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GLOBAL ERROR ESTIMATION WITH RUNGE–KUTTA TRIPLES

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Abstract—The applications of Runge–Kutta (RK) interpolation to global error estimation using the Zadunaisky and related techniques are considered. It is shown that the pseudo-problem can be based on dense output values within any one step and reliable global error estimates can be obtained at the integration mesh-points by using special RK formulae. Some special formulae of orders 2–6 are presented together with numerical results

1. INTRODUCTION

In earlier papers [1, 2] the application of the Zadunaisky technique [3, 4] of global error estimation with explicit Runge–Kutta (RK) formulae was considered. Recently several authors [5–10] have investigated the development of RK interpolation. This paper considers the application of RK interpolation to global error estimation.

Without loss of generality [11] the first order system of autonomous ordinary differential equations

$$\mathbf{y}'(x) = \mathbf{f}[\mathbf{y}(x)], \quad \text{with } \mathbf{y}(x_0) \text{ known}, \tag{1}$$

can be considered. This system can be solved using an embedded RK $q(p)$ process with formulae of order q and p ($q > p$) of the form:

$$\begin{aligned} \hat{\mathbf{y}}_{n+1} &= \hat{\mathbf{y}}_n + h_n \hat{\boldsymbol{\Phi}}(\hat{\mathbf{y}}_n, h_n) = \hat{\mathbf{y}}_n + h_n \sum_{i=1}^{s} \hat{b}_i \mathbf{g}_i, \\ \mathbf{y}_{n+1} &= \hat{\mathbf{y}}_n + h_n \boldsymbol{\Phi}(\hat{\mathbf{y}}_n, h_n) = \hat{\mathbf{y}}_n + h_n \sum_{i=1}^{s} b_i \mathbf{g}_i, \end{aligned} \tag{2}$$

where

$$\mathbf{g}_i = \mathbf{f}\left(\hat{\mathbf{y}}_n + h_n \sum_{j=1}^{i-1} a_{ij} \mathbf{g}_j\right), \quad i = 1, 2, \ldots, s,$$

$x_{n+1} = x_n + h_n$, $h_n = \theta(x_n)h$, $0 < \theta(x) \leqslant 1$ and usually $\hat{\mathbf{y}}_0 = \mathbf{y}(x_0)$.

The embedded process is applied in local extrapolation or higher order mode [12] and yields numerical approximations $\hat{\mathbf{y}}_n$ to $\mathbf{y}(x_n)$ at the mesh points x_n, $n = 0, 1, \ldots, N$. Without loss of generality the FSAL idea [9] is assumed in which the last function evaluation at any step is the same as the first at the next step. Assuming appropriate smoothness of $\mathbf{f}$ the local truncation error, $\hat{\mathbf{t}}_{n+1}$, at x_{n+1}, of the RKq process may be written [1]:

$$\begin{aligned} \hat{\mathbf{t}}_{n+1} &= \mathbf{y}(x_n) + h_n \hat{\boldsymbol{\Phi}}[\mathbf{y}(x_n), h_n] - \mathbf{y}(x_{n+1}) \\ &= \sum_{i=q}^{q+w} h_n^{i+1} \sum_{j=1}^{n_{i+1}} \hat{\tau}_j^{(i+1)} \mathbf{F}_j^{(i+1)}[\mathbf{y}(x_n)] + O(h_n^{q+w+2}), \end{aligned}$$

where the $\mathbf{F}_j^{(i+1)}$ and the $\hat{\tau}_j^{(i+1)}, j = 1, 2, \ldots, i+1$, are the elementary differentials of order $i+1$ of $\mathbf{f}$ [11] and the RK truncation error coefficients [1] respectively.

The global error, ϵ_n at x_n, of process (2) is defined by

$$\epsilon_n = \hat{\mathbf{y}}_n - \mathbf{y}(x_n), \quad n = 0, 1, \ldots, N.$$

The Zadunaisky technique for estimation of ϵ_n is based on the construction of a neighbouring problem (NP), with known true solution $\mathbf{y}_h(x)$, which is "close" to the main problem (MP) (1). The basic idea is to integrate the NP with the same RKq formula and same step sequence as for the MP to produce a numerical solution $\mathbf{y}_{hn}$. The known error $\epsilon_{hn} = \mathbf{y}_{hn} - \mathbf{y}_h(x_n)$ is then used as an estimate of ϵ_n. There are a number of ways to construct the NP. One form discussed in Ref. [2] is

$$\mathbf{y}_h'(x) = \mathbf{f}_h[\mathbf{y}_h(x)] = \mathbf{f}[\mathbf{y}_h(x)] + \mathbf{d}_h(x),$$

$$\mathbf{y}_h(x_0) = \mathbf{y}(x_0) = \mathbf{P}(x_0) \tag{3}$$

and

$$\mathbf{d}_h(x) = \mathbf{P}'(x) - \mathbf{f}[\mathbf{P}(x)],$$

whose solution is $\mathbf{y}_h(x) = \mathbf{P}(x)$. In Ref. [2] $\mathbf{P}(x)$ was chosen as a piecewise polynomial function which interpolated the numerical solution of equation (1) in subintervals of $[x_0, x_N]$. Each subinterval or block was of size m, i.e. consisted of $m + 1$ points, and three cases were discussed:

(i) interpolation of $\mathbf{y}_i$ values;
(ii) interpolation of $\mathbf{f}(\mathbf{y}_i)$ values

and

(iii) Hermite interpolation using both the $\mathbf{y}_i$ and $\mathbf{f}(\mathbf{y}_i)$ values.

Frank [13] analysed the estimation process for case (i) with constant steps and further considerations can be found in Prince [14] and in Dormand and Prince [1, 2]. Valid asymptotic estimates of ϵ_n are obtained if $\mathbf{E}_n = \epsilon_{hn} - \epsilon_n$ is $O(h^r)$, where $r > q$. In Ref. [2] it was shown that in cases (i) and (ii) valid estimation is possible if $m > q$ and $m > q - 1$, respectively, but that in case (iii) $\mathbf{E}_n$ is $O(h^q)$ irrespective of m. In each of the three cases an order bound for $\| \mathbf{E}_n \|$ was obtained in Ref. [2] which is dependent on an order bound for $\| \mathbf{d}_h^{(j)}(x) \|$. Because the defect bound depends on the truncation error coefficients, $\hat{\tau}_j^{(i)}$, it was found to be possible to construct special RKq processes in which certain of the $\hat{\tau}_j^{(i)}$ are zero with the consequence that for certain values of m an asymptotically valid estimate is obtained in case (iii). The same attack leads to better estimation in cases (i) or (ii). Despite these encouraging theoretical results, high order processes have been found to provide useful estimates only at very stringent local error tolerances. This is because high order RK formulae require large blocks, particularly in cases (i) and (ii), resulting in high degree polynomial interpolation. As might be expected, this causes problems, particularly when unequal step sizes are used.

