	0.46E-11	22	5.86	0.36E-08	19	7.69	51	5.66
0.1E-08	0.48E-12	32	6.02	0.22E-09	27	7.96	73	7.80
0.1E-09	0.49E-13	46	6.26	0.10E-10	42	6.97	109	7.68
0.1E-10	0.51E-14	68	5.79	0.10E-11	70	4.47	167	5.35
0.1E-11	0.56E-15	99	5.91	0.99E-13	124	4.08	266	5.01
0.1E-12	0.56E-15	147	0.00	0.71E-14	225	4.43	434	5.39
0.1E-13	0.56E-15	233	0.00	0.67E-15	404	4.04	737	4.47

Table 3: problem 1 , using Gauss(3) $t \in [0, 5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.41E-09	11		0.41E-09	9		38	
0.1E-03	0.43E-10	15	7.23	0.14E-09	9	∞	46	5.64
0.1E-04	0.46E-11	22	5.87	0.12E-09	9	∞	58	0.67
0.1E-05	0.48E-12	32	6.03	0.60E-10	9	∞	76	2.50
0.1E-06	0.49E-13	46	6.27	0.11E-09	9	∞	102	-2.01
0.1E-07	0.50E-14	68	5.84	0.77E-10	9	∞	140	1.10
0.1E-08	0.67E-15	99	5.36	0.67E-10	9	∞	195	0.40
0.1E-09	0.44E-15	147	1.03	0.26E-10	10	8.90	280	2.59
0.1E-10	0.67E-15	243	-0.81	0.22E-10	14	0.59	446	0.43

Table 4: problem 1 , using Gauss(3) $t \in [0, 5]$, $\lambda = -10^6$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.67E-06	42		0.70E-05	12		62	
0.1E-03	0.70E-07	89	3.02	0.67E-05	14	0.261	120	0.609E-01
0.1E-04	0.71E-08	191	2.99	0.26E-05	21	2.40	248	1.34
0.1E-05	0.72E-09	410	3.00	0.28E-06	53	2.41	541	2.85
0.1E-06	0.72E-10	883	3.00	0.21E-07	237	1.71	1287	2.96
0.1E-07	0.72E-11	1901	3.00	0.64E-09	1004	2.43	3264	3.77
0.1E-08	0.72E-12	4095	3.00	0.81E-11	3133	3.83	8001	4.86
0.1E-09	0.79E-13	8882	2.85	0.20E-12	7995	3.94	18542	4.39

Table 5: problem 1 , using Radau IA $t \in [0, 5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.72E-09	410		0.69E-08	9		526	
0.1E-03	0.72E-10	883	3.00	0.66E-08	9	∞	1109	0.544E-01
0.1E-04	0.72E-11	1901	3.00	0.71E-08	9	∞	2365	-0.102
0.1E-05	0.72E-12	4095	3.00	0.71E-08	9	∞	5070	0.129E-02
0.1E-06	0.78E-13	8881	2.88	0.72E-08	9	∞	10955	-0.521E-02

Table 6: problem 1 , using Radau IA $t \in [0, 5]$, $\lambda = -10^6$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.67E-06	42		0.67E-06	12		62	
0.1E-03	0.70E-07	89	3.02	0.70E-07	14	14.7	120	3.43
0.1E-04	0.71E-08	191	2.99	0.71E-08	19	7.47	246	3.18
0.1E-05	0.72E-09	410	3.00	0.44E-08	28	1.24	516	0.649
0.1E-06	0.72E-10	883	3.00	0.42E-08	49	0.736E-01	1099	0.545E-01
0.1E-07	0.72E-11	1901	3.00	0.24E-08	96	0.848	2356	0.748
0.1E-08	0.72E-12	4095	3.00	0.28E-09	207	2.80	5076	2.81
0.1E-09	0.75E-13	8881	2.93	0.22E-10	532	2.67	11079	3.23

Table 7: problem 1 , using Radau IIA $t \in [0, 5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.72E-09	410		0.69E-08	9		526	
0.1E-03	0.72E-10	883	3.00	0.66E-08	9	∞	1109	0.544E-01
0.1E-04	0.72E-11	1901	3.00	0.71E-08	9	∞	2365	-0.102
0.1E-05	0.72E-12	4095	3.00	0.71E-08	9	∞	5070	0.129E-02
0.1E-06	0.78E-13	8881	2.88	0.72E-08	9	∞	10955	-0.521E-02

