

# Parallel Derivation of Efficient Continuous/Discrete Explicit Runge-Kutta Methods

P.J. Prince

Guisborough,  
TS14 6NP, U.K.

September 6, 2018

## Abstract

New discrete and continuous explicit Runge-Kutta methods are developed which employ the FSAL (first-same-as-last) technique and other than possibly the FSAL evaluation no additional evaluations are required for the continuous methods. Efficiency is measured from a practical point of view by consideration of cost (function evaluations) against global accuracy. The free parameters which are associated with the new methods are chosen to satisfy this efficiency criterion. Numerical tests are carried out on a number of standard problems and these show that the new higher order methods offer significant practical advantages.

## 1 Introduction

This work has been largely influenced by the suggestion made (page 194) in [9] that new methods should be looked for which use all stages associated with the discrete and continuous processes.

Consideration is given to the first order system of non-stiff initial value ordinary differential equations

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

which may be solved using a Runge-Kutta (RK) triple [4], denoted by  $\text{RKT}q(p)q^*$ , of the form:

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

where  $\mathbf{g}_i = \mathbf{f}[x_n + c_i h_n, \widehat{\mathbf{y}}_n + h_n \sum_{j=1}^{i-1} a_{ij} \mathbf{g}_j]$ ,  $i = 1, 2, \dots, s^*$ , and in which  $x_{n+1} = x_n + h_n$ ,  $h_n = \theta(x_n)h$ ,  $0 \leq \theta(x_n) \leq 1$ ,  $\widehat{\mathbf{y}}_0 = \mathbf{y}(x_0)$ ,  $x_{n+\sigma} = x_n + \sigma h_n$ , the discrete embedded pair are of orders  $q$  and  $p$  ( $q > p$ ), the dense formula is of order  $q^*$  and it is assumed that  $\mathbf{g}_{s^*}$  is the FSAL 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  $\widehat{\mathbf{y}}_n$  to the true solution  $\mathbf{y}(x_n)$ , is the preferred mode of operation [3] and is therefore assumed. Thus the lower order discrete process is only used to control the step size. The FSAL assumption requires

$$c_{s^*} = 1, \quad \widehat{b}_{s^*} = 0, \quad a_{s^*j} = \widehat{b}_j, \quad j = 1, 2, \dots, s = s^* - 1.\tag{2}$$

Under appropriate conditions, the local truncation errors  $\widehat{\mathbf{t}}_{n+1}$  and  $\mathbf{t}_{n+1}$ , at  $x = x_{n+1}$ , of the  $\text{RK}q$  and  $\text{RK}p$  processes and the local truncation error  $\mathbf{t}_{n+\sigma}$  of the continuous  $\text{RK}q^*$  process at  $x_{n+\sigma}$  may be written [1]

$$\begin{aligned}\widehat{\mathbf{t}}_{n+1} &= \sum_{i=q+1}^{\infty} h_n^i \sum_{j=1}^{n_i} \widehat{\tau}_j^{(i)} \mathbf{F}_j^{(i)}[x_n, \mathbf{y}(x_n)], \\ \mathbf{t}_{n+1} &= \sum_{i=p+1}^{\infty} h_n^i \sum_{j=1}^{n_i} \tau_j^{(i)} \mathbf{F}_j^{(i)}[x_n, \mathbf{y}(x_n)], \\ \mathbf{t}_{n+\sigma} &= \sum_{i=q^*+1}^{\infty} (\sigma h_n)^i \sum_{j=1}^{n_i} \tau_j^{*(i)} \mathbf{F}_j^{(i)}[x_n, \mathbf{y}(x_n)],\end{aligned}$$

where the  $\mathbf{F}_j^{(i)}$  are the elementary differentials of  $\mathbf{f}$  and the  $\widehat{\tau}_j^{(i)}$ ,  $\tau_j^{(i)}$  and  $\tau_j^{*(i)}$  are truncation error coefficients, which are dependent on the parameters

$c_i, a_{ij}, \widehat{b}_i, b_i$  and  $b_i^*$  and the global errors at  $x_n$  and  $x_{n+\sigma}$  are  $\boldsymbol{\varepsilon}_n = \widehat{\boldsymbol{y}}_n - \boldsymbol{y}(x_n)$  and  $\boldsymbol{\varepsilon}_{n+\sigma} = \boldsymbol{y}_{n+\sigma}^* - \boldsymbol{y}(x_{n+\sigma})$  respectively. The ordering of the elementary differentials is that adopted by Dormand and Prince [3] to generate the RK equations of condition. The difference  $\widehat{\boldsymbol{y}}_{n+1} - \boldsymbol{y}_{n+1}$  is an estimate of  $\boldsymbol{t}_{n+1}$  and can be used to monitor the step size. Usually  $p = q - 1$  but sometimes  $p = q - 2$  [5] or a pair of lower order formulae [9] can be used successfully to give "stretched" estimation.

The development of embedded RKq(p) pairs involves a number of free parameters. Prince and Dormand [13] outlined a number of criteria as to how these parameters should best be chosen. The main criterion was to choose those parameters which affected the higher order formula so that the norm of the principal truncation error terms was small since this tended to give better global accuracy. Additionally the RK coefficients should not be very large and they should not lead to a lower order formula which gave poor local error estimation. The initial development of RK embedded pairs was carried out without any reference to continuous processes and this resulted in such processes being "added on" at a later stage to the embedded pair which, except for very low orders, implied that  $s^* > s$  and significantly so for high order pairs. The order ( $q^*$ ) of the continuous process is a significant factor in determining the value of  $s^*$ . Dormand and Prince [4] point out that it is sufficient for  $q^* = q - 1$  to have both the discrete and continuous global errors of  $O(h^q)$ . However as pointed out in [7] other applications may require  $q^* = q$  so that the local error in the continuous process is asymptotically negligible compared to the global error at the discrete points. Frequently, therefore, in the development of continuous processes for known embedded pairs there were additional RK parameters available which only affected the continuous process. The question then arose as to how best to choose these additional parameters. Clearly emphasis needs to be placed on the norm of the principal truncation error coefficients in the continuous process and this has been considered by Calvo et al. [2] who have used the additional free parameters to obtain a small value for

$$I_C = \int_0^1 \|\sigma^{q^*+1} \boldsymbol{\tau}^{*(q^*+1)}\|_2 d\sigma \quad (3)$$