The basic idea of this paper is to form $\mathbf{P}(x)$ using RK interpolation. The main advantage is that the estimation process can be applied at each integration step and not after a block of m steps. Following Dormand and Prince [9] a third RK formula (called a *dense* formula) will be used to approximate the solution of equation (1) between x_n and x_{n+1}. This is accomplished by taking a step of size σh_n $(0 < \sigma < 1)$ from x_n. The dense formula, of order p^* and employing s^* stages, may be written

$$\mathbf{y}^*_{n+\sigma} = \hat{\mathbf{y}}_n + \sigma h_n \sum_{i=1}^{s^*} b_i^* \mathbf{g}_i, \tag{4}$$

and produces estimates $\mathbf{y}^*_{n+\sigma}$ of $\mathbf{y}(x_n + \sigma h_n)$, $n = 0, 1, \ldots, N - 1$. It should be noted that common function evaluations with the embedded pair have been assumed [5, 6, 9] and that if $s_m = \max(s, s^*) > s$ then $\hat{b}_i = b_i = 0$, $i = s + 1, s + 2, \ldots, s_m$. The embedded pair together with the dense formula constitute an RK triple using s_m stages. Dormand and Prince [9] discuss the RKp^* equations of condition and also point out that for $\epsilon^*_{n+\sigma} = \mathbf{y}^*_{n+\sigma} - \mathbf{y}(x_n + \sigma h_n)$ to be $O(h^q)$ then

$p^* \geqslant q-1$. As pointed out by several authors [6, 9, 15] continuity of $\mathbf{y}^*_{n+\sigma}$ as a function of σ is desirable. The function $\mathbf{y}^*_{n+\sigma}$ is C^1 continuous if

$$b_i^*(\sigma=1)=\hat{b}_i,$$

$$b_i^*(\sigma=0)=\delta_{i1} \tag{5}$$

and

$$\hat{b}_i+\frac{\mathrm{d}b_i^*}{\mathrm{d}\sigma}(\sigma=1)=\delta_{is},$$

where

$$\delta_{ij}=\begin{cases}0, & i\neq j,\\ 1, & i=j,\end{cases}\quad i,j=1,2,\ldots,s_m.$$

Various possibilities exist for the determination of $\mathbf{P}(x)$ within each step, $[x_n, x_{n+1}]$:

(A) interpolation using only $\hat{\mathbf{y}}_n$, $\hat{\mathbf{y}}_{n+1}$ and $\mathbf{y}^*_{n+\sigma}$ values;
(B) interpolation using $\mathbf{f}(\hat{\mathbf{y}}_n)=\mathbf{g}_1$, $\mathbf{f}(\hat{\mathbf{y}}_{n+1})=\mathbf{g}_s$ and $\mathbf{f}(\mathbf{y}^*_{n+\sigma})$ values

and

(C) interpolation using both $\mathbf{y}$ and $\mathbf{f}$ values.

Possibility (B) is less attractive in practice since extra function evaluations, $\mathbf{f}(\mathbf{y}^*_{n+\sigma})$, are necessary. The modified Hermite form of (C) using $\mathbf{y}$ values and just the two known end values of $\mathbf{f}$ would seem to be the most attractive since no extra function evaluations are required. Peterson [16] considered the Zadunaisky technique as discussed in Refs [1, 2] and concluded that modified Hermite or Hermite–Birkhoff interpolation was preferable, these tending to require a smaller block size. A dense formula is a valuable addition to any RK code. Here we exploit it to reduce the block size to one.

In Section 2 we will obtain bounds for $\|\mathbf{E}_n\|$ in the more practical cases (A) and (C) and indicate that as in Ref. [2] special RK processes can be developed giving valid asymptotic global error estimation. Section 3 is concerned with the more efficient process of directly solving for the error estimate. Some new estimation formulae are derived in Section 4 and numerical tests are presented in Section 5.

2. ERROR BOUNDS

Consider the step interval $I_n=[x_n, x_{n+1}]$ and let $\mathbf{P}_n(x)$, $x\in I_n$, be the polynomial of degree $m\leqslant R$ which interpolates at the $R+1$ points $(x_{n+\sigma_k}, \mathbf{y}^*_{n+\sigma_k})$, $k=1,2,\ldots,r_1$, $(x_{n+\sigma_k}, \mathbf{f}[\mathbf{y}^*_{n+\sigma_k}])$, $k=1,2,\ldots,r_2$, where $R=r_1+r_2-1$, $\sigma_k\in[0,1]$, $\sigma_1=0$, $\sigma_2=1$, $\mathbf{y}^*_{n+\sigma_1}=\hat{\mathbf{y}}_n$ and $\mathbf{y}^*_{n+\sigma_2}=\hat{\mathbf{y}}_{n+1}$ [see equations (2), (4) and (5)]. Thus the cases discussed in Section 1 are now: (A) in which $r_2=0$, (B) in which $r_1=0$ and (C) in which $r_1>0$ and preferably $r_2=2$. If the dense output formula is such that all the a_{ij} are independent of σ then the b_i^* and hence $\mathbf{y}^*_{n+\sigma}$ are polynomials in σ. In this case, assuming $\mathbf{y}^*_{n+\sigma}$ is of degree d in σ, the continuity conditions (5) are satisfied, $R+1\geqslant d$ and $r_2\leqslant 2$, we have $\mathbf{P}(x)\equiv\mathbf{y}^*_{n+\sigma}$ and $m=d$. Let $\mathbf{V}_n(x)$ be the polynomial of degree m which interpolates the true solution and derivative at the same points. Then

$$\mathbf{P}_n(x)=\sum_{k=1}^{r_1}L_k(x)\mathbf{y}^*_{n+\sigma_k}+\sum_{k=1}^{r_2}M_k(x)\mathbf{f}(\mathbf{y}^*_{n+\sigma_k}), \tag{6}$$

$$\begin{aligned}\mathbf{V}_n(x)&=\sum_{k=1}^{r_1}L_k(x)\mathbf{y}(x_{n+\sigma_k})+\sum_{k=1}^{r_2}M_k(x)\mathbf{y}'(x_{n+\sigma_k})\\ &=\sum_{k=1}^{r_1}L_k\sum_{i=0}^{q+w}(\sigma_k h_n)^i\mathbf{y}^{(i)}(x_n)/i!+\sum_{k=1}^{r_2}M_k\sum_{i=0}^{q+w}(\sigma_k h_n)^i\mathbf{y}^{(i+1)}(x_n)/i!+O(h^{q+w+1})\end{aligned} \tag{7}$$

assuming suitable smoothness. Now $\mathbf{V}_n(x)$ is exact for all polynomials of degree less than $m+1$ and so with $x = x_n + \sigma h_n$

$$\sum_{k=1}^{r_1} L_k \sigma_k^t + \sum_{k=1}^{r_2} M_k t \sigma_k^{t-1}/h_n = \sigma^t, \quad t = 0, 1, \ldots, m. \tag{8}$$