Table 8: problem 1 , using Radau IIA $t \in [0, 5]$, $\lambda = -10^6$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.73E-06	58		0.57E-03	79		148	
0.1E-03	0.73E-07	125	2.99	0.16E-04	583	1.80	732	2.25
0.1E-04	0.73E-08	271	2.98	0.54E-06	2708	2.20	3031	2.37
0.1E-05	0.73E-09	584	3.00	0.11E-07	8234	3.55	8932	3.65
0.1E-06	0.73E-10	1260	3.00	0.69E-09	20586	2.97	22091	3.00
0.1E-07	0.73E-11	2715	3.00	0.17E-10	47382	4.43	50627	4.45
0.1E-08	0.73E-12	5850	3.00	0.12E-11	105192	3.38	112184	3.39

Table 9: problem 2 , using DIRK $t \in [0, 5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.73E-09	584		0.35E-03	80		814	
0.1E-03	0.73E-10	1260	3.00	0.11E-04	761	1.53	2333	3.27
0.1E-04	0.73E-11	2715	3.00	0.33E-06	7562	1.55	10952	2.30
0.1E-05	0.73E-12	5850	3.00	0.15E-07	73145	1.36	80551	1.55

Table 10: problem 2 , using DIRK $t \in [0, 5]$, $\lambda = -10^6$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.13E-05	3		0.29E-03	10		15	
0.1E-03	0.89E-07	5	5.31	0.16E-03	12	3.11	19	2.40
0.1E-04	0.58E-08	7	8.12	0.20E-04	15	9.39	25	7.63
0.1E-05	0.49E-09	9	9.86	0.96E-06	24	6.48	38	7.27
0.1E-06	0.47E-10	13	6.39	0.62E-07	44	4.51	63	5.41
0.1E-07	0.52E-11	19	5.81	0.35E-08	83	4.52	111	5.06
0.1E-08	0.49E-12	28	6.08	0.21E-09	161	4.23	201	4.72
0.1E-09	0.50E-13	41	5.99	0.10E-10	306	4.77	365	5.13
0.1E-10	0.52E-14	60	5.91	0.53E-12	555	4.94	641	5.22
0.1E-11	0.11E-14	87	4.17	0.37E-13	953	4.92	1078	5.12
0.1E-12	0.67E-15	130	1.27	0.11E-14	1559	7.19	1745	7.35
0.1E-13	0.44E-15	203	0.91	0.67E-15	2456	1.06	2746	1.06
0.1E-14	0.11E-14	297	-2.41	0.11E-14	4426	-0.87	4860	-0.90

Table 11: problem 2 , using Gauss(3) $t \in [0,5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	N	order	error	N	order	N	order
0.1E-02	0.59E-09	9		0.39E-03	9		36	
0.1E-03	0.51E-10	13	6.63	0.16E-03	11	4.28	45	3.85
0.1E-04	0.48E-11	19	6.22	0.17E-04	14	9.37	59	8.34
0.1E-05	0.48E-12	28	5.95	0.14E-05	21	6.21	82	7.64
0.1E-06	0.49E-13	41	5.98	0.10E-06	40	4.02	123	6.39
0.1E-07	0.50E-14	60	6.02	0.69E-08	77	4.14	194	5.96
0.1E-08	0.44E-15	87	6.51	0.38E-09	161	3.91	327	5.53
0.1E-09	0.67E-15	131	-0.99	0.23E-10	340	3.76	581	4.89
0.1E-10	0.56E-15	207	0.40	0.11E-11	797	3.56	1173	4.32
0.1E-11	0.67E-15	422	-0.26	0.15E-12	1817	2.44	2505	2.65

Table 12: problem 2 , using Gauss(3) $t \in [0,5]$, $\lambda = -10^6$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.66E-06	33		0.53E-03	91		131	
0.1E-03	0.69E-07	71	2.95	0.15E-04	595	1.91	680	2.18
0.1E-04	0.71E-08	152	2.99	0.62E-06	2275	2.36	2455	2.46
0.1E-05	0.72E-09	326	3.00	0.99E-08	6162	4.16	6549	4.22
0.1E-06	0.72E-10	701	3.00	0.40E-09	14586	3.73	15419	3.75
0.1E-07	0.72E-11	1509	3.00	0.16E-10	32737	3.95	34531	3.96
0.1E-08	0.72E-12	3250	3.00	0.11E-11	71839	3.42	75702	3.42

Table 13: problem 2 , using Radau IA $t \in [0,5]$, $\lambda = -10^3$

tol	Transient $[x_0$,T]			Smooth $[.01, xend]$			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.72E-09	326		0.76E-03	93		506	
0.1E-03	0.72E-10	701	3.00	0.19E-04	878	1.64	1755	2.96
0.1E-04	0.72E-11	1509	3.00	0.51E-06	8732	1.58	10618	2.02
0.1E-05	0.72E-12	3250	3.00	0.14E-07	83749	1.57	87928	1.68

