

Discrete and continuous global error estimation with globally embedded Runge-Kutta methods

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Abstract

Global error estimation processes applied to the first order system of non-stiff initial value ordinary differential equations are described. New methods are developed based on existing Runge-Kutta triples and new special *estimator* formulae to yield both discrete and continuous global error estimation. Such methods can be seen to be equivalent to a more efficient estimation procedure based on global extrapolation and global embedding.

1 Introduction

In previous work ([4], [9], [10], [5]) the solution of an associated problem has been used to provide global error estimation with explicit Runge-Kutta (RK) processes. This paper reviews and further clarifies this work, extending it to provide continuous global error estimation when dense output is employed.

The first order system of initial value ordinary differential equations

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

is considered. This system may be solved using a Runge-Kutta triple [8], denoted by $\text{RKT}q(p)q^*$, of the form:

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

where $\mathbf{f}_i = \mathbf{f}[x_n + c_i h_n, \hat{\mathbf{y}}_n + h_n \sum_{j=1}^{i-1} a_{ij} \mathbf{f}_j]$, $i = 1, 2, \dots, s^*$, and in which $x_{n+1} = x_n + h_n$, $h_n = \theta(x_n)h$, $0 \leq \theta(x_n) \leq 1$, $\hat{\mathbf{y}}_0 = \mathbf{y}(x_0)$, $x_{n+\sigma} = x_n + \sigma h_n$, the discrete embedded pair are of orders q and p ($q > p$), the dense formula is of order q^* and it is assumed that \mathbf{f}_{s^*} is the FSAL (First Same As Last) evaluation so that $\mathbf{y}_{n+\sigma}^*$ is C^1 on $[x_n, x_{n+1}]$. Local extrapolation, in which the integration is propagated from the higher order approximation $\hat{\mathbf{y}}_n$ to the true solution $\mathbf{y}(x_n)$, is the preferred mode of operation [6] and is therefore assumed. Thus the lower order discrete process is only used to control the step size. The FSAL assumption requires

$$c_s = 1, \quad \hat{b}_s = 0, \quad a_{s,j} = \hat{b}_j, \quad j = 1, 2, \dots, s-1.$$

Under appropriate conditions, the local truncation error $\hat{\mathbf{t}}_{n+1}$, at $x = x_{n+1}$, of the RK q process may be written [3]

$$\hat{\mathbf{t}}_{n+1} = \sum_{i=q+1}^{\infty} h_n^i \sum_{j=1}^{n_i} \hat{\tau}_j^{(i)} \mathbf{F}_j^{(i)}[x_n, \mathbf{y}(x_n)],$$

where the $\mathbf{F}_j^{(i)}$ are the elementary differentials of \mathbf{f} , the $\hat{\tau}_j^{(i)}$ are the truncation error coefficients, which are dependent on the RK parameters c_i , a_{ij} and \hat{b}_i , and the global error at x_n is $\boldsymbol{\varepsilon}_n = \hat{\mathbf{y}}_n - \mathbf{y}(x_n)$. The assumed ordering of the truncation error coefficients and elementary differentials is that adopted by Harris [13] in the generation of the equations of condition. The global error can be estimated by solving a differential system associated with (1), two forms of which have been considered previously [9]: these are

$$\begin{aligned}
\mathbf{y}'_h(x) &= \mathbf{f}_h[x, \mathbf{y}_h(x)] = \mathbf{f}[x, \mathbf{y}_h(x)] + \mathbf{d}_h(x) \\
\mathbf{d}_h(x) &= \mathbf{P}'(x) - \mathbf{f}[x, \mathbf{P}(x)], \\
\mathbf{y}_h(x_0) &= \mathbf{y}(x_0) = \mathbf{P}(x_0)
\end{aligned} \tag{3}$$

and

$$\begin{aligned}\boldsymbol{\varepsilon}'_h(x) &= \bar{\mathbf{f}}[x, \boldsymbol{\varepsilon}_h(x)] = \mathbf{P}'(x) - \mathbf{f}[x, \mathbf{P}(x) - \boldsymbol{\varepsilon}_h(x)], \\ \boldsymbol{\varepsilon}_h(x_0) &= \boldsymbol{\varepsilon}_{h0} = \mathbf{P}(x_0) - \mathbf{y}(x_0).\end{aligned}\quad (4)$$

The solution of the system (3) is $\mathbf{y}_h(x) = \mathbf{P}(x)$ and so, assuming \mathbf{P} is defined, its numerical solution by the RK q from (2) yields $\{\mathbf{y}_{hn}\}$ with known global error $\boldsymbol{\varepsilon}_{hn} = \mathbf{y}_{hn} - \mathbf{y}_h(x_n)$ which can be used to approximate $\boldsymbol{\varepsilon}_n$. System (4), which has solution $\boldsymbol{\varepsilon}_h(x) = \mathbf{P}(x) - \mathbf{y}(x)$, can be solved numerically using *any* RK process, say one of order \bar{q} , to produce $\boldsymbol{\varepsilon}_{hn}$ directly as an estimate of $\boldsymbol{\varepsilon}_n$. Practical testing [9] has shown the latter technique is preferable.

2 Discrete estimation

Asymptotically valid estimates of $\boldsymbol{\varepsilon}_n$ are obtained if $\mathbf{E}_n = \boldsymbol{\varepsilon}_{hn} - \boldsymbol{\varepsilon}_n = O(h^r)$, where $r > q$. The analysis in [3], based on the associated form (3), has shown that the order of \mathbf{E}_n is governed by that of

$$\mathbf{u}_n = \sum_{i=q+1}^{n_i} h_n^{i-1} \sum_{j=1}^{n_i} \hat{\tau}_j^{(i)} \mathbf{H}_j^{(i)}[x_n, \mathbf{y}(x_n)],$$

where $\mathbf{H}_j^{(i)}[x_n, \mathbf{y}(x_n)] = \mathbf{F}_{hj}^{(i)}[x_n, \mathbf{y}(x_n)] - \mathbf{F}_j^{(i)}[x_n, \mathbf{y}(x_n)]$. A similar analysis [4] has shown that for the form (4) the order of \mathbf{E}_n is dependent on that of

$$\mathbf{T}_n = \sum_{i=\bar{q}+1}^{n_i} h_n^{i-1} \sum_{j=1}^{n_i} \bar{\tau}_j^{(i)} \bar{\mathbf{F}}_j^{(i)}[x_n, \boldsymbol{\varepsilon}_h(x_n)], \quad (5)$$

where $\bar{\tau}_j^{(i)}$ and $\bar{\mathbf{F}}_j^{(i)}$ are the truncation coefficients and elementary differentials relating to the RK \bar{q} process applied to the associated equation (4). Peterson [14] has related the elementary differentials associated with (1), (3) and (4).