Using this together with the Taylor expansion of $\mathbf{y}(x_n + \sigma h_n)$ then equation (7) gives

$$\mathbf{V}_n(x) - \mathbf{y}(x) = \sum_{i=m+1}^{q+w} h_n^i \mathbf{y}^{(i)}(x_n)\left[\sum_{k=1}^{r_1} L_k \sigma_k^i + \sum_{k=1}^{r_2} M_k i \sigma_k^{i-1}/h_n - \sigma^i\right]\Big/ i! + O(h^{q+w+1}),$$

and since $L_k^{(j)}$ and $M_k^{(j)}$ are $O(h-j)$ and $O(h^{1-j})$ respectively for $j \leqslant m$ [6, 14], and both are zero for $j > m$, it follows that

$$\| \mathbf{V}_n^{(j)}(x) - \mathbf{y}^{(j)}(x) \|_{x\in I_n} \begin{cases} \leqslant K_1^{(j)} h^{m+1-j}, & j = 0, 1, \ldots, m, \\ \leqslant K_{1n}^{(j)}, & j > m. \end{cases} \tag{9}$$

Following Butcher [11] and the analysis in Ref. [1]

$$\mathbf{y}^*_{n+\sigma_k} = \hat{\mathbf{y}}_n + \sigma_k \sum_{i=1}^{q+w} (\sigma_k h_n)^i/(i-1)! \sum_{j=1}^{n_i} \beta_j^{(i)} \psi_j^{(i)*}(\sigma_k) \mathbf{F}_j^{(i)}(\hat{\mathbf{y}}_n) + O(h^{q+w+1})$$

and

$$\mathbf{y}(x_{n+\sigma_k}) = \mathbf{y}(x_n) + \sigma_k \sum_{i=1}^{q+w} (\sigma_k h_n)^i/i! \sum_{j=1}^{n_i} \alpha_j^{(i)} \mathbf{F}_j^{(i)}[\mathbf{y}(x_n)] + O(h^{q+w+1})$$

and so

$$\begin{aligned} \epsilon^*_{n+\sigma_k} &= \mathbf{y}^*_{n+\sigma_k} - \mathbf{y}(x_{n+\sigma_k}) \\ &= \epsilon_n + \sum_{i=1}^{q} (\sigma_k h_n)^i \sum_{j=1}^{n_i} \tau_j^{(i)*}(\sigma_k) \mathbf{F}_j^{(i)}[\mathbf{y}(x_n)] + O(h^{q+1}). \end{aligned}$$

Now the dense formula is of order p^* and so

$$\tau_j^{(i)*}(\sigma_k) = 0, \quad i = 1, 2, \ldots, p^*, \quad j = 1, 2, \ldots, n_i,$$

and when $k = 2$

$$\tau_j^{(i)*} = \hat{\tau}_j^{(i)} = 0, \quad i = 1, 2, \ldots, q, \quad j = 1, 2, \ldots, n_i.$$

Thus

$$\epsilon^*_{n+\sigma_k} = \epsilon_n + O(h^{\min[p^*, q]+1}),$$

and so, differentiating equation (8) when $t = 0$, equations (6) and (7) yield

$$\| \mathbf{P}_n^{(j)}(x) - \mathbf{V}_n^{(j)}(x) \|_{x\in I_n} \begin{cases} \leqslant K_{2n}^{(0)} h^{\min[q, p^*+1]}, & j = 0, \\ \leqslant K_{2n}^{(j)} h^{\min[q, p^*]+1-j}, & 1 \leqslant j \leqslant m, \\ = 0, & j > m. \end{cases}$$

Use of this with equation (9) now gives

$$\| \mathbf{P}_n^{(j)}(x) - \mathbf{y}^{(j)}(x) \|_{x\in I_n} \begin{cases} \leqslant K_{3n}^{(0)} h^{\min[q, p^*+1, m+1]}, & j = 0, \\ \leqslant K_{3n}^{(j)} h^{\min[q, p^*, m]+1-j}, & 1 \leqslant j \leqslant m, \\ \leqslant K_{3n}^{(j)}, & j > m. \end{cases}$$

Similar to the analysis in Ref. [2] the following bounds are now obtained on $\| \mathbf{d}_n^{(j)}(x) \|$ and $\| \mathbf{E}_n(x) \|$.

$$\| \mathbf{d}_n^{(j)}(x) \|_{x\in[x_0, x_N]} \begin{cases} \leqslant N_j h^{\min[q, p^*, m]-j}, & 0 \leqslant j \leqslant m-1, \\ \leqslant N_j h^{\min[0, q-m+1, p^*-m+1]}, & j \geqslant m, \end{cases}$$

and

$$\max_{0\leqslant n\leqslant N} \| \mathbf{E}_n \| \begin{cases} \leqslant A h^q, & q \geqslant m, \\ \leqslant A h^{\min[q, p^*]}, & q < m, \end{cases} \tag{10}$$

where it has been assumed that $p^* \geqslant q - 1$. Thus in either case (A) or (C) it would seem that asymptotically viable global error estimation is not possible. Note that in Ref. [2] estimation was possible, for certain values of m, using interpolation on the $\mathbf{y}_i$ values. Numerical tests have confirmed result (10).