However, Baker et al. [1], point out that the choice of these parameters should be made according to how they affect the continuous global error and therefore should be chosen to give a small value for

$$I_B = \int_0^1 \|\sigma^{q^*+1} \boldsymbol{\tau}^{*(q^*+1)} - \sigma \widehat{\boldsymbol{\tau}}^{(q^*+1)}\|_2 d\sigma \quad (4)$$

where it should be noted that if  $q^* = q - 1$  then  $I_C$  and  $I_B$  are identical since all the  $\hat{\tau}_j^{(q)}$  are zero. Thus when  $s^* > s$  and there are additional free parameters which do not affect the main discrete process it seems preferable to devise the processes such that  $A^{(q+1)} = \|\hat{\boldsymbol{\tau}}^{(q+1)}\|_2$  is small which tends to give smaller discrete global error and to choose the additional parameters so that  $I_B$  is small (while also taking into account the size of the RK coefficients and the affect on the local error estimation process).

Initially this work will assume that  $q^* = q$  so that  $I_C$  and  $I_B$  are not the same and from (1) and (2) there are no additional parameters that do not affect the main discrete process. The question arises therefore as to whether the free parameters should be chosen mainly to give small  $A^{(q+1)}$  or whether in addition the size of  $I_B$  should be taken into account. From Baker et al. [1] the continuous global error can be expressed as

$$\boldsymbol{\varepsilon}_{n+\sigma} = \boldsymbol{\varepsilon}_n + \mathbf{G}_{n+\sigma} + \mathbf{t}_{n+\sigma}^* + O(h^{q+2})$$

showing that the continuous global error is directly dependent on that at the discrete points which suggests that the priority should be for small  $A^{(q+1)}$ .

In considering the various values of  $q = q^*$  this work was guided by the entries for  $N_q$ ,  $D_q$  and  $C_q$  in Table 1 where  $N_q$  is the number of RK equations of condition for order  $q$ ,  $D_q$  is the minimum number of stages for an explicit discrete RK process and  $C_q$  is the minimum number of stages for an explicit continuous RK process. The values of  $C_q$ ,  $q = 1, 2, \dots, 6$ , in Table 1 are

Table 1: Values of  $N_q$ ,  $D_q$  and  $C_q$  for  $q = 1, 2, \dots, 10$

$q$	1	2	3	4	5	6	7	8	9	10
$N_q$	1	2	4	8	17	37	85	200	486	1205
$D_q$	1	2	3	4	6	7	9	11	$\leq 15$	$\leq 16$
$C_q$	1	2	4	6	8	11	$\leq 14$	$\leq 18$	$\leq 22$	

those given by Enright et al. [7]. The entries for  $C_7$ ,  $C_8$  and  $C_9$  are obtained from the analysis in the other sections of this work. Note that the values of  $D_9$  and  $D_{10}$  are not precisely known. From the work of Hairer [8] it was known that  $D_{10} \leq 17$  but this entry can now be replaced by  $\leq 16$  since a 16-stage RK10 process is given in Table 2 but it should be noted that all the free parameters have been chosen randomly. The process is only presented in order to show that such a process is possible.

Table 2: A 16-stage explicit RK10 process where  $a_{17j} = b_j$ ,  $j = 1, 2, \dots, 16$ ,

$$c_i = \sum_{j=1}^{i-1} a_{ij}, \quad i = 1, 2, \dots, 16 \text{ and the table only contains the non-zero } a_{ij}.$$

$i$	$j$	$Numerator(a_{ij})$	$Denominator(a_{ij})$	$i$	$j$	$Numerator(a_{ij})$	$Denominator(a_{ij})$
2	1	1	9	13	4	-144031	9768285
3	1	-5	6	13	5	4025343400	2690185689
3	2	25	18	13	6	94166721047	23473655658
4	1	5	24	13	7	7335448531	8595710442
4	3	5	8	13	8	-44196265055873	56837005275636
5	1	121397	1318200	13	9	-51978654834616	10620609181875
5	3	25721	878800	13	10	-211398749870620672	226295508183215625
5	4	-32657	2636400	13	11	101535598	486253125
6	1	121	3060	13	12	-1082198294528	133223113814175
6	4	1	20340	14	1	2899	96
6	5	2197	17289	14	2	25	18
7	1	161	340	14	6	9022833	58667
7	4	9	565	14	7	2685	77
7	5	-10985	5763	14	8	-6413500779	180382240
7	6	23	12	14	9	-3445903488009	24066350000
8	1	426932	1428595	14	10	-50803557531648	1236558640625
8	4	82872	9495955	14	11	17425287	1750000
8	5	-111080320	96858741	14	12	-255879168	687061375
8	6	64192	50421	14	13	-4201227	444080
8	7	2312	16807	15	1	1	9
9	1	-15694499	482751380	15	3	-1	18
9	4	-2369871	802219205	15	14	1	18
9	5	1196310440	2727545297	16	1	-9379980173	534775120
9	6	-12236093	48275138	16	2	493920	393217
9	7	112607	2839714	16	3	92610	393217
9	8	-1241317	96550276	16	4	16192827	222167605
10	1	53529428429	45634027520	16	5	-16719820312	2266109571
10	4	7464384207	151666032640	16	6	-2287318770977	19773310062
10	5	-466500093865	96687095808	16	7	-5088054879	268173994
10	6	251090729	100663296	16	8	145283084168551	7092936326608
10	7	-1972264857	2952790016	16	9	2267252583356677	19312852955000
10	8	5553817927	25232932864	16	10	1593601199469232128	61523723464121875
10	9	218123025995	138781130752	16	11	-59691112677	9830425000
11	1	95553638	44883315	16	12	4309516947456	7718977505525
11	4	1325104	11049705	16	13	5558223321	2494568648
11	5	-3865665440	338120973	16	14	-92610	393217
11	6	-71919334	86774409	16	15	-493920	393217
11	7	-97709266	60020433	17	1	887	14112
11	8	27036181984	35017962363	17	2	1	20
11	9	20183684860	1910973141	17	3	1	40
11	10	268435456000	275804802441	17	6	120528	50575
12	1	9506527619197	1855976898560	17	7	-34208	107415
12	4	-6581911077	192762306560	17	8	11166419537	24351602400
12	5	423361032185	122885970432	17	9	-70322610762721	30323601000000
12	6	2238520211347	59363966976	17	10	-140737488355328	3747412280390625
12	7	1247928517773	232679456768	17	11	528039	8750000
12	8	-471699954635119	85178422132736	17	12	43670044672	216424333125
12	9	-276460201705587	7055441592320	17	13	4201227	8881600
12	10	-615042605056	77689354975	17	14	-1	40
12	11	520936699437	272937779200	17	15	-1	20
13	1	3919624801	9998920260	17	16	393217	11113200