With either of the associated equations the choice of $\mathbf{P}(x)$ is crucial. The following choices have been analysed: ([4], [9], [7])

- (i) take $\mathbf{P}(x)$ to be the degree m piecewise polynomial interpolant of $(x_i, \hat{\mathbf{y}}_i)$ based on blocks of m steps;
- (ii) as (i) but interpolating $(x_i, \mathbf{f}[x_i, \hat{\mathbf{y}}_i])$;
- (iii) as above but using Hermite interpolants based on $\hat{\mathbf{y}}$ and \mathbf{f} ;
- (iv) use the RK triple (2) to form $\mathbf{P}(x)$ in a single step with the following possibilities:

- (A) $\mathbf{P}(x)$ interpolates $(x_{n+\sigma_j}, \mathbf{y}_{n+\sigma_j}^*)$, $j = 0, 1, \dots, m$;
- (B) as (A) but using $\mathbf{f}[x_{n+\sigma_j}, \mathbf{y}_{n+\sigma_j}^*]$ values;
- (C) using some (not necessarily all) of the $\mathbf{y}_{n+\sigma_j}^*$ and $\mathbf{f}[x_{n+\sigma_j}, \mathbf{y}_{n+\sigma_j}^*]$ from (A) and (B).

A major advantage of case (iv) is that the estimation process can be applied after each step of the numerical integration rather than following a block of m steps. This case includes the situation

$$\mathbf{P}(x) \equiv \mathbf{y}_{n+\sigma}^*,$$

which offers computational advantages [4] over the other modes and so the remainder of this paper assumes that this is the case and thus the degree, m , of $\mathbf{P}(x)$ is predetermined by the particular dense formula being used. In most cases $m = q^*$ and usually [8] q^* is either q or $q - 1$. In what follows the term *integrator* is adopted for the RK triple defined by (2) and applied to equation (1) and the term *estimator* for the RK process used with (4).

Consideration of \mathbf{T}_n from (5) shows that the order of \mathbf{E}_n is dependent on the $\bar{\tau}_j^{(i)}$ and the $\bar{\mathbf{F}}_j^{(i)}$ with the latter being dependent on the derivatives of $\mathbf{U}(x) = \mathbf{P}(x) - \mathbf{y}(x)$ for which the following bounds hold [4]

$$\|\mathbf{U}^{(k)}(x)\| \leq \begin{cases} N_k h^{\min[q, q^*+1, m+1]}, & k = 0 \\ N_k h^{\min[q, q^*, m]+1-k}, & 1 \leq k \leq m \\ N_k, & k > m \end{cases}, \quad (6)$$

Examination of the $\bar{\mathbf{F}}_j^{(i)}$, $j = 1, 2, \dots, n_i$, shows that for fixed i only $\bar{\mathbf{F}}_1^{(i)}$ contains the highest derivative $\mathbf{U}^{(i)}$ which corresponds to the *quadrature* type RK equations of condition. The remaining $\bar{\mathbf{F}}_j^{(i)}$ contain $\mathbf{U}^{(i-1)}$ and lower derivatives. Table 1 gives the \mathbf{U} derivative dependency for $i = 2, 3, \dots, 10$. It will be useful to introduce the quantity $S_r^{(i)}$ defined as the set of RK truncation error coefficients of order i corresponding to the $\bar{\mathbf{F}}_j^{(i)}$ containing the highest derivative $\mathbf{U}^{(i-r+1)}$. Thus

$$\begin{aligned} S_1^{(i)} &= \{\bar{\tau}_1^{(i)}\}, \quad \forall i, \\ S_2^{(3)} &= \{\bar{\tau}_2^{(3)}\}, \quad S_2^{(4)} = \{\bar{\tau}_3^{(4)}\}, \quad S_2^{(5)} = \{\bar{\tau}_5^{(5)}\}, \quad \dots, \\ S_3^{(4)} &= \{\bar{\tau}_2^{(4)}, \bar{\tau}_4^{(4)}\}, \quad S_3^{(5)} = \{\bar{\tau}_4^{(5)}, \bar{\tau}_8^{(5)}\}, \dots, \\ S_4^{(5)} &= \{\bar{\tau}_j^{(5)}, j = 2, 3, 6, 7, 9\}, \quad \dots, \end{aligned}$$

Table 1: Highest derivatives of \mathbf{U} occurring in $\bar{\mathbf{F}}_j^{(i)}$.

i	j	Highest deriv.	i	j	Highest deriv.
2	1	2	8	1	8
3	1	3		15	7
	2	2		14, 53	6
4	1	4		12, 13, 51, 52, 89	5
	3	3	9	1	9
	2, 4	2		22	8
5	1	5	21, 98	7	
	5	4	19, 20, 96, 97, 191	6	
	4, 8	3	10	1	10
	2, 3, 6, 7, 9	2		30	9
6	1	6	29, 177	8	
	7	5	27, 28, 175, 176, 402	7	
	6, 15	4			
	4, 5, 13, 14, 19	3			
7	1	7			
	11	6			
	10, 29	5			
	8, 9, 27, 28, 42	4			

It is instructive to set $\bar{q} = 1$ and to consider the contribution of truncation coefficients to \mathbf{T}_n which can be seen by replacing $\bar{\mathbf{F}}_j^{(i)}$ by the corresponding highest derivative of \mathbf{U} and introducing the $S_r^{(i)}$. This gives

$$\mathbf{E}_n \sim \sum_{i=1} \sum_{k=1} h^{i+k-1} \mathbf{U}^{(k+1)} S_i^{(i+k)},$$

which, using the appropriate order of $\mathbf{U}^{(k)}(x)$ from (6), may be used to show which $S_r^{(i)}$, and hence which $\bar{\tau}_j^{(i)}$, affect the principal terms in \mathbf{E}_n . Thus

$$\|\mathbf{E}_n\| \sim \sum_{i=1} h^i V_i, \quad (7)$$

where the V_i are dependent on q , q^* , m and the $S_r^{(k)}$.

Zeroisation of the elements of the appropriate V_i will now lead to a suitable estimator. So the estimation process where $\mathbf{P}(x) \equiv \mathbf{y}_{n+\sigma}^*$ will allow global error estimation to be obtained at the end of every step of the integration

process. Usually q^* is either $q - 1$ or q and m is either q^* or $q^* + 1$. It is found from (7) that

$$\begin{aligned} V_i &= 0, \quad i = 1, 2, \dots, q^* - 1, \\ V_{q^*} &= V_{q^*} \{S_1^{(k)} = \bar{\tau}_1^{(k)}, \quad k = 1, 2, \dots, q^* + 1\}, \\ V_{q^*+1} &= V_{q^*+1} \{S_1^{(k)}, \quad k = 1, 2, \dots, q^* + 2; S_2^{(k)}, \quad k = 3, 4, \dots, q^* + 2\}, \\ &\dots \end{aligned} \quad (8)$$

and so it is clearly preferable where possible to have $q^* = q$. Thus from (8), if $q^* = q$ and $\bar{\tau}_1^{(k)} = 0$ where

$$\bar{\tau}_1^{(k)} = \frac{1}{(k-1)!} \sum_{i=1}^{\bar{s}} \bar{b}_i \bar{c}_i^{k-1} - \frac{1}{k!}, \quad k = 1, 2, \dots, q+1, \quad (9)$$

then $\|\mathbf{E}_n\|$ will be at least $O(h^{q+1})$. Using (8) again it can be seen that 2-term asymptotic estimation is possible if

$$\bar{\tau}_1^{(k)} = 0, \quad k = 1, 2, \dots, q+2 \quad \text{and} \quad \sum_{i=2}^{\bar{s}} \bar{b}_i \bar{Q}_{i,k} = 0, \quad k = 1, 2, \dots, q. \quad (10)$$

The $\bar{Q}_{i,k}$ are functions of the RK parameters $\bar{a}_{i,j}$ and \bar{c}_i [15]. If $q^* = q - 1$ then additional truncation coefficients need to be zero.