We do not present the analysis for approach (B) here, but it can be found in Ref. [17] where the following bound on $\| \mathbf{E}_n \|$ was obtained:

$$\max_{0 \leqslant n \leqslant N} \| \mathbf{E}_n \| \begin{cases} \leqslant Ah^q, & q \geqslant m, \\ \leqslant Ah^{(\min[q+1, p^*+1]}, & q < m. \end{cases} \tag{11}$$

A consideration of condition (11) reveals that in case (B) valid asymptotic estimation is possible if $q < m$ *and* $p^* \geqslant q$. Computational results have confirmed the validity of condition (11). Although it would seem that valid estimation using dense output is only possible in this latter case, it was shown in Ref. [1] that the order of $\mathbf{E}_n$ for $q > 1$ was governed by the expression

$$\sum_{i=q+1}^{2q} h^{i-1} \sum_{j=1}^{n_i} \hat{\tau}_j^{(i)} \{ \mathbf{F}_{hj}^{(i)}[\mathbf{y}(x_n)] - \mathbf{F}_j^{(i)}[\mathbf{y}(x_n)] \} + O(h^{2q}), \tag{12}$$

where the term in brackets is a function of $\mathbf{f}$, $\mathbf{d}_h$ and their derivatives. Similar to the analysis in Ref. [2], it is found that, depending on q, m, p^* and the resulting order of $\mathbf{d}_h^{(j)}(x)$, only certain of the $\hat{\tau}_j^{(i)}$ will appear in the leading terms in expression (12). By choosing an RK process with appropriate $\hat{\tau}_j^{(i)}$ made zero, the order of $\mathbf{E}_n$ can be improved over that predicted by conditions (10) or (11). To facilitate this, the $\hat{\tau}_j^{(i)}$ occurring in the h^q and h^{q+1} terms of expression (12) are given in Table 1 for $q = 2, \ldots, 6$ and various m for those cases when $\| \mathbf{E}_n \|$ is $O(h^q)$ in condition (10) and $p^* = q - 1$ or $p^* = q$. A table of corresponding $\hat{\tau}_j^{(i)}$ is not presented for the less practical case (B).

3. SOLVING FOR THE ERROR ESTIMATE

Peterson [16] compared the Zadunaisky block technique with other correction type methods and in particular with the idea of "solving for the correction" discussed by Skeel in Ref. [18]. This approach is concerned with the differential system

$$\epsilon_h'(x) = \bar{\mathbf{f}}[\epsilon_h(x)] = \mathbf{P}'(x) - \mathbf{f}[\mathbf{P}(x) - \epsilon_h(x)],$$

$$\epsilon_h(x_0) = \epsilon_{h0} = \mathbf{P}(x_0) - \mathbf{y}(x_0), \tag{13}$$

Table 1. RK truncation coefficients for cases (A) or (C)

p^*	q	m	h^q	h^{q+1}
1	2	2	$\hat{\tau}_i^{(3)}$, $i = 1, 2$	$\hat{\tau}_i^{(3)}$, $i = 1, 2$; $\hat{\tau}_i^{(4)}$, $i = 1, 2, 3, 4$
2	3	2, 3	$\hat{\tau}_i^{(4)}$, $i = 1, 3$	$\hat{\tau}_i^{(4)}$, $i = 1, 2, 3, 4$; $\hat{\tau}_i^{(5)}$, $i = 1, 4, 5, 8$
3	4	2	$\hat{\tau}_i^{(5)}$, $i = 1, 4, 5, 8$	
		3, 4	$\hat{\tau}_i^{(5)}$, $i = 1, 5$	$\hat{\tau}_i^{(5)}$, $i = 1, 4, 5, 8$; $\hat{\tau}_i^{(6)}$, $i = 1, 6, 7, 15$
		2		
4	5	3	$\hat{\tau}_i^{(6)}$, $i = 1, 6, 7, 15$	
		4, 5	$\hat{\tau}_i^{(6)}$, $i = 1, 7$	$\hat{\tau}_i^{(6)}$, $i = 1, 6, 7, 15$; $\hat{\tau}_i^{(7)}$, $i = 1, 10, 11, 29$
		2, 3		
5	6	4	$\hat{\tau}_i^{(7)}$, $i = 1, 10, 11, 29$	
		5, 6	$\hat{\tau}_i^{(7)}$, $i = 1, 11$	$\hat{\tau}_i^{(7)}$, $i = 1, 10, 11, 29$; $\hat{\tau}_i^{(8)}$, $i = 1, 14, 15, 53$
2	2	2, 3	$\hat{\tau}_1^{(3)}$	$\hat{\tau}_i^{(3)}$, $i = 1, 2$; $\hat{\tau}_i^{(4)}$, $i = 1, 3$
		2	$\hat{\tau}_i^{(4)}$, $i = 1, 3$	$\hat{\tau}_i^{(4)}$, $i = 1, 2, 3, 4$; $\hat{\tau}_i^{(5)}$, $i = 1, 4, 5, 8$
3	3	3, 4	$\hat{\tau}_1^{(4)}$;	$\hat{\tau}_i^{(4)}$, $i = 1, 3$; $\hat{\tau}_i^{(5)}$, $i = 1, 5$
		5	$\hat{\tau}_1^{(4)}, \hat{\tau}_1^{(5)}$;	$\hat{\tau}_i^{(4)}$, $i = 1, 3$; $\hat{\tau}_i^{(5)}$, $i = 1, 5$; $\hat{\tau}_i^{(6)}$, $i = 1, 7$
		2	$\hat{\tau}_i^{(5)}$, $i = 1, 4, 5, 8$	
4	4	3	$\hat{\tau}_i^{(5)}$, $i = 1, 5$	$\hat{\tau}_i^{(5)}$, $i = 1, 4, 5, 8$; $\hat{\tau}_i^{(6)}$, $i = 1, 6, 7, 15$
		4, 5	$\hat{\tau}_1^{(5)}$;	$\hat{\tau}_i^{(5)}$, $i = 1, 5$; $\hat{\tau}_i^{(6)}$, $i = 1, 7$
		2		
		3	$\hat{\tau}_i^{(6)}$, $i = 1, 6, 7, 15$	
5	5	4	$\hat{\tau}_i^{(6)}$, $i = 1, 7$	$\hat{\tau}_i^{(6)}$, $i = 1, 6, 7, 15$; $\hat{\tau}_i^{(7)}$, $i = 1, 10, 11, 29$
		5, 6	$\hat{\tau}_1^{(6)}$	$\hat{\tau}_i^{(6)}$, $i = 1, 7$; $\hat{\tau}_i^{(7)}$, $i = 1, 11$
		2, 3		
		4	$\hat{\tau}_i^{(7)}$, $i = 1, 10, 11, 29$	
6	6	5	$\hat{\tau}_i^{(7)}$, $i = 1, 11$	$\hat{\tau}_i^{(7)}$, $i = 1, 10,11, 29$; $\hat{\tau}_i^{(8)}$, $i = 1, 14, 15, 53$
		6, 7	$\hat{\tau}_1^{(7)}$	$\hat{\tau}_i^{(7)}$, $i = 1, 11$; $\hat{\tau}_i^{(8)}$, $i = 1, 15$

whose solution is $\epsilon_h(x) = \mathbf{P}(x) - \mathbf{y}(x)$. This system is solved using a RK method of order $\bar{q}$ employing $\bar{s}$ stages for the numerical solution ϵ_{hn} which is then used as an estimate of ϵ_n. Usually $\bar{q} = q$ but this formula need not be the same as the main RK integration formula. Similar to the analysis carried out in Ref. [1] we have