Much of the previous development of discrete embedded RK $q(p)$  pairs has involved the simultaneous solution of the RK equations of condition for both orders  $q$  and  $p$  where usually  $p = q - 1$ . Except for low orders the necessity of embedding increased the number of stages required from that of  $D_q$  given in Table 1. The strategy in this work is to initially ignore the requirement for a lower order embedded process and to develop discrete and continuous RK processes of order  $q^*$  with  $s^*$  common stages. The RK equations of condition for the continuous process may be written [9]

$$\Phi B = G$$

where  $\Phi$  is a matrix with  $N_{q^*}$  rows and  $s^*$  columns and is dependent on the RK parameters,  $c_i$  and  $a_{ij}$ ,  $B$  is a matrix with  $s^*$  rows and  $q^*$  columns whose elements are  $B_{ij}$  where  $b_i^*(\sigma) = \sum_{j=0}^{q^*-1} B_{ij} \sigma^j$ ,  $i = 1, 2, \dots, s^*$  and  $G$  is a matrix with constant coefficients that are associated with the RK equations of condition. From Owren and Zennaro [11] it is required that

$$\text{rank}(\Phi) = \text{rank}(\Phi \mid G) \quad (5)$$

For each process of order  $q^*$  the equations of condition will be solved using  $s^*$  stages to obtain a continuous process. The discrete process, of order  $q = q^*$ , will then be obtained by satisfying the FSAL conditions (2) which will ensure  $C^1$  smoothness of the continuous process. The lower order process (or processes if "stretched" estimation is used) is then considered so that local error estimation can be obtained. The free parameters are then chosen with small  $A^{(q+1)}$  as the main priority but with consideration also given to the size of the parameters, to the affect on the local error estimation process and to the size of  $J^{(q^*+1)}$  where

$$J^{(q^*+1)} = \sqrt{\int_0^1 \sum_{j=1}^{N_{q^*+1}-N_{q^*}} [\sigma^{q^*+1} \tau_j^{*(q^*+1)} - \sigma \hat{\tau}_j^{(q^*+1)}]^2 d\sigma} \quad (6)$$

which is an easier to compute comparable measure to  $I_B$ . An additional point to note regarding the lower order discrete embedded process is that the error estimation process should preferably involve the function evaluation at the endpoint of the step so that the situation as outlined by Hairer et al. [9] in relation to the RK8(6) process of [5] does not occur.

## 2 RK triple processes

Owren and Zennaro [12] have developed triple processes of orders 3, 4 and 5 in which  $I_C$  has been minimised and which have been tested on a selection of

problems from the DETEST package [10] using an efficiency criterion based on expected global accuracy. These triples will be considered and new triples of orders 3, 4, . . . , 9 will be developed but all testing will be carried out using the efficiency criterion of actual global accuracy against cost.

## 2.1 Order 3

From Table 1  $s^* = 4$  is required and the 4 equations of condition for the continuous process are easily solved [12]. The FSAL assumption (2) then leads to a 2-parameter ( $c_2$  and  $c_3$ ) family of discrete/continuous processes. As usual with such models there are certain restrictions on the values of  $c_2$  and  $c_3$ . The expressions for the principal truncation error terms for the continuous process are

$$\begin{aligned}\tau_1^{*(4)} &= \frac{-3\sigma^2 + \sigma(12c_2c_3 - 8(c_2 + c_3) + 12) - 18c_2c_3 + 12(c_2 + c_3) - 12}{72\sigma^2}, \\ \tau_2^{*(4)} &= \frac{-3\sigma^2 - 4\sigma(2c_3 - 3) - 12(1 - c_3)}{24\sigma^2}, \\ \tau_3^{*(4)} &= \frac{-\sigma^2 + 4\sigma(1 - c_2) - 2(2 - 3c_2)}{24\sigma^2} \quad \text{and} \quad \tau_4^{*(4)} = \frac{-(\sigma - 2)^2}{24\sigma^2}.\end{aligned}$$