3 Continuous estimation

Applying the RK process of order \bar{q} with \bar{s} stages together with an associated dense process of order \bar{q}^* and \bar{s}^* stages to system (4) gives

$$\boldsymbol{\varepsilon}_{hn+1} = \boldsymbol{\varepsilon}_{hn} + h_n \sum_{i=1}^{\bar{s}} \bar{b}_i \bar{\mathbf{f}}_i \quad \text{and} \quad \boldsymbol{\varepsilon}_{hn+\sigma}^* = \boldsymbol{\varepsilon}_{hn} + \sigma h_n \sum_{i=1}^{\bar{s}^*} \bar{b}_i^*(\sigma) \bar{\mathbf{f}}_i \quad (11)$$

where

$$\bar{\mathbf{f}}_i = \bar{\mathbf{f}}[x_n + \bar{c}_i h_n, \boldsymbol{\varepsilon}_{hn} + h_n \sum_{j=1}^{i-1} \bar{a}_{ij} \bar{\mathbf{f}}_j], \quad i = 1, 2, \dots, \bar{s}^*. \quad (12)$$

It is assumed that $\bar{q}^* = \bar{q} - 1$ or \bar{q} , the FSAL evaluation is utilised so that C^1 continuity is obtained and $\bar{s}^* \geq \bar{s} + 1$. Equation (11) yields a numerical solution $\boldsymbol{\varepsilon}_{hn+\sigma}^*$ approximating $\boldsymbol{\varepsilon}_h(x_{n+\sigma})$ and using the true solution of (4) with $\mathbf{P}(x) \equiv \mathbf{y}_{n+\sigma}^*$, this leads to

$$\boldsymbol{\varepsilon}_h(x_{n+\sigma}) = \mathbf{y}_{n+\sigma}^* - \mathbf{y}(x_{n+\sigma}).$$

Similar to the analysis of ([4], [3]) the following result for $\mathbf{E}_{n+\sigma}^*$ is easily deduced:

$$\mathbf{E}_{n+\sigma}^* = \boldsymbol{\varepsilon}_{hn+\sigma}^* - \boldsymbol{\varepsilon}_h(x_{n+\sigma}) \sim O(\|\mathbf{E}_n\|) + \mathbf{T}_n^*,$$

where

$$\mathbf{T}_n^* = \sigma h_n \sum_{i=\bar{q}^*+1} (\sigma h_n)^{i-1} \sum_{j=1}^{n_i} \bar{\tau}_j^{*(i)}(\sigma) \bar{\mathbf{F}}_j^{(i)}[x_n, \boldsymbol{\varepsilon}_h(x_n)]. \quad (13)$$

Since the dense output solutions $\mathbf{y}_{n+\sigma}^*$ and $\boldsymbol{\varepsilon}_{hn+\sigma}^*$ are not propagated beyond step n the expression (13) is effectively a local contribution to $\mathbf{E}_{n+\sigma}^*$. The similarity between (13) and (5) allows a determination of which truncation error coefficients $\bar{\tau}_j^{*(i)}(\sigma)$, relating to the RK \bar{q}^* , affect the leading few terms of \mathbf{T}_n^* . Taking $\bar{q}^* = 1$ these can be determined in a similar manner to those in the discrete case. From an asymptotic point of view it is required that $\mathbf{E}_{n+\sigma}^*$ should be at least $O(h_n^{q^*+1})$.

4 Global extrapolation and global embedding

Having obtained estimates for the discrete and continuous global errors the extrapolated (higher order) values are $\tilde{\mathbf{y}}_n = \hat{\mathbf{y}}_n - \boldsymbol{\varepsilon}_{hn}$ and $\tilde{\mathbf{y}}_{n+\sigma}^* = \mathbf{y}_{n+\sigma}^* - \boldsymbol{\varepsilon}_{hn+\sigma}^*$ and consideration has been given to the discrete value in [5]. The following analysis considers the continuous situation. With $x \in [x_n, x_{n+1}]$ it is found that

$$\mathbf{P}(x) = \mathbf{P}(x_n + \sigma h) = \mathbf{y}_{n+\sigma}^* \text{ and } \mathbf{P}'(x_n + \sigma h) = \sum_{i=1}^{s^*} d_i^*(\sigma) \mathbf{f}_i$$

where

$$b_i^*(\sigma) = \sum_{j=0}^{m-1} B_{i,j} \sigma^j \quad \text{and} \quad d_i^*(\sigma) = b_i^*(\sigma) + \sigma \frac{d}{d\sigma} b_i^*(\sigma) = \sum_{j=0}^{m-1} B_{i,j} (1+j) \sigma^j.$$

Consideration of the expression for $\bar{\mathbf{f}}_i$ from (12) shows that

$$\bar{\mathbf{f}}_1 = \mathbf{f}_1 - \mathbf{f}(x_n, \tilde{\mathbf{y}}_n) = \mathbf{f}_1 - \mathbf{f}_{s^*+1}$$

and

$$\bar{\mathbf{f}}_k = \sum_{i=1}^{s^*} d_i^*(\bar{c}_k) \mathbf{f}_i - \mathbf{f}_{s^*+k}, \quad k = 1, 2, \dots, \bar{s}^*,$$

where

$$\mathbf{f}_{s^*+k} = \mathbf{f}[x_n + \bar{c}_k h_n, \tilde{\mathbf{y}}_n + h_n \sum_{j=1}^{s^*+k-1} a_{s^*+k,j} \mathbf{f}_j], \quad k = 1, 2, \dots, \bar{s}^*,$$

and

$$a_{s^*+k,j} = \begin{cases} \bar{c}_k b_j^*(\bar{c}_k) - \sum_{i=1}^{k-1} \bar{a}_{k,i} d_j^*(\bar{c}_i), & j = 1, 2, \dots, s^*, \quad k = 1, 2, \dots, \bar{s}^* \\ \bar{a}_{k,j-s^*}, & j = s^* + 1, s^* + 2, \dots, s^* + k - 1, \quad k = 1, 2, \dots, \bar{s}^* \end{cases} \quad (14)$$