$$\epsilon_{hn+1} - \epsilon_h(x_{n+1}) = \epsilon_{hn} - \epsilon_h(x_n) + \sum_{i=1}^{\bar{q}+\bar{w}} h_n^i \sum_{j=1}^{n_i} \{\bar{\zeta}_j^{(i)} \bar{\mathbf{F}}_j^{(i)}[\epsilon_{hn}] - \delta_j^{(i)} \bar{\mathbf{F}}_j^{(i)}[\epsilon_h(x_n)]\} + O(h^{\bar{q}+\bar{w}+1}), \tag{14}$$

where $\bar{\mathbf{F}}_j^{(i)}$ are the elementary differentials of $\bar{\mathbf{f}}$,

$$\bar{\zeta}_j^{(i)} = \beta_j^{(i)} \bar{\Psi}_j^{(i)}/(i-1)! \quad \text{and} \quad \delta_j^{(i)} = \alpha_j^{(i)}/i!.$$

Now $\epsilon_n(x_n) = \mathbf{P}_n(x_n) - y(x_n) = \epsilon_n$, assuming $\mathbf{P}_n(x)$ interpolates at $(x_n, \hat{\mathbf{y}}_n)$, and so $\epsilon_{hn} - \epsilon_h(x_n) = \mathbf{E}_n$. Hence, similar to the analysis in Ref. [1], equation (14) may be written

$$\mathbf{E}_{n+1} = \mathbf{E}_n + h\mathbf{G}_n(\mathbf{E}_n) + h\mathbf{T}_n, \quad \mathbf{E}_0 \text{ known},$$

where

$$\mathbf{T}_n = \sum_{i=\bar{q}+1}^{\bar{q}+\bar{w}} h^{i-1} \sum_{j=1}^{n_i} \bar{\tau}_j^{(i)} \bar{\mathbf{F}}_j^{(i)}(\epsilon_n) + O(h^{\bar{q}+\bar{w}}), \tag{15}$$

and $\bar{\tau}_j^{(i)} = \bar{\zeta}_j^{(i)} - \delta_j^{(i)}$ are the truncation coefficients pertaining to the RK formula used to integrate system (13). From the analysis in Ref. [1], it is this expression which governs the order of $\|\mathbf{E}_n\|$. Now $\mathbf{y}(x) = \mathbf{P}(x) - \epsilon_h(x)$ and from system (3) $\mathbf{f}_h[\mathbf{P}(x)] = \mathbf{P}'(x)$ thus $\bar{\mathbf{f}}[\epsilon_h(x)] = \mathbf{f}_h[\mathbf{P}(x)] - \mathbf{f}[\mathbf{y}(x)]$ and as indicated by Peterson [16] the linear independence of the elementary differentials implies that

$$\bar{\mathbf{F}}_j^{(i)}[\epsilon_h(x)] = \mathbf{F}_{hj}^{(i)}[\mathbf{P}(x)] - \mathbf{F}_j^{(i)}[\mathbf{y}(x)],$$

which with $x = x_n$ shows the similarity between equations (12) and (15). This allows the possibility of special RK$\bar{q}$ processes being used in which certain of the truncation error terms are zero. In the case where $\mathbf{P}(x)$ is based on dense output points these can be obtained from Table 1 in the case $\bar{q} = q$ simply by replacing $\hat{\tau}_j^{(i)}$ by $\bar{\tau}_j^{(i)}$.

Comparing this technique of solving for the error estimate with that of Section 2, we see that it costs about 2s **f** evaluations per step compared to 3s. This is because system (13) only requires one **f** evaluation against the two required when using system (3). Also it is not necessary to integrate system (13) with the same RK formula used to integrate equation (1) as is the case if using system (3) with equation (1). Thus in addition to being more efficient this process of solving for the error estimate also allows greater flexibility with regard to the choice of the various RK processes.

This means that we can integrate equation (1) with *any* RK$q(p)$ process, form $\mathbf{P}(x)$ using a dense output RK process and then integrate system (13) with a RK$\bar{q}$ process. It seems preferable to have $\bar{q}$ as small as possible provided an asymptotically valid error estimate is available. If $\bar{q} = q$ then the process must have the appropriate $\bar{\tau}_j^{(i)}$ zero. If $\bar{q} > q$, an asymptotically valid global error estimate is directly available. This, however, is usually more costly. If $\bar{q} < q$ then more of the truncation error coefficients will have to be zero for an estimate to be possible. Thus, an estimate ϵ_{hn+1}, of the global error, ϵ_{n+1}, at any mesh point, x_{n+1}, $n = 0, 1, \ldots, N-1$, can be obtained as follows:

(i) Use the RK$q(p)$ process, form (2), to obtain an acceptable (on local error grounds) estimate, $\hat{\mathbf{y}}_{n+1}$, of $\mathbf{y}(x_{n+1})$.
(ii) Use the dense formula, equation (4), to obtain the required non-mesh point values, $\mathbf{y}^*_{n+\sigma_k}$, for specific values of k, and possibly intermediate **f** values.
(iii) Using the values from (ii) together with the end point values form the polynomial $\mathbf{P}_n(x)$.
(iv) Use a RK$\bar{q}$ process to obtain from system (13) the estimate ϵ_{hn+1}.

If $\mathbf{P}_n(x) \equiv \mathbf{y}^*_{n+\sigma}$ then the above procedure is even simpler and since $\bar{\mathbf{f}}$ in system (13) is evaluated at $x_n + \bar{c}_j h_n$, i.e. at $\sigma = \bar{c}_j$, this allows the possibility that $b_i^*(\bar{c}_j)$ and $\mathrm{d}b_i^*/\mathrm{d}\sigma^i(\bar{c}_j)$ can be pre-determined with savings on the overhead of divided differences and numerical differentiation.

4. SPECIAL RK FORMULAE GIVING GLOBAL ERROR ESTIMATION

In the method of Section 3 no restrictions are necessary on the $\hat{\tau}_j^{(i)}$, only on the $\bar{\tau}_j^{(i)}$ of the RK$\bar{q}$ used as the estimator formula. Thus it seems preferable to follow the strategy of Dormand and Prince [1] and Prince and Dormand [19] and use RK$q(p)$ processes with small principal error truncation coefficients for the integration of equation (1). All the dense formulae used in the following discussions satisfy the continuity conditions (5) and each polynomial $\mathbf{P}_n(x)$ required by system (13) is equal to the corresponding $\mathbf{y}^*_{n+\sigma}$.