The corresponding expressions for the principal truncation error terms of the discrete process can be obtained by putting  $\sigma = 1$  which yields the following expression for  $A^{(4)} = \|\hat{\tau}^{(4)}\|_2$

$$A^{(4)} = \sqrt{\frac{(9c_2^2 - 12c_2 + 40)c_3^2 - (12c_2^2 - 17c_2 + 60)c_3 + 13c_2^2 - 15c_2 + 27}{1296}}$$

Choosing  $(c_2, c_3) = (\frac{1}{2}, \frac{3}{4})$  gives a near minimal value for  $A^{(4)}$  of  $\approx 4.18 \times 10^{-2}$  with  $J^{(4)} \approx 6.43 \times 10^{-3}$ . To complete the triple it is easiest to obtain a discrete formula of order 2 which requires the solution of 2 equations of condition. This involves either 3 or 4 unknown weights ( $b_i$ ) depending on whether or not the FSAL evaluation is utilised. Owren and Zennaro [12] suggest that  $b_4$  should be zero so that the FSAL evaluation is not used for the error estimation process and therefore one less evaluation will be lost in the case of any step rejections. However, if neither  $c_2$  or  $c_3$  is 1, then without the FSAL evaluation the error estimation process could lead to poor results on problems such as EULR [9] and, in any case, it may possibly be preferable to utilise the FSAL evaluation if better error estimation is obtained. A careful choice of the free weights (with  $b_4 \neq 0$ ) gives the triple process in Table 3. Owren and Zennaro [12] in looking for a small value for  $I_C$  chose  $(c_2, c_3) = (\frac{12}{23}, \frac{4}{5})$

and  $b_4 = 0$  for their triple giving  $A^{(4)} \approx 4.26 \times 10^{-2}$  and  $J^{(4)} \approx 6.46 \times 10^{-3}$ . It might be expected therefore that, from the global error/cost efficiency point of view, there would be little difference in general between the two triples.

Table 3: RKT3(2)3

$c_i$	$a_{ij}$			$\hat{b}_i$	$b_i$	$b_i^*$
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	$\frac{1}{9}$	$\sigma(\sigma - 1)$

## 2.2 Order 4

From Table 1  $s^* = 6$  is required and so the 8 equations of condition for the continuous process can now be solved. The FSAL assumption (2) leaves the following free parameters:  $c_2, c_3, c_4, c_5$  and  $a_{32}$ . Unfortunately the expressions for some of the  $a_{ij}$  are exceedingly large. It is however possible to make progress by choosing  $Q_{31} = 0$  where

$$Q_{ik} = \sum_{j=1}^{i-1} a_{ij} c_j^k - \frac{c_i^{k+1}}{k+1}, \quad i = 2, 3, \dots, s^*, \quad k = 1, 2, \dots \quad (7)$$

and this has the affect of making  $Q_{i1} = 0$ ,  $i = 4, 5$  and  $\hat{b}_2 = b_2^* = 0$  which greatly simplifies the analysis. Examination of the principal truncation error terms for the discrete process now shows that only  $\hat{\tau}_4^{(5)}$  and  $\hat{\tau}_8^{(5)}$  are dependent on  $c_2$  which can only therefore play a minor role in the determination of  $A^{(5)}$ . Hence the standard choice of  $c_2 = \frac{2}{3}c_3$  is made giving

$$\hat{\tau}_1^{(5)} = \frac{30c_3c_4c_5 - 20(c_3c_4 + c_4c_5 + c_5c_3) + 15(c_3 + c_4 + c_5) - 12}{1440},$$

$$\hat{\tau}_2^{(5)} = 6\hat{\tau}_1^{(5)}, \quad \hat{\tau}_3^{(5)} = 3\hat{\tau}_1^{(5)}, \quad \hat{\tau}_4^{(5)} = 4\hat{\tau}_1^{(5)}, \quad \hat{\tau}_7^{(5)} = 3\hat{\tau}_5^{(5)}, \quad \hat{\tau}_8^{(5)} = \hat{\tau}_5^{(5)},$$

$$\hat{\tau}_5^{(5)} = -\frac{10(c_3c_4 - 5(c_3 + c_4) + 3)}{360}, \quad \hat{\tau}_9^{(5)} = -\frac{(10c_4c_5 - 5c_4 + 1)}{120}$$



$$\text{and } \widehat{\tau}_6^{(5)} = \frac{30c_3c_4c_5 - 20c_4(c_3 + c_5) + 5c_5 + 15c_4 - 4}{120}.$$

The expressions for the  $\tau_j^{*(5)}$ ,  $j = 1, 2, \dots, 9$  are similarly related but involve  $\sigma$  and are much larger and therefore not given here. It turns out that  $A^{(5)} = 0$  with  $c_3 = \frac{2}{5}$ ,  $c_4 = 1$  and  $c_5 = 1$ . Unfortunately  $c_4 \neq c_5$  is one of the restrictions for this 3-parameter family. With small  $A^{(5)}$  as a priority a reasonable choice is  $c_3 = \frac{2}{5}$ ,  $c_4 = \frac{24}{25}$  and  $c_5 = 1$  giving  $A^{(5)} \approx 6.37 \times 10^{-4}$  and  $J^{(5)} \approx 3.85 \times 10^{-3}$ . For error estimation a discrete process of order 3 can be obtained by solving 4 equations involving the 6 weights  $b_i$ ,  $i = 1, 2, \dots, 6$ . Practical tests show that there is no obvious advantage in utilising the FSAL evaluation in the error estimation process and a suitable triple is given in Table 4. Owren and Zennaro [12] chose  $c_2 = \frac{1}{6}$ ,  $c_3 = \frac{11}{37}$ ,  $c_4 = \frac{11}{17}$ ,  $c_5 = \frac{13}{15}$  and  $b_6 = 0$  giving  $A^{(5)} \approx 3.16 \times 10^{-3}$  with  $J^{(5)} \approx 1.74 \times 10^{-3}$  and so their error estimation process does not involve the endpoint evaluation. The difference in the  $A^{(5)}$  values is such that it might be expected, from a global error/cost point of view, that there would be a significant difference in the practical results particularly at the more stringent tolerances.