Using equations (2), (11) and (12) it is found that

$$\tilde{\mathbf{y}}_{n+\sigma}^* = \tilde{\mathbf{y}}_n + \sigma h_n \left\{ \sum_{i=1}^{s^*} b_i^*(\sigma) \mathbf{f}_i - \sum_{i=1}^{\bar{s}^*} \bar{b}_i^*(\sigma) \bar{\mathbf{f}}_i \right\}$$

which using the expressions for $\bar{\mathbf{f}}_i$ gives

$$\tilde{\mathbf{y}}_{n+\sigma}^* = \tilde{\mathbf{y}}_n + \sigma h_n \sum_{i=1}^{\bar{s}^*} \bar{b}_i^*(\sigma) \mathbf{f}_{s^*+i} - \sigma h_n \sum_{i=1}^{s^*} Y_i^*(\sigma) \mathbf{f}_i$$

where

$$Y_i^* = \sum_{k=1}^{\bar{s}^*} \bar{b}_k^*(\sigma) d_i^*(\bar{c}_k) - b_i^*(\sigma), \quad i = 1, 2, \dots, s^*$$

and substitution for $d_i^*(\bar{c}_k)$ gives

$$Y_i^* = \sum_{j=0}^{m-1} (1+j) B_{i,j} \left\{ \sum_{k=1}^{\bar{s}^*} \bar{b}_k^*(\sigma) \bar{c}_k^j - \sigma^j / (j+1) \right\} = \sum_{j=0}^{m-1} (1+j) B_{i,j} \sigma^j j! \bar{\tau}_1^{*(j+1)}(\sigma)$$

where $\bar{\tau}_1^{*(j+1)}(\sigma)$, $j = 0, 1, \dots, m-1$ are the quadrature truncation coefficients associated with the continuous process of order \bar{q}^* which are required zero for valid asymptotic estimation. Thus $Y_i^* = 0$, $i = 1, 2, \dots, s^*$ leading to

$$\tilde{\mathbf{y}}_{n+\sigma}^* = \tilde{\mathbf{y}}_n + \sigma h_n \sum_{i=1}^{\bar{s}^*} \bar{b}_i^*(\sigma) \mathbf{f}_{s^*+i} \quad \text{and} \quad \tilde{\mathbf{y}}_{n+1} = \tilde{\mathbf{y}}_n + h_n \sum_{i=1}^{\bar{s}} \bar{b}_i \mathbf{f}_{s^*+i} \quad (15)$$

where $\tilde{\mathbf{y}}_0 = \mathbf{y}(x_0)$ and the latter result from (15) has been obtained by putting $\sigma = 1$ giving the result for the discrete extrapolated value from [5]. This may be written

$$\tilde{\mathbf{y}}_{n+1} = \tilde{\mathbf{y}}_n + h_n \sum_{i=1}^{\bar{s}} \bar{b}_i \mathbf{f}_i, \quad \tilde{\mathbf{y}}_{n+\sigma}^* = \tilde{\mathbf{y}}_n + \sigma h_n \sum_{i=1}^{\bar{s}^*} \bar{b}_i^*(\sigma) \mathbf{f}_i \quad \text{and}$$

$$\mathbf{f}_i = \begin{cases} \mathbf{f}(x_n + c_i h_n, \hat{\mathbf{y}}_n + h_n \sum_{j=1}^{i-1} a_{i,j} \mathbf{f}_j), & i = 1, 2, \dots, s^*, \\ \mathbf{f}(x_n + c_i h_n, \tilde{\mathbf{y}}_n + h_n \sum_{j=1}^{i-1} a_{i,j} \mathbf{f}_j), & i = s^* + 1, s^* + 2, \dots, \bar{s}^* \end{cases} \quad (16)$$

where

$$\begin{aligned} \tilde{s} &= s^* + \bar{s}, & \tilde{s}^* &= s^* + \bar{s}^*, & c_{s^*+i} &= \bar{c}_i, & i &= 1, 2, \dots, \bar{s}^*, \\ \tilde{b}_i &= \tilde{b}_i^* = 0, & i &= 1, 2, \dots, s^*, & \tilde{b}_i &= \bar{b}_{i-s^*}, & \tilde{b}_i^* &= \bar{b}_{i-s^*}^*, & i &= s^*+1, s^*+2, \dots, \tilde{s}^*. \end{aligned}$$

Thus the extrapolation process (16) is rather like a standard RK formula. The difference being that the function evaluations with extrapolation utilise both $\hat{\mathbf{y}}_n$ and $\tilde{\mathbf{y}}_n$. In what follows the term *Extrapolator* will be adopted for this process. After using the integrator at each step to obtain values $\hat{\mathbf{y}}_n$ and $\mathbf{y}_{n+\sigma}^*$ by solving the system (1) there are two approaches that can be used to obtain the required global error estimates. First the estimator can be applied to solve the error correction system (4) giving global error estimates $\boldsymbol{\varepsilon}_{hm}$ and $\boldsymbol{\varepsilon}_{hn+\sigma}^*$. Alternatively the extrapolator can be used to give error estimates $\hat{\mathbf{y}}_n - \tilde{\mathbf{y}}_n$ and $\mathbf{y}_{n+\sigma}^* - \tilde{\mathbf{y}}_{n+\sigma}^*$. Clearly this latter approach is to be preferred since it significantly reduces the complexity of the overall estimation process by eliminating the need for the second system (4) to be solved numerically. *Global Embedding* is the term that has been adopted for this approach [5] and Fortran 90 code associated with the estimation procedure can be found in [2]. Since the processes (2) and (16) utilise common function evaluations the error estimation procedure is extremely cost effective. Assuming no step rejections the whole procedure, after the first step, costs $\tilde{s}^* - 2$ function evaluations per step since there are effectively two applications of the FSAL strategy. This compares very favourably against Richardson extrapolation which costs $3S$ function evaluations per step where S is the cost of a basic step integration. Richardson extrapolation has the advantage of estimating the global error in the more accurate integration but the global extrapolation process can obtain far better estimates by careful choice of the estimator/extrapolator as will be demonstrated in §5.

5 Global error estimation processes

This section is concerned with the construction of RK estimation processes with consideration being given to obtaining *both* discrete and continuous estimates.

5.1 Integrator of order 3

Any third order RK triple in the form of (2) can be used as the integrator. The RKT3(2)3 of [15] (see Table 2) where $q = 3$, $q^* = 3$, and $s = s^* = 4$ is one such possibility.

Table 2: Integrator RKT3(2)3

c_i	a_{ij}			\widehat{b}_i	b_i	b_i^*
0				$\frac{2}{9}$	$\frac{7}{36}$	$\frac{5\sigma^2-12\sigma+9}{9}$
$\frac{1}{2}$	$\frac{1}{2}$			$\frac{1}{3}$	$\frac{19}{36}$	$\frac{\sigma(3-2\sigma)}{3}$
$\frac{3}{4}$	0	$\frac{3}{4}$		$\frac{4}{9}$	$\frac{1}{6}$	$\frac{4\sigma(3-2\sigma)}{9}$
1	$\frac{2}{9}$	$\frac{1}{3}$	$\frac{4}{9}$	0	$\frac{1}{9}$	$\sigma(\sigma - 1)$

Since the RKT3(2)3 has $q^* = q$ then from (9) $\bar{\tau}_1^{(k)} = 0$, $k = 1, 2, \dots, 4$, will yield 1-term discrete estimation. Assuming distinct \bar{c}_i , $i = 1, 2, 3$, the $\bar{\tau}_1^{(k)}$ can be zeroed with $\bar{s} = 3$ and it requires $\bar{c}_3 = (4\bar{c}_2 - 3)/(2(3\bar{c}_2 - 2))$ and leaves $\bar{a}_{3,2}$ and \bar{c}_2 as degrees of freedom. For the continuous estimator \bar{s}^* is taken as 4 where stage 4 is the FSAL stage which implies

$$\bar{c}_4 = 1, \quad \bar{b}_4 = 0 \quad \text{and} \quad \bar{a}_{4,j} = \bar{b}_j, \quad j = 1, 2, 3.$$

