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ROBUST DEFECT CONTROL WITH RUNGE–KUTTA SCHEMES*

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Abstract. Enright [Numerical Analysis Report 122, University of Manchester, Manchester, U.K., 1986] implements a Runge–Kutta method for solving the initial value problem using an alternative to the standard local error control scheme. The aim is to control the defect associated with a local interpolant by sampling its value at one or more fixed points within each step. However, in general, the quality of a sample point is problem-dependent and also varies from step to step. Two classes of interpolant are presented for which the asymptotic behaviour of the defect is known a priori, allowing optimal sample points to be chosen.

Key words. Runge–Kutta formula, defect, interpolation

AMS(MOS) subject classification. 65L05

1. Introduction. We consider the numerical solution of a nonstiff system of ordinary differential equations

$$(1.1)\qquad \begin{aligned} &y'(x)=f(x, y(x)), \qquad y(x_0)=y_0,\\ &f:\mathbf{R}\times\mathbf{R}^N\to\mathbf{R}^N, \end{aligned}$$

using an explicit Runge–Kutta method. Given $y_n \approx y(x_n)$, such a method takes a step of length h $(=h_n)$ and produces an approximation y_{n+1} to $y(x_n+h)$. Most popular codes attempt to control the local error $u(x_n+h)-y_{n+1}$, where the local solution $u(x)$ satisfies $u'(x)=f(x, u(x))$ and $u(x_n)=y_n$. Recently several authors have shown that it is possible, at reasonable cost, to produce a function $p(x)$ that approximates the local solution over the entire step [1], [4], [6], [8]–[10]. It is then natural to consider the *defect* of $p(x)$,

$$(1.2)\qquad \delta(x):=p'(x)-f(x, p(x)),$$

that is, the amount by which $p(x)$ fails to satisfy the differential equations. Enright [2] suggests that it may be preferable to control the defect on each step rather than the local error. This approach is shown to offer several advantages, particularly from the user's point of view. Further analysis of defect control strategies is given in [3]. We are concerned here with the problem of reliably estimating the defect.

One of the defect control schemes proposed in [2] is motivated by the desire to bound $\max_{\tau\in[0,1]}\|\delta(x_n+\tau h)\|_\infty$. The defect is sampled at the points $\{x_n+\tau_i^* h\}_{i=1}^k$, where the $\{\tau_i^*\}_{i=1}^k$ are fixed in $(0,1)$, and the step is accepted if and only if $\max_{1\le i\le k}\|\delta(x_n+\tau_i^* h)\|_\infty<\mathrm{TOL}$, for some user-supplied parameter TOL. The simplest case, $k=1$, is implemented in [2], and an asymptotic expansion of $\delta(x)$ is used there to gain insight into the performance of this type of scheme. We now consider this expansion.

To begin, we suppose that the approximation $p(x)$ has local order $l+1$, that is,

$$(1.3)\qquad p(x)-u(x)=O(h^{l+1}).$$

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Assuming that f satisfies a Lipschitz condition on $[x_n, x_n + H]$, where $h < H$, we then have

$$(1.4)\qquad \begin{aligned} \delta(x) &= p'(x) - u'(x) + f(x, u(x)) - f(x, p(x)) \\ &= p'(x) - u'(x) + O(h^{l+1}). \end{aligned}$$

Using local interpolants derived in [4] for the function $p(x)$, Enright notes that for sufficiently smooth f, (1.4) may be written in the form

$$(1.5)\qquad \delta(x_n + \tau h) = h^l \sum_{j=1}^{m_l} q_j'(\tau) F_j + O(h^{l+1}).$$

Here F_j is an elementary differential that depends only on f, x_n, and y_n, and $q_j'(\tau)$ is a polynomial in τ whose coefficients depend only on the Runge-Kutta interpolation scheme. Enright recommends that for a particular scheme a sample point τ^* should be chosen so that each $|q_j'(\tau^*)|$ is relatively large. This means that if one of the F_j's is dominant, then it will be allowed to make a significant contribution to the leading term. However, he points out that for any fixed τ^* there always exists the possibility of cancellation in the sum $\sum_{j=1}^{m_l} q_j'(\tau^*) F_j$, caused by the problem-dependent F_j's. Hence the size of the defect at $x_n + \tau^* h$ can be an arbitrarily poor indication of its maximum value over $[x_n, x_n + h]$.