Table 4: RKT4(3)4

$c_i$	$a_{ij}$				$\widehat{b}_i$	$b_i$	$b_i^*$
0					$\frac{73}{576}$	$\frac{1}{12}$	$-\frac{375\sigma^3 - 1180\sigma^2 + 1308\sigma - 576}{576}$
$\frac{4}{15}$	$\frac{4}{15}$				0	0	0
$\frac{2}{5}$	$\frac{1}{10}$	$\frac{3}{10}$			$\frac{575}{1008}$	$\frac{25}{36}$	$\frac{25\sigma(75\sigma^2 - 196\sigma + 144)}{1008}$
$\frac{24}{25}$	$\frac{528}{625}$	$-\frac{1944}{625}$	$\frac{2016}{625}$		$\frac{3125}{4032}$	0	$-\frac{3125\sigma(3\sigma - 2)(5\sigma - 6)}{4032}$
1	$\frac{337}{272}$	$-\frac{645}{136}$	$\frac{2175}{476}$	$-\frac{125}{1904}$	$-\frac{17}{36}$	$\frac{2}{9}$	$\frac{17\sigma(705\sigma^2 - 1324\sigma + 576)}{1548}$
1	$\frac{73}{576}$	0	$\frac{575}{1008}$	$\frac{3125}{4032}$	$-\frac{17}{36}$	0	$\frac{\sigma(\sigma - 1)(115\sigma - 72)}{43}$

### 2.3 Order 5

From Table 1  $s^* = 8$  is required. The solution of the 17 equations associated with the continuous process has been investigated in detail by Owren and Zennaro ([11] and [12]). Together with the FSAL conditions (2) this leads

of a family of processes with  $c_2, c_3, c_6, c_7$  and  $a_{54}$  as the free parameters. It should be noted that the model requires

$$c_4 = c_5 = 2c_3, \quad b_2^* = \widehat{b}_2 = 0, \quad Q_{i1} = 0, \quad i = 1, 3, 4, \dots, s^* \quad (8)$$

Consideration of the expressions for the 20 principal truncation error terms in the fifth order discrete process shows that none are dependent on  $a_{54}$ , only  $\widehat{\tau}_j^{(6)}$ ,  $j = 4, 5, 13, 14, 19$  are dependent on  $c_2$  and that  $\widehat{\tau}_j^{(6)}$ ,  $j = 15, 18$  are only dependent on  $c_3$ . Investigations show that the smallest possible value of  $A^{(6)}$  is approximately  $9.2 \times 10^{-4}$ . Choosing  $c_2 = \frac{1}{5}$ ,  $c_3 = \frac{3}{10}$ ,  $c_6 = \frac{2}{5}$ ,  $c_7 = \frac{9}{10}$  gives  $A^{(6)} \approx 9.53 \times 10^{-4}$  with  $J^{(6)} \approx 9.04 \times 10^{-4}$  and a suitable fourth order discrete embedded formula is easily found leading to the triple in Table 5. The 5(4) formula of Owren and Zennaro [12] has  $c_2 = \frac{1}{6}$ ,  $c_3 = \frac{1}{4}$ ,  $c_6 = \frac{9}{14}$ ,  $c_7 = \frac{7}{8}$  and  $b_8 = 0$  giving  $A^{(6)} \approx 1.09 \times 10^{-3}$  with  $J^{(6)} \approx 1.92 \times 10^{-4}$  and so it might be expected therefore that, from the global error/cost efficiency point of view, there would be little difference in general between the two triples.

It is interesting to compare these triples, as far as the cost is concerned, with the RK5(4)7FM (sometimes referred to as DOPRI5) of [3] which uses 7 stages (including the FSAL stage) per step with  $A^{(6)} \approx 3.99 \times 10^{-4}$  and which was originally developed without any continuous process. Subsequently it was provided with both a fourth order continuous process using the 7 stages [4] and a fifth order continuous process using 9 stages [1].

Table 5: RKT5(4)5

$c_i$	$a_{ij}$						$\widehat{b}_i$	$b_i$	$b_i^*$
0							$\frac{29}{324}$	$\frac{73}{1620}$	$\frac{(1895\sigma^4 - 5080\sigma^3 + 5007\sigma^2 - 2412\sigma + 648)}{648}$
$\frac{1}{5}$	$\frac{1}{5}$						0	0	0
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					$\frac{5}{9}$	$\frac{11}{9}$	$-\frac{5\sigma(185\sigma^3 - 415\sigma^2 + 281\sigma - 54)}{27}$
$\frac{3}{5}$	$\frac{3}{10}$	$-\frac{9}{10}$	$\frac{6}{5}$				$\frac{25}{162}$	$-\frac{185}{3078}$	$\frac{25\sigma(35\sigma^3 - 55\sigma^2 + 3\sigma + 18)}{162}$
$\frac{3}{5}$	$\frac{1}{10}$	0	$\frac{2}{5}$	$\frac{1}{10}$			$\frac{35}{162}$	$\frac{1432}{1539}$	$-\frac{5\sigma(2785\sigma^3 - 4640\sigma^2 + 981\sigma + 846)}{648}$
$\frac{2}{5}$	$\frac{8}{135}$	$\frac{4}{15}$	$\frac{8}{135}$	$\frac{2}{45}$	$-\frac{4}{135}$		$-\frac{1}{4}$	$-\frac{5}{4}$	$\frac{\sigma(365\sigma^3 - 760\sigma^2 + 429\sigma - 36)}{8}$
$\frac{9}{10}$	$-\frac{14}{95}$	$\frac{261}{760}$	$\frac{196}{95}$	$-\frac{17}{380}$	$\frac{27}{20}$	$-\frac{405}{152}$	$\frac{19}{81}$	$\frac{1}{81}$	$\frac{19\sigma(5\sigma^3 + 5\sigma^2 - 27\sigma + 18)}{81}$
1	$\frac{29}{324}$	0	$\frac{5}{9}$	$\frac{25}{162}$	$\frac{35}{162}$	$-\frac{1}{4}$	$\frac{19}{81}$	$\frac{1}{10}$	$\frac{\sigma(\sigma - 1)(5\sigma^2 - 15\sigma + 18)}{8}$