This permits the parameters $\bar{b}_i^*(\sigma)$, $i = 1, 2, \dots, 4$, to be found by zeroisation of the $\bar{\tau}_1^{*(k)}(\sigma)$, $k = 1, 2, \dots, 4$. The coefficients of the extrapolator can now be found from (14). It is noticed that *if all the function evaluations were to be evaluated using the same value of \mathbf{y}* , say \mathbf{Y} where $\mathbf{Y}_0 = \mathbf{y}(x_0)$, then the extrapolator coefficients give rise to an *associated* standard fourth order RK process. This would mean that 1-term global error estimates, $\hat{\mathbf{y}}_n - \mathbf{Y}_n$, in the RKT3(2)3 integrator could be obtained using this fourth order associated process but it would be at a significant cost since the process would not now be using common function evaluations. A couple of obvious possibilities arise as to how the two degrees of freedom should be chosen. First they could be chosen to obtain a small contribution from those truncation error terms, $\bar{\tau}_j^{(i)}$, which would generally have to be made zero if 2-term estimation was required. This, however, raises a problem in that these consist of terms of differing orders and it is not clear how any weighting associated with the terms should be applied. For example should the terms with small i values be given more weight? A second possibility is to consider the associated RK process and choose the free parameters to give a small norm of the principal truncation error terms, $\tilde{\tau}_j^{(5)}$, $j = 1, 2, \dots, 9$. It is easily found that the $\bar{\tau}_j^{(i)}$ and the $\tilde{\tau}_j^{(5)}$ are related. For example

$$\tilde{\tau}_1^{(5)} = \bar{\tau}_1^{(5)} \quad \text{and} \quad \tilde{\tau}_9^{(5)} = \frac{\bar{\tau}_2^{(3)}}{3} - \bar{\tau}_3^{(4)} + \bar{\tau}_5^{(5)}.$$

Practical investigations show that the second possibility is preferable. This leads to the choice $\bar{a}_{3,2} = 7/8$ and $\bar{c}_2 = 1/3$ and results in the estimator EST1 and extrapolator XTR1 (see Tables 3 and 4). Notice how coefficients from the integrator and estimator appear in the extrapolator tableau. The estimation process using (2) and (16) effectively uses 6 function evaluations per step, assuming no rejected steps, where it can be seen that the fourth evaluation at step n will be the same as the first evaluation at step n+1 and that the last evaluation at step n will be the same as the fifth evaluation at step n+1. The coefficients of the integrator-extrapolator process can also be found in the file rkcoeffs.pdf at <https://www.petepreece.co.uk/>.

Table 3: Estimator EST1

\bar{c}_i	\bar{a}_{ij}			\bar{b}_i	\bar{b}_i^*
0				$\frac{1}{10}$	$\frac{10-26\sigma+26\sigma^2-9\sigma^3}{10}$
$\frac{1}{3}$	$\frac{1}{3}$			$\frac{1}{2}$	$\frac{\sigma(9\sigma^2-22\sigma+15)}{4}$
$\frac{5}{6}$	$-\frac{1}{24}$	$\frac{7}{8}$		$\frac{2}{5}$	$\frac{-2\sigma(9\sigma^2-16\sigma+6)}{5}$
1	$\frac{1}{10}$	$\frac{1}{2}$	$\frac{2}{5}$	0	$\frac{\sigma(\sigma-1)(9\sigma-5)}{4}$

Table 4: Extrapolator XTR1 based upon the integrator RKT3(2)3

c_i	a_{ij}						\tilde{b}_i	\tilde{b}_i^*
0							0	0
$\frac{1}{2}$	$\frac{1}{2}$						0	0
$\frac{3}{4}$	0	$\frac{3}{4}$					0	0
1	$\frac{2}{9}$	$\frac{1}{3}$	$\frac{4}{9}$				0	0
0	0	0	0	0		$\frac{1}{10}$	$\frac{10-26\sigma+26\sigma^2-9\sigma^3}{10}$	
$\frac{1}{3}$	$-\frac{31}{243}$	$\frac{7}{81}$	$\frac{28}{243}$	$-\frac{2}{27}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{\sigma(9\sigma^2-22\sigma+15)}{4}$	
$\frac{5}{6}$	$\frac{11}{972}$	$-\frac{13}{162}$	$-\frac{26}{243}$	$\frac{19}{108}$	$-\frac{1}{24}$	$\frac{7}{8}$	$\frac{-2\sigma(9\sigma^2-16\sigma+6)}{5}$	
1	0	0	0	0	$\frac{1}{10}$	$\frac{1}{2}$ $\frac{2}{5}$	$\frac{\sigma(\sigma-1)(9\sigma-5)}{4}$	

Higher order discrete estimation can be obtained using (8) and (10) to zeroise more of the appropriate discrete truncation error terms. This has been done with both $\bar{s} = 4$ and $\bar{s} = 5$ to give 2-term and 3-term discrete estimators respectively. The zeroisation of truncation coefficients is generally more costly in the continuous case and for higher order processes this may have a significant affect on the size of \bar{s}^*/\tilde{s}^* . These estimators, EST2 and EST3, and corresponding extrapolators, XTR2 and XTR3, can be found in Tables 5, 6, 7 and 8 respectively and the extrapolator coefficients can be found in the file rkcoeffs.pdf. The overall estimation processes using XTR2 and XTR3 use effectively 7 and 8 f evaluations respectively per step.

Table 5: Estimator EST2

\bar{c}_i	\bar{a}_{ij}				\bar{b}_i	\bar{b}_i^*
0					$\frac{5}{48}$	$\frac{48-126\sigma+128\sigma^2-45\sigma^3}{48}$
$\frac{1}{3}$	$\frac{1}{3}$				$\frac{27}{56}$	$\frac{27\sigma(5\sigma^2-12\sigma+8)}{56}$
$\frac{4}{5}$	$-\frac{19}{25}$	$\frac{39}{25}$			$\frac{125}{336}$	$-\frac{125\sigma(9\sigma^2-16\sigma+6)}{336}$
1	$\frac{38}{7}$	$-\frac{87}{14}$	$\frac{25}{14}$		$\frac{1}{24}$	$-\frac{\sigma(2-3\sigma)(6-5\sigma)}{24}$
1	$\frac{5}{48}$	$\frac{27}{56}$	$\frac{125}{336}$	$\frac{1}{24}$	0	$\frac{\sigma(\sigma-1)(5\sigma-3)}{2}$