(a) RK2(1)

Following Prince [14] the RK2(1)3FM can be used as the main integration pair. This processes has $s = 3$ and uses the FSAL idea. Reference to Table 1 shows that an estimation process with $\bar{q} = 2$ and $p^* = 1$ is not possible since this would require both $\bar{\tau}_1^{(3)}$ and $\bar{\tau}_2^{(3)}$ to be zero, and this would imply a third order process. Consideration of the case where $p^* = 2$ shows that principal term estimation is possible if $\bar{\tau}_1^{(3)} = 0$ and $m = 2$ or 3. A dense formula, with $s^* = 3$, $p^* = 2$ and $d = 3$, with common function evaluations is possible. Since the main integration formula is such that $\hat{\tau}_1^{(3)} = 0$ this can also be used as the estimator. Thus we have a RK2 estimator with $\bar{q} = 2$ and $\bar{s} = 2$. The resulting process is presented in Table 2 as the RK2(1)3FD process.

(b) RK3(2)

In this case a process, using FSAL and $s = 4$, in which $p^* = 3$, $s^* = 4$ and $d = 3$ is possible. From Table 1, assuming $\bar{q} = 3$, with $m = 3$ we require $\bar{\tau}_1^{(4)} = 0$ so that one term estimation is possible. Since $\hat{\tau}_1^{(4)} = 0$ it is convenient to use the same formula as both integrator and estimator and so $\bar{s} = 3$. The resulting process is presented in Table 2 as the RK3(2)4FD.

(c) RK4(3)

As in Ref. [1] it is possible to use an embedded process employing FSAL with $s = 5$, but the process with $s = 6$ is found to be superior since it allows $p^* = 4$ and is capable of two term error estimation. A new 4(3) pair has been developed following the criteria outlined in Prince and Dormand [19]. For the dense process $s^* = 6$ and $d = 4$ and thus reference to Table 1 with $m = 4$ shows that, assuming $\bar{q} = 4$, we need an estimator with $\bar{\tau}_1^{(5)} = \bar{\tau}_5^{(5)} = \bar{\tau}_1^{(6)} = \bar{\tau}_7^{(6)} = 0$.

This is possible with $\bar{s} = 5$ and the recommended process is presented as the RK4(3)6FD in Table 3.

Table 2. Embedded RK processes for global error estimation using dense output

c_i	$a_{ij} = \bar{a}_{ij}$	$\hat{b}_i = \bar{b}_i$	b_i	b_i^*
		(i) RK2(1)3FD		
0		$\frac{1}{4}$	1	$\frac{2\sigma^2 - 5\sigma + 4}{4}$
$\frac{2}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0	$\frac{3\sigma(3 - 2\sigma)}{4}$
1	$\frac{1}{4}\quad\frac{3}{4}$	0	0	$\sigma(\sigma - 1)$
		(ii) RK3(2)4FD		
0		$\frac{1}{6}$	0	$\frac{4\sigma^2 - 9\sigma + 6}{6}$
$\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{3}$	1	$\frac{2\sigma(3 - 2\sigma)}{3}$
1	$-1\quad 2$	$\frac{1}{6}$	0	$\frac{\sigma(3 - 2\sigma)}{6}$
1	$\frac{1}{6}\quad\frac{2}{3}\quad\frac{1}{6}$	0	0	$\sigma(\sigma - 1)$

For (i) RK2(1)3FD. One term estimation is obtained: $q = 2$, $s = 4$, $p = 1$, $p^* = 2$, $s^* = 3$, $d = m = 3$, $\bar{q} = 2$, $\bar{s} = 2$.
For (ii) RK3(2)4FD. One term estimation is obtained: $q = 3$, $s = 4$, $p = 2$, $p^* = 3$, $s^* = 4$, $d = m = 3$, $\bar{q} = 3$, $\bar{s} = 3$.

Table 3. The RK4(3)6FD process for global error estimation

c_i	a_{ij}					$\hat{b}_i$	b_i	b_i^*
Embedded integrator and dense output formula								
0						$\frac{29}{238}$	$\frac{363}{2975}$	$\frac{-(162\sigma^3 - 504\sigma^2 + 551\sigma - 238)}{238}$
$\frac{7}{27}$	$\frac{7}{27}$					0	0	0
$\frac{7}{18}$	$\frac{7}{72}$	$\frac{7}{24}$				$\frac{216}{385}$	$\frac{981}{1750}$	$\frac{27\sigma(27\sigma^2 - 70\sigma + 51)}{385}$
$\frac{17}{18}$	$\frac{3043}{3528}$	$\frac{-3757}{1176}$	$\frac{1445}{441}$			$\frac{54}{85}$	$\frac{2709}{4250}$	$\frac{-27\sigma(27\sigma^2 - 50\sigma + 21)}{85}$
1	$\frac{17617}{11662}$	$\frac{-4023}{686}$	$\frac{9372}{1715}$	$\frac{-66}{595}$		$\frac{-7}{22}$	$\frac{-3}{10}$	$\frac{7\sigma(2232\sigma^2 - 4166\sigma + 1785)}{3278}$
1	$\frac{29}{238}$	0	$\frac{216}{385}$	$\frac{54}{85}$	$\frac{-7}{22}$	0	$\frac{-1}{50}$	$\frac{\sigma(\sigma - 1)(387\sigma - 238)}{149}$
$\bar{c}_i$	$\bar{a}_{ij}$					$\bar{b}_i$		
Estimation formula								
0						$\frac{1}{144}$		
$\frac{1}{10}$	$\frac{1}{10}$					$\frac{1000}{4347}$		
$\frac{3}{7}$	$\frac{-198}{343}$	$\frac{345}{343}$				$\frac{16807}{43056}$		
$\frac{4}{5}$	$\frac{654}{275}$	$\frac{-756}{253}$	$\frac{8918}{6325}$			$\frac{1375}{4368}$		
1	$-\frac{233}{25}$	$\frac{10503}{805}$	$\frac{-28518}{7475}$	$\frac{99}{91}$		$\frac{25}{432}$		

Two terms estimation is obtained: $q = 4$, $s = 6, p = 3, p^* = 4, s^* = 6, d = m = 4, \bar{q} = 4, \bar{s} = 5$.