In this paper we introduce some alternative interpolants for use with a defect control scheme. For these interpolants the associated defect has the form (1.5), but the important additional feature is that each $q_j'(\tau)$ is a multiple of a known polynomial $\Phi(\tau)$ so that

$$(1.6)\qquad \delta(x_n + \tau h) = h^l \Phi(\tau) K + O(h^{l+1})$$

where K is independent of τ and h. (In fact we shall prove this result directly by interpolation theory rather than by using (1.5).) It follows that a sample point is available that is asymptotically optimal for any problem, namely, a τ^* that maximises $|\Phi(\tau)|$ over $[0, 1]$.

In the next section we present two classes of interpolant that have this property and give some specific examples. The corresponding defect control schemes incur a higher cost per step than those of [2] and [3]. This is discussed in § 3. The final section describes the results of some numerical experiments that support the theory.

2. The interpolants. The interpolants considered below fall within the framework of Shampine [9] and Gladwell et al. [6]. We suppose that there are distinct points $\{\xi_i\}_{i=1}^m$ in $[x_n, x_n + h]$ with corresponding approximations $u_i \in \mathbf{R}^N$ satisfying

$$u_i - u(\xi_i) = O(h^{q+1}), \qquad i = 1, \cdots, m,$$

and that $u_i' = f(\xi_i, u_i) \in \mathbf{R}^N$ is available for $i = 1, \cdots, r \leqq m$, whence

$$u_i' - u'(\xi_i) = O(h^{q+1}), \qquad i = 1, \cdots, r$$

for Lipschitzian f. The data $\{u_i\}_{i=1}^m$ and $\{u_i'\}_{i=1}^r$ is said to be of local order $q+1$. We then take $p(x): \mathbf{R} \to \mathbf{R}^N$ to be the unique Hermite interpolating polynomial of degree less than or equal to $m + r - 1$ that satisfies

$$(2.1)\qquad \begin{aligned} p(\xi_i) &= u_i, \qquad i = 1, \cdots, m, \\ p'(\xi_i) &= u_i', \qquad i = 1, \cdots, r. \end{aligned}$$

We insist that $\xi_1 = x_n$, $u_1 = y_n$, $\xi_r = x_n + h$, and $u_r = y_{n+1}$, ensuring that the piecewise polynomial interpolant is continuously differentiable over the range of integration and hence that the defect (1.2) is properly defined.

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Shampine [9] (see also [6]) has examined the accuracy of this interpolant, and its derivatives, by splitting the error into two components in the following way. Let $Q(x)$ denote the Hermite polynomial that interpolates to the *exact* local values:

$$Q(\xi_i) = u(\xi_i), \qquad i = 1, \cdots, m,$$

$$Q'(\xi_i) = u'(\xi_i), \qquad i = 1, \cdots, r.$$

We assume that u has $m+r$ continuous derivatives and write

$$p^{(k)}(x) - u^{(k)}(x) = [p^{(k)}(x) - Q^{(k)}(x)] + [Q^{(k)}(x) - u^{(k)}(x)]. \tag{2.2}$$

Shampine shows that the first term on the right-hand side of (2.2), the "data error," is $O(h^{q+1-k})$ while the second term, the "interpolation error," is $O(h^{m+r-k})$. We make use of this result with $k=0$ and $k=1$ to examine the asymptotic behaviour of the defect in two special cases.

2.1. Case I. We suppose that the interpolation scheme has been set up so that the interpolation error is dominant in (2.2), that is, $m+r<q+1$. It then follows from (1.3) and (1.4) that

$$\delta(x) = Q'(x) - u'(x) + O(h^{m+r}) \tag{2.3}$$

with

$$Q'(x) - u'(x) = O(h^{m+r-1}).$$

The precise form of $Q'(x)-u'(x)$ can be found by applying classical interpolation theory. We denote by $u_t(x)$ and $Q_t(x)$ the tth components of $Q(x)$ and $u(x)$, respectively, and examine the term $Q_t'(x)-u_t'(x)$. The following theorem summarises some results from [12, pp. 1-5].