Table 6: Estimator EST3

\bar{c}_i	\bar{a}_{ij}					\bar{b}_i	\bar{b}_i^*
0						$\frac{53}{702}$	$\frac{702-2685\sigma+4436\sigma^2-3360\sigma^3+960\sigma^4}{702}$
$\frac{1}{4}$	$\frac{1}{4}$					$\frac{44}{117}$	$-\frac{2\sigma(240\sigma^3-765\sigma^2+854\sigma-351)}{117}$
$\frac{13}{20}$	$-\frac{4759183}{6982500}$	$\frac{2324452}{1745625}$				$\frac{100}{273}$	$\frac{50\sigma(48\sigma^3-129\sigma^2+110\sigma-27)}{273}$
$\frac{9}{10}$	$\frac{4500387}{1163750}$	$-\frac{10646649}{2327500}$	$\frac{45}{28}$			$\frac{50}{351}$	$-\frac{50\sigma(96\sigma^3-228\sigma^2+170\sigma-39)}{351}$
1	$-\frac{7313669}{907725}$	$\frac{3399923}{302575}$	$-\frac{33}{13}$	$\frac{14}{39}$		$\frac{5}{126}$	$-\frac{\sigma(4496\sigma^3-10865\sigma^2+8292\sigma-1948)}{630}$
1	$\frac{53}{702}$	$\frac{44}{117}$	$\frac{100}{273}$	$\frac{50}{351}$	$\frac{5}{126}$	0	$\frac{\sigma(\sigma-1)(1328\sigma^2-1767\sigma+529)}{90}$

Table 7: Extrapolator XTR2 based upon the integrator RKT3(2)3

c_i	a_{ij}								\tilde{b}_i	\tilde{b}_i^*
0									0	0
$\frac{1}{2}$	$\frac{1}{2}$								0	0
$\frac{3}{4}$	0	$\frac{3}{4}$							0	0
1	$\frac{2}{9}$	$\frac{1}{3}$	$\frac{4}{9}$						0	0
0	0	0	0	0					$\frac{5}{48}$	$\frac{48-126\sigma+128\sigma^2-45\sigma^3}{48}$
$\frac{1}{3}$	$-\frac{31}{243}$	$\frac{7}{81}$	$\frac{28}{243}$	$-\frac{2}{27}$	$\frac{1}{3}$				$\frac{27}{56}$	$\frac{27\sigma(5\sigma^2-12\sigma+8)}{56}$
$\frac{4}{5}$	$\frac{119}{225}$	$-\frac{148}{375}$	$-\frac{592}{1125}$	$\frac{49}{125}$	$-\frac{19}{25}$	$\frac{39}{25}$			$\frac{125}{336}$	$\frac{-125\sigma(9\sigma^2-16\sigma+6)}{336}$
1	$-\frac{409}{126}$	$\frac{53}{21}$	$\frac{212}{63}$	$-\frac{37}{14}$	$\frac{38}{7}$	$-\frac{87}{14}$	$\frac{25}{14}$		$\frac{1}{24}$	$-\frac{\sigma(3\sigma-2)(5\sigma-6)}{24}$
1	0	0	0	0	$\frac{5}{48}$	$\frac{27}{56}$	$\frac{125}{336}$	$\frac{1}{24}$	0	$\frac{\sigma(\sigma-1)(5\sigma-3)}{2}$

Table 8: Extrapolator XTR3 based upon the integrator RKT3(2)3

c_i	a_{ij}								\tilde{b}_i	\tilde{b}_i^*
0									0	0
$\frac{1}{2}$	$\frac{1}{2}$								0	0
$\frac{3}{4}$	0	$\frac{3}{4}$							0	0
1	$\frac{2}{9}$	$\frac{1}{3}$	$\frac{4}{9}$						0	0
0	0	0	0	0					$\frac{53}{702}$	$\frac{702-2685\sigma+4436\sigma^2-3360\sigma^3+960\sigma^4}{702}$
$\frac{1}{4}$	$-\frac{43}{576}$	$\frac{5}{96}$	$\frac{5}{72}$	$-\frac{3}{64}$	$\frac{1}{4}$				$\frac{44}{117}$	$-\frac{2\sigma(240\sigma^3-765\sigma^2+854\sigma-351)}{117}$
$\frac{13}{20}$	$\frac{113369191}{335160000}$	$-\frac{14519609}{55860000}$	$-\frac{14519609}{41895000}$	$\frac{5993689}{22344000}$	$-\frac{4759183}{6982500}$	$\frac{2324452}{1745625}$			$\frac{100}{273}$	$\frac{50\sigma(48\sigma^3-129\sigma^2+110\sigma-27)}{273}$
$\frac{9}{10}$	$-\frac{927519}{581875}$	$\frac{3044619}{2327500}$	$\frac{1014873}{581875}$	$-\frac{678807}{465500}$	$\frac{4500387}{1163750}$	$-\frac{10646649}{2327500}$	$\frac{45}{28}$		$\frac{50}{351}$	$-\frac{50\sigma(96\sigma^3-228\sigma^2+170\sigma-39)}{351}$
1	$\frac{692786}{209475}$	$-\frac{194813}{69825}$	$-\frac{779252}{209475}$	$\frac{14909}{4655}$	$-\frac{7313669}{907725}$	$\frac{3399923}{302575}$	$-\frac{33}{13}$	$\frac{14}{39}$	$\frac{5}{126}$	$-\frac{\sigma(4496\sigma^3-10865\sigma^2+8292\sigma-1948)}{630}$
1	0	0	0	0	$\frac{53}{702}$	$\frac{44}{117}$	$\frac{100}{273}$	$\frac{50}{351}$	$\frac{5}{126}$	$\frac{\sigma(\sigma-1)(1328\sigma^2-1767\sigma+529)}{90}$

One way to compare the efficiency of the three extrapolators associated with the RKT3(2)3 is to compare cost (in terms of function evaluations) against global accuracy. The RKT3(2)3 provides third order estimates, $\hat{\mathbf{y}}_n$ and $\mathbf{y}_{n+\sigma}^*$, of $\mathbf{y}(x_n)$ and $\mathbf{y}(x_{n+\sigma})$ at $x = x_n$ and $x = x_{n+\sigma}$ respectively where the step sequence is determined by local error estimates. Each extrapolator, XTR1, XTR2 and XTR3, can then be used to obtain the global errors, $\tilde{\mathbf{e}}_n$ and

$\tilde{\epsilon}_{n+\sigma}^*$, in the $\tilde{\mathbf{y}}_n$ and $\tilde{\mathbf{y}}_{n+\sigma}^*$ approximations. For a given initial value problem, range of integration and a sequence of tolerances it is possible to plot $\log_{10}M$ against cost where M is the maximum absolute value of the global error (ϵ_n for the integrator or $\tilde{\epsilon}_n$ for the extrapolators) over all steps and equation components. To test continuous estimation the plots of $\log_{10}M^*$ against cost are used where M^* is the maximum absolute value of the global error at the mid-point of each step ($\epsilon_{n+1/2}^*$ or $\tilde{\epsilon}_{n+1/2}^*$). This has been done using a sample of the problems from the DETEST suite [12] and from those used by Hairer et al. [11]. On the vast majority of the test problems all three extrapolators gave good estimates for both the discrete and continuous global errors over the range of integration. Each problem considered the various $\log_{10}M$ or $\log_{10}M^*$ values generated using a range of local error tolerances from 10^{-3} down to 10^{-5} to control the local error estimates from the RKT3(2)3 integrator. Since the estimation procedure depends on asymptotic applicability any problems tended to occur at the more lax tolerances where in some cases the results for XTR1 were rather poor. Unless very accurate estimation is required XTR2 is recommended. To illustrate the situation two example plots are considered. Figure 1 shows the plots of the various $\log_{10}M$ values for the integrator, RKT3(2)3, and the three extrapolators, XTR1, XTR2 and XTR3, against function evaluations for DETEST problem D3 and Figure 2 shows the plots of the various $\log_{10}M^*$ values for the AREN problem of [11].