Table 14: problem 2 , using Radau IA $t \in [0,5]$, $\lambda = -10^6$

tol	Transient [x_0,T]			Smooth [.01, $xend$]			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.66E-06	33		0.61E-04	11		51	
0.1E-03	0.69E-07	71	2.95	0.39E-04	13	2.60	98	0.664
0.1E-04	0.71E-08	152	2.99	0.21E-04	19	1.67	200	0.889
0.1E-05	0.72E-09	326	3.00	0.91E-06	65	2.55	453	3.83
0.1E-06	0.72E-10	701	3.00	0.28E-07	388	1.95	1222	3.52
0.1E-07	0.72E-11	1509	3.00	0.82E-09	1653	2.43	3447	3.40
0.1E-08	0.72E-12	3250	3.00	0.13E-10	4755	3.89	8620	4.48
0.1E-09	0.84E-13	7200	2.70	0.66E-12	11542	3.39	20064	3.56

Table 15: problem 2 , using Radau IIA $t \in [0,5]$, $\lambda = -10^3$

tol	Transient [x_0,T]			Smooth [.01, $xend$]			Whole Interval	
	error	n	order	error	n	order	n	order
0.1E-02	0.72E-09	326		0.61E-07	9		422	
0.1E-03	0.72E-10	701	3.00	0.42E-07	9	∞	885	0.498
0.1E-04	0.72E-11	1509	3.00	0.83E-07	9	∞	1881	-0.902
0.1E-05	0.72E-12	3250	3.00	0.51E-07	9	∞	4028	0.631
0.1E-06	0.80E-13	7203	2.77	0.43E-07	9	∞	8854	0.209

Table 16: problem 2 , using Radau IIA $t \in [0,5]$, $\lambda = -10^6$

magnitude, for a fixed accuracy. The transient region is decreasing in size as $5/\lambda$. The stepsize h therefore changes as $O(1/(N\lambda))$. Full order is expected in the transient since $h\lambda = O(1/N)$ is small.

Using the DIRK full classical order is achieved on the whole interval. At $\lambda = 10^{-6}$ we still have tolerance proportionality, but the observed order has been reduced to 1.36 (see table 10) in the smooth region. In this case $h\lambda \approx 68$ and some order reduction is occurring. The predicted worst case S-stability order is 1. The overall order is 1.55. This is better than in the smooth region, because full order is achieved in the transient where a significant amount of the work is done, although it is also clear, that for strict tolerances most of the work is associated with the smooth region.

The Radau IA has an observed reduced order of 2 only for $\lambda = -10^6$ and $\tau = 10^{-6}$. For the same achieved accuracy as the DIRK the Radau IA costs more for $\lambda = -10^3$ and less for $\lambda = -10^6$. The Radau IIA attains better than classical order and cost far less than the DIRK for the same accuracy if we ignore the cost advantage of the DIRK (see tables 13-16).

The Gauss(3) formula produced similar results with respect to the predicted reduced order from $2s$ to s. The observed order $\bar{p}$ is in the interval [4.17-6.5], [3.9-4.92], [5.2-5.5] over the transient, smooth and over the whole interval respectively (see tables 11 and 12). Full accuracy is essentially achieved when tolerance $= 10^{-10}$.

When the program terminates for this problem before $\tau = 10^{-14}$, it is due to $h < \mu$ for DIRK, and it is because too many steps are taken for Gauss(3). The Radau IA takes too many steps and the Radau IIA has $h < \mu$.

For both problems and all formulas, the achieved accuracy behaved like $\tau/|\lambda|$ in the transient region. In the smooth region tolerance proportionality was still maintained with a constant of proportionality less than or near one and independent of $|\lambda|$. In many cases especially for large values of $|\lambda|$, the stepsize in this region was determined by the rule to never more than double the stepsize, rather than accuracy and consequently the observed order results are not appropriate.

5 Conclusion

In this paper we have reviewed the concepts of stability, stiffness and order reduction and investigated numerically the extent of order reduction for variable step implicit RK methods. We have derived the general local error expression for RK formulas applied to the S-stable test problem and determined these terms explicitly for five A-stable formulas. A global measure of order was introduced, which we have called the 'observed order' that was thought to better reflect the relationship between accuracy and cost. This measure was used in experiments on the formulas introduced and detailed results for two test problems were reported.

The results of more extensive testing are contained in [1] including tables for a linear and a non-linear vector problem. The linear problem displayed no order reduction for any formula. The other results were consistent with those reported here.

The lack of S-stability in these formulas did not reduce this measure of order to the worst case fixed stepsize S-stable order over the interval of integration, although some degradation of order was observed. Variable stepsize methods based on formulas that are A-stable, have higher observed order than suggested by stiff-order analysis for some problems. The observed order is a more appropriate measure of the performance of adaptive step methods but it may be too sensitive to the particular test problem to allow general observations or conclusions.

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