THEOREM 1. *If $u_t \in C^{m+r}[x_n, x_n+h]$, then for $x_n \leqq x \leqq x_n+h$*

$$Q_t(x) - u_t(x) = -\pi(x) G_t(x) \tag{2.4}$$

where

$$\pi(x) = \prod_{i=1}^{r} (x-\xi_i)^2 \prod_{i=r+1}^{m} (x-\xi_i)$$

and

$$G_t(x) = \frac{u_t^{(m+r)}(\theta(x))}{(m+r)!}$$

for some $x_n \leqq \theta(x) \leqq x_n+h$. Furthermore, $G_t'(x)$ is continuous on $[x_n, x_n+h]$.

Now write $\xi_i = x_n + \sigma_i h$ and let $x = x_n + \tau h$, so that

$$\pi(x) = \prod_{i=1}^{r} (\tau-\sigma_i)^2 h^2 \prod_{i=r+1}^{m} (\tau-\sigma_i) h$$

$$\equiv h^{m+r} r(\tau).$$

Differentiating (2.4) and using the additional fact that

$$G_t(x) = \frac{u_t^{(m+r)}(x_n)}{(m+r)!} + O(h),$$

we obtain

$$Q_i'(x) - u_i'(x) = -h^{m+r-1} \frac{dr(\tau)}{d\tau} \frac{u_i^{(m+r)}(x_n)}{(m+r)!} + O(h^{m+r}),$$

for each $1 \leqq i \leqq N$. Substituting this expression into (2.3), we find

$$\delta(x_n + \tau h) = -h^{m+r-1} \frac{dr(\tau)}{d\tau} \frac{u^{(m+r)}(x_n)}{(m+r)!} + O(h^{m+r}), \tag{2.5}$$

which has the required form (1.6), and shows that, asymptotically, the defect behaves as does a multiple of $dr(\tau)/d\tau$ over the step.

We now consider some specific interpolation schemes of this type. It is traditional to measure the cost of a Runge–Kutta-interpolation scheme in terms of the number of f evaluations required per step. We will use the notation $s(+1)$ to mean that a scheme requires $(s+1)f$ evaluations to form y_{n+1}, $\{u_i\}_{i=1}^m$, and $\{u_i'\}_{i=1}^r$ and sample the defect at a single point; the "+1" appears in brackets because, after a successful step, one of the f values, $f(x_{n+1}, y_{n+1})$, can be reused at the start of the next step.

The simplest example is the cubic Hermite interpolant to y_n, $f(x_n, y_n)$, y_{n+1}, and $f(x_n + h, y_{n+1})$, corresponding to $m = r = 2$ in (2.1). A fourth-order, four-stage Runge–Kutta formula could be used to generate a y_{n+1} of local order five. This leads to an overall cost of $5(+1)$ f evaluations. The polynomial $dr(\tau)/d\tau$ in (2.5) becomes

$$\frac{dr(\tau)}{d\tau} = 2\tau(\tau - 1)(2\tau - 1), \tag{2.6}$$

as plotted in Fig. 1. There are two local extrema of equal magnitude at $\tau = \frac{1}{2} \pm \sqrt{3}/6$.

Next we consider the case $m = 3$, $r = 2$. Using a result of Horn [8] we could employ the higher-order formula of the well-known Fehlberg pair to form y_{n+1} and then generate a data point u_2 of the correct local order at any point $\xi_2 = x_n + \sigma_2 h$ for a total of $9(+1)$ evaluations. In this case

$$\frac{dr(\tau)}{d\tau} = \tau(\tau - 1)(5\tau^2 - [3 + 4\sigma_2]\tau + 2\sigma_2). \tag{2.7}$$

From (2.5) we see that the most efficient scheme, asymptotically, is found by choosing σ_2 in $(0, 1)$ to minimise $\max_{\tau \in [0,1]} |dr(\tau)/d\tau|$. A computer search revealed that this is achieved at $\sigma_2 = \frac{1}{2}$. The graph resulting from (2.7) is plotted in Fig. 2 and has a pleasing