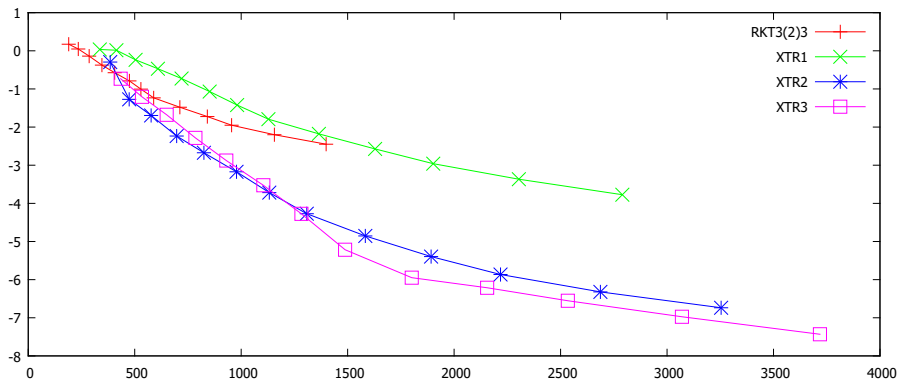


Figure 1: DETEST Problem D3: $\log_{10}M$ against Function Evaluations.

5.2 Higher order integrators

The global extrapolation process has been applied to integrators of higher order. For example, the fourth order integrator, RKT4(3)4 of [15], where $q = q^* = 4$, $s = 5$ and $s^* = 6$ has been utilised to obtain extrapolators,

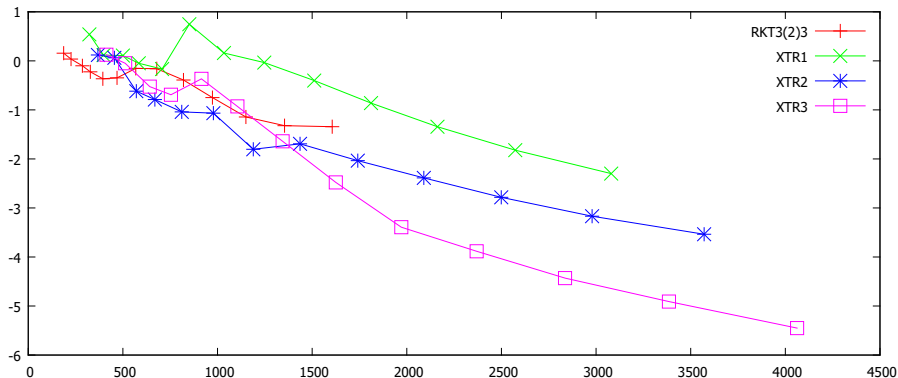


Figure 2: AREN Problem: $\log_{10}M^*$ against Function Evaluations.

XTR4, XTR5 and XTR6 following a similar analysis to that in §5.1 (see file rkcoeffs.pdf). These respectively yield 1-term, 2-term and 3-term discrete error estimation and respectively have $(\bar{s}, \bar{s}^*) = (10, 11)$, $(11, 12)$ and $(12, 14)$. Alternatively EST1 and EST2 could be used to obtain extrapolators based on the RKT4(3)4 which respectively yield 1-term and 2-term discrete global error estimation.

Among the possible integrators of order 5 are the RKT5(4)5 of [15] where $q = q^* = 5$, $s = s^* = 8$ which effectively uses 7 function evaluations per step and the RK5(4)7FM of [6] (frequently referred to as DOPRI5) which has dense processes of orders 5 and 4 ([1], [8]) where with the fifth order dense formula this process has $s = 7$ and $s^* = 9$ (effectively using 8 evaluations per step) and with the fourth order dense formula has $s = s^* = 7$ (effectively using 6 evaluations per step). Since practical testing [15] has shown that the RK5(4)7FM is generally to be preferred to the RKT5(4)5 based on global error versus cost considerations the RK5(4)7FM will be considered as the integrator and consideration will be given to both cases where $q^* = 5$ and $q^* = 4$. With $q^* = 5$ the required continuous global error estimates will need to be at least $O(h^6)$ whereas for $q^* = 4$ they will need to be at least $O(h^5)$. It is important to note that the value of q^* will govern the values of \bar{s} , \bar{s}^* and the quality of estimation. With $q^* = 5$ the extrapolator XTR7 has been produced where $\bar{s} = 6$, $\bar{s}^* = 8$ which implies that $\tilde{s} = 15$ and $\tilde{s}^* = 17$ whereas with $q^* = 4$ the extrapolator XTR8 has been produced where $\bar{s} = 7$, $\bar{s}^* = 9$ which implies that $\tilde{s} = 14$ and $\tilde{s}^* = 16$. For both XTR7 and XTR8 the use of (2) and (16) will yield 3-term discrete estimation. The coefficients for both XTR7 and XTR8 can be found in the file rkcoeffs.pdf. Over a wide range of problems and tolerances the process involving XTR8 is significantly better

than that utilising XTR7 for discrete estimation. For continuous estimation the difference between the two is not as great as in the discrete case. To illustrate the estimation process three example plots are considered where local error tolerances from 10^{-3} down to 10^{-9} were used. Figure 3 shows the plots of the various $\log_{10}M$ values for the integrator, RK5(4)7FM, and the two extrapolators, XTR7 and XTR8, against function evaluations for the AREN problem of [11]. Figure 4 shows the plots of the various $\log_{10}M^*$ values for the BRUS problem of [11] and Figure 5 shows the plots of the various $\log_{10}M$ values for the DETEST problem D3.

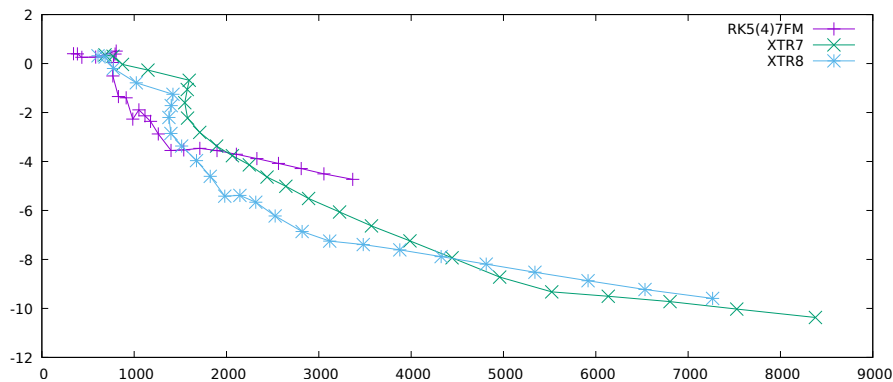


Figure 3: AREN Problem: $\log_{10}M$ against Function Evaluations.