## 2.4 Order 6

From Table 1  $s^* = 11$  is required and the solution of the 37 equations of condition for the continuous process utilises the requirements (8) and leads to a significant restriction in that either

$$a_{76} = 0 \quad (9)$$

or

$$c_7 = c_6 \quad (10)$$

At this point in the analysis the continuous process is of order 6 with degrees of freedom  $c_2, c_5, c_6, c_8, c_9, c_{10}, c_{11}, a_{54}, a_{82}, a_{92}, a_{98}, a_{102}, a_{108}, a_{109}, a_{112}, a_{118}, a_{119}, a_{1110}$  and either  $c_7$  or  $a_{76}$ . It should be noted that (9) and (10) cannot both be true. In either case after applying the FSAL assumption (2) and consideration of the discrete process there are still a considerable number of degrees of freedom left. Since small  $A^{(7)}$  is the priority these are chosen accordingly. In fact it is found that  $A^{(7)}$  can be made zero. Thus  $\hat{\tau}_j^{(7)} = 0, j = 1, 2, \dots, 85$ , making the discrete process of order 7. It should be noted that  $\hat{\tau}_{15}^{(7)}$  is rather difficult to deal with since, after applying (8), it involves a term of the form  $\sum_{i=2}^{10} \hat{b}_i a_{i2}^2$ . Although a model is possible based on either (9) or (10) the analysis is far easier if (10) is true and for this model the following are satisfied

$$\begin{aligned} a_{54} &= \frac{c_5}{6}, \quad \hat{b}_i = b_i^* = b_i = 0, \quad i = 2, 3, 4, 6, \\ Q_{i1} &= Q_{i2} = 0, \quad i = 3, 4, \dots, s^*, \\ Q_{i3} &= a_{i2} = 0, \quad i = 5, 7, 8, \dots, s^*, \end{aligned} \quad (11)$$

and

$$\hat{R}_{0j} = 0, \quad j = 1, 2, \dots, s, \quad (12)$$

where

$$\hat{R}_{kj} = \sum_{i=j+1}^s \hat{b}_i c_i^k a_{ij} - \frac{\hat{b}_j (1 - c_j^{(k+1)})}{k+1}, \quad j = 1, 2, \dots, s, \quad k = 0, 1, \dots \quad (13)$$

and where  $c_9$  is restricted as follows

$$c_9 = \frac{35c_5c_6c_8 - 21(c_5c_6 + c_6c_8 + c_8c_5) + 14(c_5 + c_6 + c_8) - 10}{7(10c_5c_6c_8 - 5(c_5c_6 + c_6c_8 + c_8c_5) + 3(c_5 + c_6 + c_8) - 2)}$$

Note that  $\widehat{R}_{010} = 0$  implies  $c_{10} = 1$  leaving the remaining degrees of freedom as  $c_5$ ,  $c_6$  and  $c_8$ . Now since the higher order discrete process has been made to be order 7, implying that  $I_C$  and  $I_B$  are identical, the question arises as to how these remaining degrees of freedom should be chosen. It seems sensible to look for a small value of  $J^{(7)}$  with possibly a small value of  $A^{(8)}$ . The choice  $c_5 = \frac{1}{2}$ ,  $c_6 = \frac{3}{16}$  and  $c_8 = \frac{3}{5}$  implies  $c_9 = \frac{6}{7}$  and gives  $J^{(7)} \approx 7.18 \times 10^{-5}$  and  $A^{(8)} \approx 5.68 \times 10^{-5}$ . With regard to the error estimation process it is not possible to obtain a distinct embedded sixth order formula using the 11 stages. This is not a significant problem since the embedded formula is only used to monitor and predict step sizes. An embedded fifth order formula is easily obtained or alternatively a combination of lower order formulae is possible so that stretched estimation can be used. A triple utilising a fifth order embedded formula is given in Table 6 which contains only the non-zero entities.

It is interesting to compare this triple, as far as the cost is concerned, with the RK6(5)9FM of [6] which yields sixth order discrete approximations and error estimates in 9 evaluations per step (including the FSAL evaluation). A tenth evaluation per step is required when using the fifth order continuous process and a total of 12 evaluations per step are necessary if sixth order continuous approximations are required [1]. The RKT7(5)6 which requires 10 evaluations per step for seventh order discrete approximations and error estimates and requires the additional FSAL evaluation per step for sixth order continuous approximations would appear to be more cost effective.

Table 6: RKT7(5)6. Note that  $c_i = \sum_{j=1}^{i-1} a_{ij}$ ,  $b_i^*(\sigma) = \sum_{k=0}^5 B_{ik} \sigma^k$ ,  $i = 1, 2, \dots, 11$  and  $\widehat{b}_j = a_{11j}$ ,  $j = 1, 2, \dots, 10$ .