(d) RK5(4)

In this case the RK5(4)7FM of Dormand and Prince [12] can be used as the main integration pair, possibly with the modification for the fourth order formula suggested by Shampine [7], and a 4th order dense formula with $s^* = 7$ and $d = 5$ is given by Dormand and Prince [9]. Alternatively one of the DPS triple forms [7] can be used which, at extra cost, allows $p^* = 5$. Assuming the embedded pair is used with the 4th order dense formula, no extra function evaluations are necessary and from Table 1, with $m = 5$ and $\bar{q} = 5$, we require an estimator with $\bar{\tau}_i^{(6)} = 0$, $i = 1, 6, 7, 15$ and $\bar{\tau}_i^{(7)} = 0$, $i = 1, 10, 11, 29$ which may be used to give two term error estimation. However, it was not found possible to obtain such a process in 6 stages. A 7 stage process is presented in Table 4 which has the above error terms zero, allowing two term estimation, and in addition has $\bar{\tau}_i^{(8)} = 0$, $i = 1, 14, 15, 53$. Although this does not significantly help the dense implementation of the global error estimation process, it means that 3 term estimation is possible if the block Hermite form in Ref. [2] is used and it also permits this estimator to be used in conjunction with our new RK6(5) pair.

Table 4. The RK5 estimator for use with the RK5(4)7FM and associated dense formula

$\bar{c}_i$	$\bar{a}_{ij}$						$\bar{b}_i$
0							$\frac{1}{20}$
$\frac{7 \pm R}{21}$	$\frac{7 \pm R}{21}$						0
$\frac{7 \pm R}{14}$	$\frac{7 \pm R}{56}$	$\frac{3(7 \pm R)}{56}$					0
$\frac{7 \mp R}{14}$	$\frac{77 \mp 16R}{28}$	$\frac{-273 \pm 60R}{28}$	$\frac{105 \mp 23R}{14}$				$\frac{49}{180}$
$\frac{1}{2}$	$\frac{-627 \pm 119R}{384}$	$\frac{651 \mp 147R}{128}$	$\frac{-329 \pm 74R}{96}$	$\frac{91 \pm 13R}{192}$			$\frac{16}{45}$
$\frac{7 \mp R}{14}$	$\frac{1239 \mp 89R}{1176}$	$\frac{-3(35 \mp 9R)}{56}$	$\frac{109 \mp 27R}{84}$	$\frac{-23 \mp 4R}{42}$	$\frac{4(7 \pm R)}{49}$		$\frac{49}{180}$
1	$\frac{-583 \pm 95R}{72}$	$\frac{7(31 \mp 7R)}{8}$	$\frac{-2541 \pm 563R}{108}$	$\frac{126 \pm 23R}{54}$	$\frac{4(1 \mp R)}{9}$	$\frac{7(7 \mp R)}{18}$	$\frac{1}{20}$

Two term estimation is obtained [also for use with the RK6(5)9FM: $q = 5$, $s = 7$, $p = 4$, $p^* = 4$, $s^* = 7$, $d = m = 5$, $\bar{q} = 5$, $\bar{s} = 7; R = \sqrt{21}$.

(e) RK6(5)

In this case we take the opportunity to re-evaluate the RK6(5) situation. Table 5 contains a new process, the RK6(5)9FM, developed following the strategy of Prince and Dormand [19], which has proved to be very competitive as an integrator particularly when compared to the RK5(4)7FM and the RK6(5)8M of Ref. [19]. However, it still appears preferable on global accuracy vs cost grounds to use a higher order process such as the RK8(7)13M for stringent tolerances.

Regarding a 5th order dense formula, it was not found possible to obtain a process in which $s^* = 9$ and all evaluations were in common with the integration pair. Thus $s^* = 10$ was considered and the resulting dense process (a_{10j} and b_i^*), with $d = 5$, is presented in Table 5. It would now be possible to consider an estimator with $\bar{q} = 6$ and using Table 1 obtain the necessary restrictions on the $\bar{\tau}_i$. However, because of the specific $\bar{\tau}_i$ that are zero in the RK5 estimator (Table 4), it is possible, with $m = 5$, to obtain two term error estimation using the 5th order formula as estimator. Thus we have $\bar{q} = 5$ and $\bar{s} = 7$.

It is interesting to compare the costs, in terms of function evaluations per step, incurred by each of the special processes, which as well as allowing global error estimation at each mesh point also permit dense output estimates to be obtained. Assuming no rejects, the number of evaluations per step, after the first step, for the 2nd–6th order processes is 4, 6, 10, 13 and 16 respectively. Orders 2 and 3 yield one term estimation whilst the others give two term estimation.

5. NUMERICAL TESTS

To evaluate the efficiency of the new global error estimation procedure we have conducted tests using the formulae presented in Section 4. These confirm the analytical predictions for the order of $\mathbf{E}_n$. We present here some results of integrations with the processes of orders 4, 5 and 6. The two standard test problems, A3 and D5, used in Ref. [2] are considered and the more economical direct approach of Peterson [16] has been employed. As we have seen this allows greater flexibility and also gives superior results at lax tolerances [16]. Variable integration steps were used and were computed according to the mixed local error per step criterion as discussed by Shampine [20].

Figure 1 refers to problem A3 and contains two curves for each process. The efficiency of the main integrator is represented by the solid curve ($\log_{10}\{\max|\epsilon_n|\}$ over all steps) while the dashed curve shows the error of the global error estimate ($\log_{10}\{\max|E_n|\}$ over all steps). Error estimation is effective in all cases and it is clear that, at the more stringent tolerances, at least three significant figures in the global error are obtained. In particular the new 6th order process yields very good efficiency with good global error estimation via the RK5 estimator (Table 4). An important property of the new method is the good performance at lax tolerances as compared with the 5th and 6th order cases presented in Ref. [2].

Figure 2 shows corresponding results for problem D5. In this case the maximum values of $\|\epsilon_n\|$ and $\|\mathbf{E}_n\|$ over all steps and variables are considered. Again it is clear that the 6th order process is most efficient, yielding better results than the other two over any reasonable range of tolerances. Since the RK6(5)9FM process offers dense output it would appear to be a more practical formula for general usage than any one previously published.

6. DISCUSSION

The results reported above confirm our previous predictions in Ref. [2] regarding use of dense output in defect formation. The use of Peterson's [16] model has further enhanced the practicality of global error estimation: a reliable estimate can now be achieved at about double the cost of an ordinary integration. It is possible that users of a package based on these techniques would be tempted to perform global extrapolation on the results. Since the estimation technique is robust such a temptation would not be dangerous provided, of course, the user is aware of the solution to which the global error estimate refers. If the 6th order formula is used an extrapolated result would have global error of order h^8. Since this takes 16 function evaluations per step it is likely to be more expensive than the RK8(7)13M of Ref. [19] which uses 13 evaluations per step.