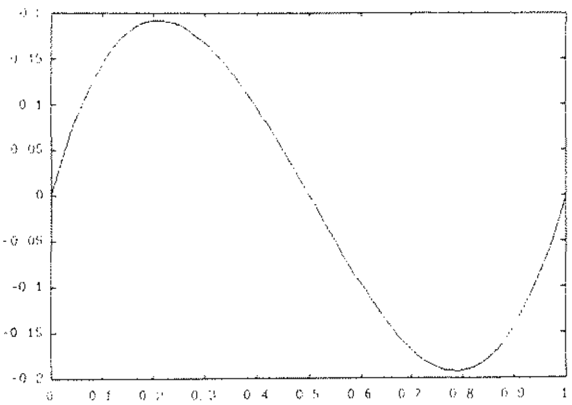

FIG. 1

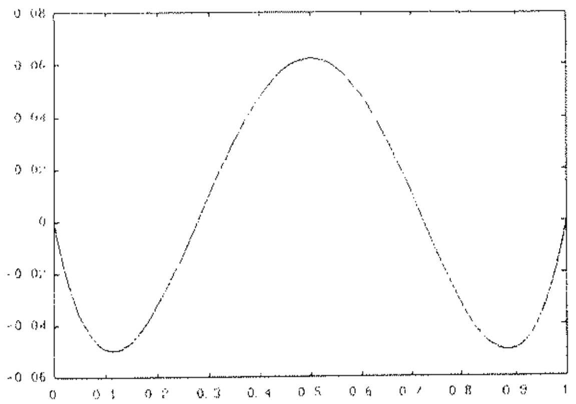

FIG. 2

shape; the peak at $\tau=\frac{1}{2}$ is 1.25 times as big as the other local extrema at $\frac{1}{2}\pm\sqrt{15}/10$. Also, for the choice $\sigma_2=\frac{1}{2}$ a similar scheme requiring one fewer function evaluation is available using the Dormand-Prince-Shampine (DPS) triple [10].

For larger values of $m+r$ the problem of finding enough data of the correct local accuracy, using a reasonable number of function evaluations, becomes more challenging [9, p. 1020]. Enright et al. [4] give an alternative to Shampine's method for constructing interpolants. Their method is perfectly general: given any Runge-Kutta formula an interpolant can be produced that has the same local accuracy. It would therefore be possible to choose a high-order Runge-Kutta formula, construct a high-order interpolant using the technique of [4] and then use this interpolant to provide the necessary data for an interpolant of the form considered here. Due to the high cost (in terms of f evaluations per step) we do not pursue such an approach in this paper.

2.2. Case II. We now examine the case where the data error dominates in (2.2). This situation has been analysed by Gladwell et al. [6] with a view to relating $u^{(k)}(x)-p^{(k)}(x)$ to the local error at x_n+h. We shall use their results to reveal the asymptotic behavior of the defect.

It has been shown [6, p. 325] that for $m+r>q+1$, (2.2) takes the form

$$p^{(k)}(x)-u^{(k)}(x)=\sum_{i=2}^{m} A_i^{(k)}(x)[u_i-u(\xi_i)]+O(h^{q+2-k})$$

where $A_i(x)$ is a fundamental interpolating polynomial that depends only on the abscissae $\{\xi_i\}_{i=1}^{m}$. From (1.3) and (1.4) we then have

$$\delta(x)=\sum_{i=2}^{m} A_i'(x)[u_i-u(\xi_i)]+O(h^{q+1}). \tag{2.8}$$

To recover a result of the form (1.6) we must reduce the summation in (2.8) to a single term. For example, the standard cubic Hermite interpolant ($m=r=2$) could be used with a second-order, two-stage Runge-Kutta formula ($q+1=3$) to give

$$\delta(x)=A_2'(x)[y_{n+1}-u(x_n+h)]+O(h^3).$$

This may be written

$$\delta(x_n+\tau h)=6\tau(1-\tau)\frac{[y_{n+1}-u(x_n+h)]}{h}+O(h^3),$$

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which is essentially the same form as (1.6). Figure 3 presents a plot of $6\tau(1-\tau)$; the single extremum in $[0, 1]$ occurs at $\tau=\frac{1}{2}$. The cost of this scheme is (3+1) evaluations per step.

For higher-order schemes we look at $m=r=3$. Interpolants of the desired form can be obtained by applying a single formula of order less than or equal to 4 over steps of length h and $h/2$ or over two steps of length $h/2$ [6, p. 326], but the resulting defect control schemes are more expensive than those of § 2.1. An alternative approach suggested in [6] that turns out to be useful in our context, is to use a fifth-order Runge–Kutta formula to generate y_{n+1}, making $u_3-u(\xi_3)=y_{n+1}-u(x_n+h)=O(h^6)$, and then to form an approximation at ξ_2 that is locally $O(h^5)$. In this way the $i=2$ term dominates the right-hand side of (2.8) to give