$i$	$j$	$Numerator(a_{ij})$	$Denominator(a_{ij})$	$i$	$j$	$Numerator(a_{ij})$	$Denominator(a_{ij})$
2	1	1	6	8	6	-14592	78125
3	1	1	16	8	7	33792	78125
3	2	3	16	9	1	51237	285719
4	1	1	4	9	3	4580136	2000033
4	2	-3	4	9	4	-419616	2000033
4	3	1	1	9	5	-2586870	2000033
5	1	1	12	9	6	-8901120	2000033
5	3	1	3	9	7	3840000	1294139
5	4	1	12	9	8	30234375	22000363
6	1	9	128	10	1	-1396	1647
6	2	135	1024	10	3	-19396	1281
6	3	-3	256	10	4	944	1281
6	4	-57	4096	10	5	105447	10675
6	5	45	4096	10	6	494336	19215
7	1	129	2048	10	7	-213085184	15852375
7	3	-117	1024	10	8	-2575625	380457
7	4	207	16384	10	9	530621	617625
7	5	-135	16384	11	1	179	3240
7	6	15	64	11	5	88	375
8	1	36	625	11	7	2097152	7239375
8	3	36	625	11	8	3125	21384
8	4	-288	15625	11	9	285719	1215000
8	5	4023	15625	11	10	61	1560

$i$	$k$	$Numerator(B_{ik})$	$Denominator(B_{ik})$	$i$	$k$	$Numerator(B_{ik})$	$Denominator(B_{ik})$
1	0	1	1	8	3	1559375	7128
1	1	-67	12	8	4	-59375	297
1	2	392	27	8	5	175000	2673
1	3	-4205	216	9	1	-16807	4500
1	4	587	45	9	2	16807	675
1	5	-280	81	9	3	-4823609	81000
5	1	-432	25	9	4	1025227	16875
5	2	528	5	9	5	-134456	6075
5	3	-5448	25	10	1	19764	302107
5	4	23696	125	10	2	-160857	604214
5	5	-896	15	10	3	-2003423	2416856
7	1	524288	53625	10	4	3669821	1510535
7	2	-3670016	96525	10	5	-1233176	906321
7	3	29360128	482625	11	1	45225	46478
7	4	-12058624	268125	11	2	-157380	23239
7	5	3670016	289575	11	3	844295	46478
8	1	3125	198	11	4	-485844	23239
8	2	-59375	594	11	5	198464	23239

$i$	1	3	4	5	6	7	8	9	10
$Numerator(b_i)$	575	1	1	-1	-128	45568	34625	31213	175
$Denominator(b_i)$	6912	2	40	5	225	96525	76032	172800	3328

## 2.5 Order 7

From Table 1 there are 85 equations of condition associated with a continuous process of order 7 and this section briefly outlines a solution of the equations with  $s^* = 14$ . The solution builds upon the analysis from the previous orders and assumes the FSAL conditions (2) together with the equations (8), (10) and (11). The first requirement of the solution is that either

$$c_9 = c_8 \quad \text{and} \quad a_{98} \neq 0 \quad \text{or} \quad a_{98} = 0 \quad \text{and} \quad c_9 \neq c_8$$

or

$$c_8 = c_3 \tag{14}$$

The analysis is greatly simplified by assuming (14) and this then leads to the following requirement that either (but not both)

$$c_{10} = c_9 \tag{15}$$

or

$$a_{109} = 0 \tag{16}$$

Following the model of order 6 it is possible using equation (12) to make the discrete formula of order 8. Having done that leaves the remaining degrees of freedom as  $c_3, c_6, c_9, c_{11}, c_{12}, a_{1413}$  ( $\widehat{b}_{13}$ ) and either  $a_{109}$  or  $c_{10}$  depending on whether equation (15) or equation (16) is imposed. It is not obvious as to how  $a_{1413}$  should best be selected so it has been chosen to zeroise  $\widehat{\tau}_1^{(9)}$  and it would seem to be more flexible to impose equation (16) and leave  $c_{10}$  free. This then permits the remaining free parameters to be chosen to give small values for  $J^{(8)}$  and  $A^{(9)}$ . Choosing  $c_3 = \frac{7}{50}, c_6 = \frac{19}{40}, c_9 = \frac{2}{25}, c_{10} = \frac{8}{15}, c_{11} = \frac{4}{5}$  and  $c_{12} = \frac{22}{25}$  gives  $J^{(8)} \approx 6.28 \times 10^{-6}$  and  $A^{(9)} \approx 4.48 \times 10^{-6}$ . Similar to the situation of the previous section it is not possible to obtain a distinct embedded seventh order formula using the 14 common stages but a sixth order formula is easily found or alternatively a combination of lower order formulae can be obtained so that stretched estimation may be employed. A triple utilising a sixth order embedded process can be found in Tables 7 and 8 which contain only the non-zero entities.

It is instructive to compare the cost of this triple with the RK8(7)13M of [13] and the RK8(6)12M of [5] (equivalently the DOP853 of [9]). The RK8(7)13M and RK8(6)12M use 13 and 12 stages respectively for discrete approximations and error estimation and then both use either an additional 4 or 7 stages (which includes the FSAL stage) for continuous approximation depending on whether  $q^* = 7$  or  $q^* = 8$  [1]. The RKT8(6)7 uses 13 stages for discrete estimation with the additional FSAL stage for seventh order continuous approximation and thus appears to be more cost effective.

Table 7: RKT8(6)7 which is continued in Table 8. Note that  $\widehat{b}_i = a_{14i}$ ,  
 $i = 1, 2, \dots, 13$  and  $b_i = a_{15i}$ ,  $c_i = \sum_{j=1}^{i-1} a_{ij}$ ,  $i = 1, 2, \dots, 14$ .