Table 5. The RK6(5)9FM process and associated dense formula

c_i	a_{ij}									$\hat{b}_i$	b_i
0										$\frac{203}{2880}$	$\frac{36567}{458800}$
$\frac{1}{9}$	$\frac{1}{9}$									0	0
$\frac{1}{6}$	$\frac{1}{24}$	$\frac{1}{8}$								0	0
$\frac{1}{4}$	$\frac{1}{16}$	0	$\frac{3}{16}$							$\frac{30208}{70785}$	$\frac{9925984}{27063465}$
$\frac{5}{9}$	$\frac{280}{729}$	0	$\frac{-325}{243}$	$\frac{1100}{729}$						$\frac{177147}{164560}$	$\frac{85382667}{117968950}$
$\frac{1}{2}$	$\frac{6127}{14680}$	0	$\frac{-1077}{734}$	$\frac{6494}{4037}$	$\frac{-9477}{161480}$					$\frac{-536}{705}$	$\frac{-310378}{808635}$
$\frac{48}{49}$	$\frac{-13426273320}{14809773769}$	0	$\frac{4192558704}{2115681967}$	$\frac{14334750144}{14809773769}$	$\frac{117092732328}{14809773769}$	$\frac{-361966176}{40353607}$				$\frac{1977326743}{3619661760}$	$\frac{262119736669}{345979336560}$
1	$\frac{-2340689}{1901060}$	0	$\frac{31647}{13579}$	$\frac{253549596}{14951869}$	$\frac{10559024082}{977620105}$	$\frac{-152952}{12173}$	$\frac{-5764801}{186010396}$			$\frac{-259}{720}$	$\frac{-1}{2}$
1	$\frac{203}{2880}$	0	0	$\frac{30208}{70785}$	$\frac{177147}{164560}$	$\frac{-536}{705}$	$\frac{1977326743}{3619661760}$	$\frac{-259}{720}$		0	$\frac{-101}{2294}$
$\frac{1}{2}$	$\frac{33797}{460800}$	0	0	$\frac{27757}{70785}$	$\frac{7923501}{26329600}$	$\frac{-927}{3760}$	$\frac{-3314760575}{23165835264}$	$\frac{2479}{23040}$	$\frac{1}{64}$		

$b_1^* = (66480\sigma^4 - 206243\sigma^3 + 237786\sigma^2 - 124793\sigma + 28800)/28800,\ b_2^* = b_3^* = 0,$

$b_4^* = -16\sigma(45312\sigma^3 - 125933\sigma^2 + 119706\sigma - 40973)/70785,$

$b_5^* = -2187\sigma(19440\sigma^3 - 45743\sigma^2 + 34786\sigma - 9293)/1645600.$

$b_6^* = \sigma(12864\sigma^3 - 30653\sigma^2 + 23786\sigma - 6533)/705.$

$b_7^* = -5764801\sigma(16464\sigma^3 - 32797\sigma^2 + 17574\sigma - 1927)/7239323520,$

$b_8^* = 37\sigma(336\sigma^3 - 661\sigma^2 + 342\sigma - 31)/1440,\ b_9^* = \sigma(\sigma - 1)(16\sigma^2 - 15\sigma + 3)/4,$

$b_{10}^* = 8\sigma(\sigma - 1)^2(2\sigma - 1).$

Two term estimation is obtained: $q = 6, s = 9, p = 5, p^* = 5, s^* = 10, d = m = 5, \bar{q} = 5, \bar{s} = 7.$

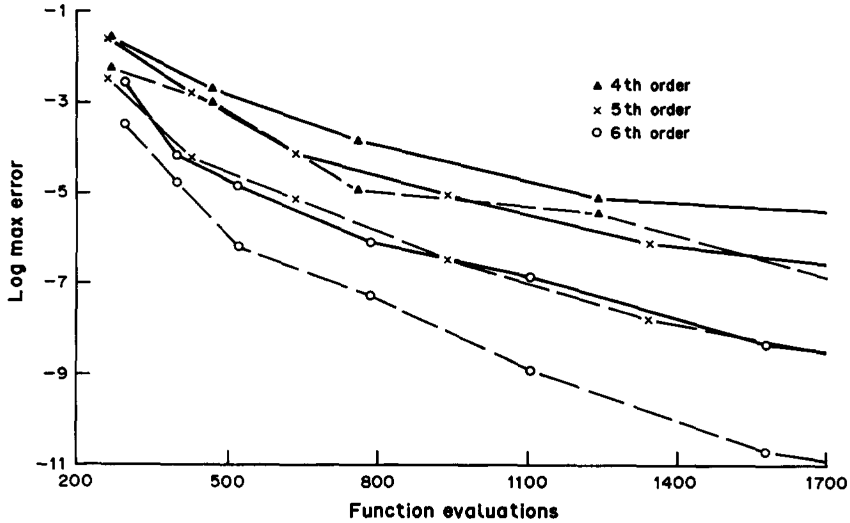

Fig. 1. Curves showing the variation of maximum global error ϵ (———) over all steps and maximum error E of ϵ (– – –), with function evaluations for three formulae applied to problem A3.

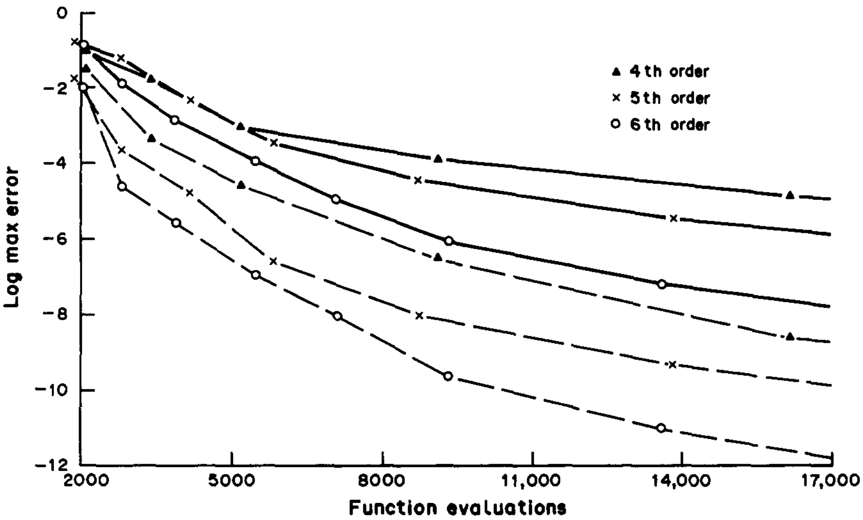

Fig. 2. Curves showing the variation of maximum global error ϵ (———) over all steps and variables and maximum error E of ϵ (– – –), with function evaluations for three formulae applied to problem D5.

Future developments of the global error estimation technique will be aimed at an 8th order process and at the provision of estimates of the global error at dense output points. This latter situation will involve derivation of dense output formulae with properties akin to those of the special formulae presented in this paper.

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