$$\delta(x)=A_2'(x)[u_2-u(\xi_2)]+O(h^5),$$

which may be written

$$\delta(x_n+\tau h)=\frac{2\tau(\tau-1)(\tau^2[5-10\sigma_2]+\tau[10\sigma_2^2-3]-5\sigma_2^2+3\sigma_2)}{\sigma_2^3(\sigma_2-1)^3}\,\frac{[u_2-u(\xi_2)]}{h}+O(h^5)$$

$$\equiv g_{\sigma_2}(\tau)\,\frac{[u_2-u(\xi_2)]}{h}+O(h^5)$$

where we recall that $\xi_2=x_n+\sigma_2 h$. With the fifth-order formula of the DPS triple it has been shown [1] that a suitable approximation u_2 can be found for any σ_2 using no extra function evaluations. The overall cost of the defect control scheme is then 8(+1) evaluations. One reasonable way of choosing $\sigma_2\in(0,1)$ is to minimise $\max_{\tau\in[0,1]}|g_{\sigma_2}(\tau)|$. The minimum was found by a computer search to occur at $\sigma_2=\frac{1}{2}$. The corresponding polynomial, $g_{1/2}(\tau)$, is an exact multiple of the right-hand side of (2.6). Similar schemes can be constructed using Horn's results for the Fehlberg fifth-order formula. With $\sigma_2=3/5$ a scheme costing 8(+1) evaluations is available while for any other σ_2 the cost increases by 1.

The idea of making one of the $[u_i-u(\xi_i)]$ terms in (2.8) dominate can be used to construct higher-order schemes but, as in Case I, this may not be practical.

3. Discussion. Apart from the low-order version in § 2.2, the schemes presented here are more expensive than their competitors. The first example in § 2.1 gives an $O(h^3)$ defect for 5(+1) evaluations per step, while the same order of accuracy could

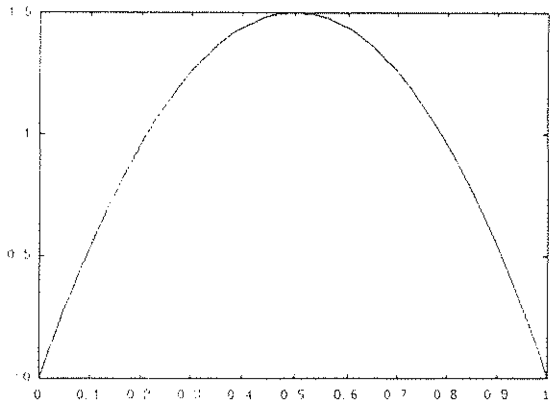

FIG. 3

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be achieved with 4(+1) evaluations by a third-order, three-stage Runge-Kutta formula and a cubic Hermite interpolant. Similarly, the 8(+1) evaluations required by the DPS based schemes of §§ 2.1 and 2.2 to obtain an $O(h^4)$ defect can be compared with the 6(+1) evaluations used by the most efficient of those in [3]. However, the extra cost is countered by the asymptotic validity of the new schemes.

It is shown in [3] that standard nonextrapolated error-per-unit-step control can also be regarded as asymptotically valid defect control. The schemes proposed in this paper, which require fewer function evaluations per step, are closely related—they are asymptotically equivalent to controlling the local error-per-unit-step in the interpolant at some method dependent point, $x_n + \hat{\tau} h$.

4. Numerical results. We have implemented the following schemes:

3/8: Case I, $m = r = 2$, with the "3/8-Rule" [7, p. 137] as the fourth-order Runge–Kutta formula.

DPS#1: Case I, $m = 3$, $r = 2$, with the fifth-order formula of RK5(4)7FM and the $O(h^6)$ midpoint approximation from [10],

DPS#2: Case II, $m = r = 3$, with the fifth-order formula of RK5(4)7FM and the $O(h^5)$ midpoint approximation from [10] (also derived in [1]).