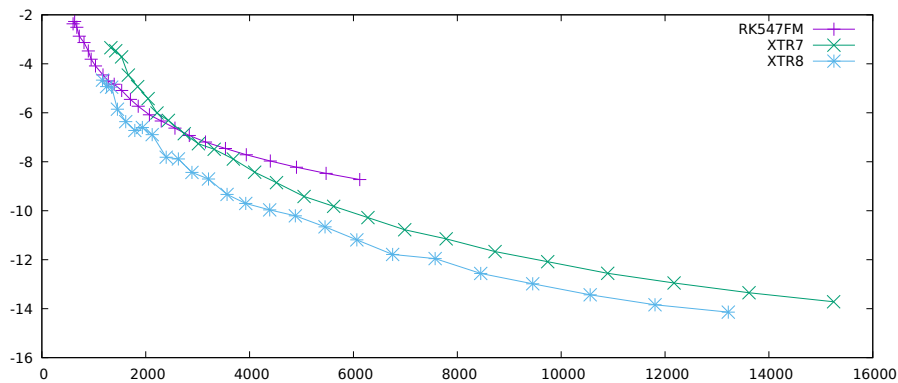


Figure 4: BRUS Problem: $\log_{10}M$ against Function Evaluations.

The RK triple RKT8(6)7 of [15] where $q = 8$, $p = 6$, $q^* = 7$, $s = 13$ and $s^* = 14$ has been considered as the integrator. With $\bar{s} = 6$ and $\bar{s}^* = 9$ an estimator and an extrapolator have been developed. The extrapolator, XTR9 (see file rkcoeffs.pdf), has $\tilde{s} = 20$ and $\tilde{s}^* = 23$. This will yield 2-term

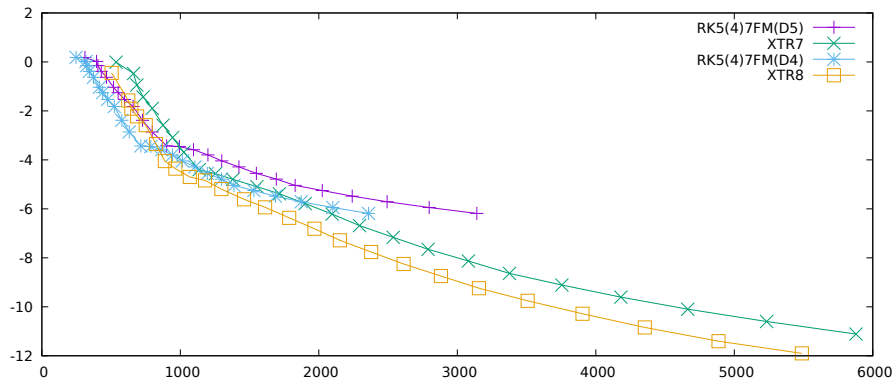


Figure 5: DETEST Problem D3: $\log_{10}M^*$ against Function Evaluations.

discrete estimation. Notice how, for large values of q , the values of \bar{s}^* and \tilde{s}^* become significantly greater than \bar{s} and \tilde{s} . Once again the estimation process is illustrated by three example plots (Figures 6, 7 and 8) where local error tolerances from 10^{-3} down to 10^{-12} were used.

6 Conclusions

The results of this work suggest that global extrapolation methods based on Runge-Kutta triples are a cost effective way of global error estimation in both the discrete and continuous cases. As might be expected the RK triple RK5(4)7FM (with fourth order dense) together with the extrapolator XTR8 seems to give best estimation when the local error tolerances are lax to medium whereas for stringent tolerances the RK triple RKT8(6)7 together with the extrapolator XTR9 is preferred.

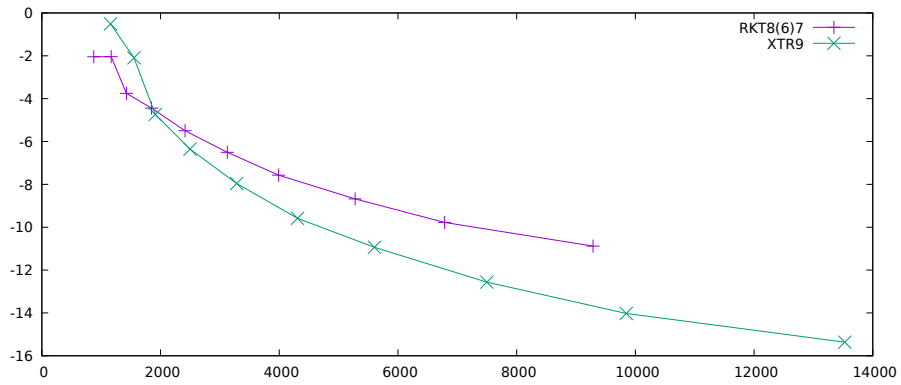


Figure 6: AREN Problem: $\log_{10} M$ against Function Evaluations.

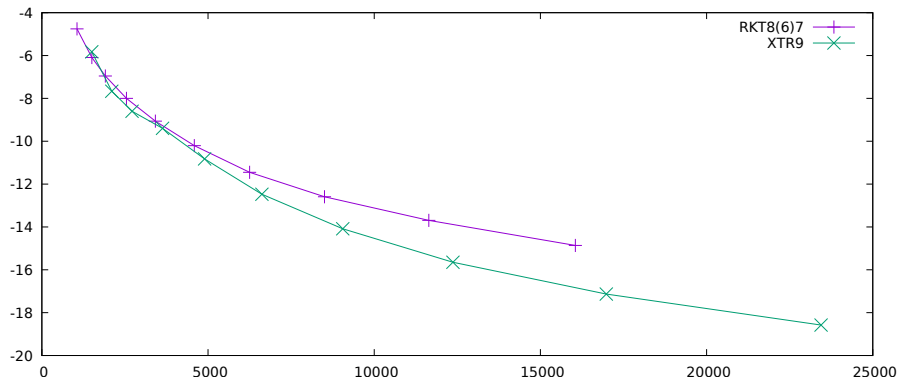


Figure 7: BRUS Problem: $\log_{10} M$ against Function Evaluations.

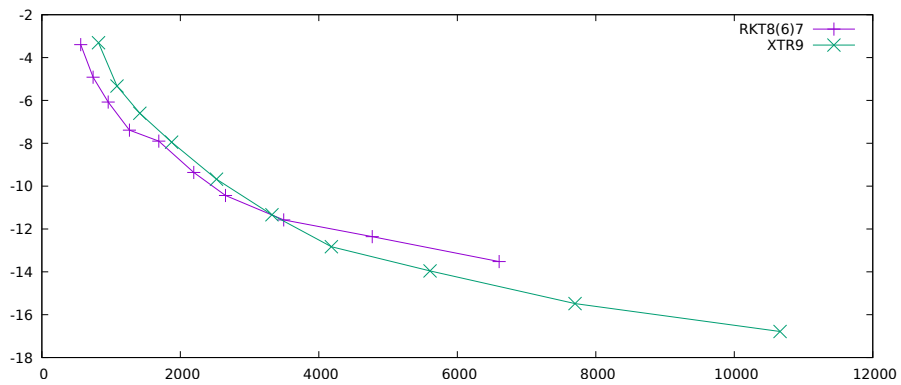


Figure 8: DETEST Problem D3: $\log_{10} M^*$ against Function Evaluations.

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