The defect was controlled by sampling at a single point: $\tau^* = \frac{1}{2} + \sqrt{3}/6$ for the 3/8 and DPS#2 schemes, and $\tau^* = \frac{1}{2}$ for the DPS#1 scheme. After each step, whether successful or not, the new stepsize was chosen according to

$$\frac{h_{\text{new}}}{h_{\text{old}}} = .9\left(\frac{\text{TOL}}{\|\delta(x_n + \tau^* h)\|_\infty}\right)^{1/p}$$

for a defect of $O(h^p)$. As a safety precaution we imposed the restriction

$$\frac{1}{10} \leqq \frac{h_{\text{new}}}{h_{\text{old}}} \leqq 5,$$

discussed in [11]. Following [2] the quantities

$$\text{R1} = \frac{\max_{j=1,\cdots,100} \|\delta(x_n + .01jh)\|_\infty}{\|\delta(x_n + \tau^* h)\|_\infty},$$

$$\text{R2} = \frac{\max_{j=1,\cdots,100} \|\delta(x_n + .01jh)\|_\infty}{\text{TOL}}$$

were computed on each step; R1MAX and R2MAX denote their respective maximum values over the range of integration. Note that R1MAX measures the quality of the sample point and R2MAX indicates how successful the code was in keeping $\|\delta(x)\|_\infty <$ TOL. Ideally we would like R1MAX $= 1$ and R2MAX $\approx< 1$.

The methods were tested on the orbit equations [5, Class D]:

$$\begin{aligned}
y_1' &= y_3, & y_1(0) &= 1 - \varepsilon, \\
y_2' &= y_4, & y_2(0) &= 0, \\
y_3' &= \frac{-y_1}{(y_1^2 + y_2^2)^{3/2}}, & y_3(0) &= 0, \\
y_4' &= \frac{-y_2}{(y_1^2 + y_2^2)^{3/2}}, & y_4(0) &= \left(\frac{1+\varepsilon}{1-\varepsilon}\right)^{1/2},
\end{aligned}$$

$$0 \leqq x \leqq 20$$

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TABLE 1
R1MAX, R2MAX *pairs for 3/8 scheme.*

TOL	10^{-2}	10^{-4}	10^{-6}	10^{-8}
$\varepsilon = .1$	3.3, 2.7	2.1, 1.6	1.4, 1.1	1.1, 0.8
$\varepsilon = .5$	1.9, 1.7	1.3, 1.1	1.1, 0.8	1.0, 0.8
$\varepsilon = .9$	1.5, 1.1	1.1, 1.0	1.0, 0.9	1.0*, 0.8*

* The integration was halted prematurely after 5,000 steps.

TABLE 2
R1MAX, R2MAX *pairs for* DPS#1 *scheme.*

TOL	10^{-2}	10^{-4}	10^{-6}	10^{-8}
$\varepsilon = .1$	3.2, 1.5	3.4, 2.2	1.3, 1.1	1.0, 0.8
$\varepsilon = .5$	4.9, 0.9	2.0, 1.0	1.0, 1.0	1.0, 0.8
$\varepsilon = .9$	1.2, 0.8	1.0, 1.0	1.0, 1.0	1.0, 0.8

TABLE 3
R1MAX, R2MAX *pairs for* DPS#2 *shceme.*

TOL	10^{-2}	10^{-4}	10^{-6}	10^{-8}
$\varepsilon = .1$	2.3, 0.9	5.1, 2.0	1.2, 0.8	1.0, 0.7
$\varepsilon = .5$	3.0, 0.9	2.2, 1.3	1.2, 1.0	1.1, 0.8
$\varepsilon = .9$	4.2, 1.0	2.1, 1.0	1.1, 1.0	1.0, 0.9

where values of .1, .5, and .9 were chosen for the eccentricity parameter ε. Tables 1–3 record the R1MAX and R2MAX values. As the analysis of § 2 predicts, we see that the performance becomes extremely good as TOL decreases. The results can be compared with those of the original defect control schemes in [2] for the orbit problems; while both sets of results are satisfactory, the new schemes are clearly more reliable at stringent tolerances. We emphasise that the price to be paid for this improvement is a higher cost per step.

To conclude, we outline some possible extensions to this work. The schemes described in § 2 allow some freedom in the choice of Runge–Kutta formula and interpolation points. By examining higher-order terms in the expansion (1.5), it may be possible to use this freedom to produce schemes for which the leading term is more likely to dominate. Finally, in some cases it may be preferable to estimate and control a measure of the defect other than $\max_{\tau\in[0,1]} \|\delta(x_n+\tau h)\|_\infty$ (see [2]). Whatever measure is used, the interpolants presented here should prove extremely useful, since an asymptotically correct approximation to the defect over the entire step can be constructed from a single sample value.

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