$i$	$j$	$a_{ij}$	$i$	$j$	$a_{ij}$
2	1	9.33333333333333333333333333333333E-2	11	7	-7.1579553906147432099663790337E0
3	1	3.5E-2	11	8	2.26593581547052770034800605954E0
3	2	1.05E-1	11	9	1.31756939077540917088647769884E1
4	1	1.4E-1	11	10	4.35147985890989745154013147945E0
4	2	-4.2E-1	12	1	2.13650273135026061952015557422E0
4	3	5.6E-1	12	3	1.22726517463837019805397194412E1
5	1	4.6666666666666666666666666666667E-2	12	4	4.57653009750266308294439689668E0
5	3	1.8666666666666666666666666666667E-1	12	5	-1.02693748349496721494231277368E1
5	4	4.666666666666666666666666666667E-2	12	6	-3.7629577005440390399992522631E-1
6	1	5.51743197278911564625850340136E-1	12	7	5.13017034156407434494186004831E0
6	2	-1.68355389030612244897959183674E0	12	8	9.62489338117485142433512784366E-2
6	3	1.28544855442176870748299319728E0	12	9	-1.03442766767566431388674762321E1
6	4	-1.02147251199586977648202137998E0	12	10	-2.59772774629732852847083885323E0
6	5	1.3428346506013119533527696793E0	12	11	2.55571177445599178571884809579E-1
7	1	6.24295812074829931972789115646E-2	13	1	-1.3576928555186849895417607979E0
7	3	1.1561591754239009036450401056E-1	13	3	-5.1848880697594401985846769119E0
7	4	-2.48173453254069484936831875607E-1	13	4	-9.44146275842569180247520769719E-1
7	5	4.76004820175838192419825072886E-1	13	5	5.7895230679047775815740126675E0
7	6	6.9123134328358208955223880597E-2	13	6	-8.78331322343203825844350417575E-2
8	1	5.31754385964912280701754385965E-2	13	7	-5.3269980917879320756691248069E0
8	3	1.07960199004975124378109452736E-1	13	8	-3.29419214246872762413611365341E0
8	4	-4.55448717948717948717948717949E-2	13	9	7.12498180803033672915227750425E0
8	5	2.13141025641025641025641025641E-2	13	10	4.23294185993291744523268528268E0
8	6	1.80954510721537509608660353975E-2	13	11	-4.04195634685480312241204160092E-1
8	7	-1.50003194428508726399201574995E-2	13	12	4.52499466462306516458275969143E-1
9	1	4.66308628714643752237737200143E-2	14	1	1.01794429109647960346134352579E-1
9	3	5.89926174413351732228314575591E-2	14	5	3.42368385444252768240392979897E-1
9	4	-3.85681391925321394464275175145E-2	14	7	-2.93579170210195254952533184107E-1
9	5	2.31207294594081206081229649243E-2	14	8	-9.95353542504925310796528261447E-2
9	6	1.33009364423326992630144289062E-2	14	9	2.07437934572206346408597479637E-1
9	7	-1.12383747568330718937876881162E-2	14	10	5.43021201240774613165496369804E-1
9	8	-1.22386322651751569775273657731E-2	14	11	1.07235531414217311653209089107E-1
10	1	5.44217687074829931972789115646E-2	14	12	1.44540738194287577003626386342E-1
10	3	5.40333156097836021965644146011E-1	14	13	3.8331290683984373526250270207E-2
10	4	1.13688418211922452259942034977E-1	15	1	-5.91293258004837089685158123242E-2
10	5	7.13352588752466984012721183007E-2	15	5	-1.14901053624678659268733720599E0
10	6	5.33742685221169022273976869374E-3	15	7	3.77974861322618360761792589719E0
10	7	1.41741045931070379958169549861E-1	15	8	7.48570483449616205367366755746E-1
10	8	-3.93523741342436902671713196074E-1	15	9	1.74577267785426015996335159381E-2
11	1	-2.5940248582906658528380592843E0	15	10	-3.00845790812659142174173541204E0
11	3	-1.77182396161676339315977974886E1	15	11	9.70820946719519308812662261486E-1
11	4	-7.20291569558395826074056304001E0	15	12	-4.0E-1
11	5	1.49881506312855377166637034571E1	15	13	1.0E-1
11	6	6.91875347236946677726180862128E-1			

Table 8: Continuation of the RKT8(6)7 from Table 7. Note that  $b_i^*(\sigma) = \sum_{k=0}^6 B_{ik} \sigma^k$ ,  $i = 1, 2, \dots, 14$ .

$i$	$k$	$B_{ik}$	$i$	$k$	$B_{ik}$
1	0	1.0E0	10	1	9.65701535222266902447206365602E-1
1	1	-1.41239093743887554093438640359E1	10	2	1.29274299904241623819239369537E1
1	2	8.4016766195696458031461586846E1	10	3	-1.00480323438077279181257364969E2
1	3	-2.51083997467010984848468599308E2	10	4	2.45834235483979601485491021852E2
1	4	3.86512292414528095658571249453E2	10	5	-2.42964579882849927174983253853E2
1	5	-2.91148854238488538278621434142E2	10	6	8.42605575125419501995439500197E1
1	6	8.48378819125746896424356746212E1	11	1	8.35557991425411575752552757343E-2
5	1	5.10665844292158893795819184009E0	11	2	-3.81989088470777655385269085515E-1
5	2	-4.00124279090280806878089311459E1	11	3	1.70967961712293483156233961215E0
5	3	1.84440467426588995836723836551E2	11	4	-5.28883927213581506454906269727E0
5	4	-3.78973592698221239000827838379E2	11	5	7.30946577097275164964837014524E0
5	5	3.41538781236289637930611683348E2	11	6	-3.32463729521741760719842416123E0
5	6	-1.11757518113106650248416549234E2	12	1	-6.33380888284421342020961449909E-2
7	1	-2.0751485626953971018794503634E0	12	2	-1.09526815610176510133599623253E0
7	2	-9.92180312887292232371883540967E0	12	3	8.61906649612399098614496017804E0
7	3	9.25598164917894535323732388042E1	12	4	-2.30612339267248796358151679261E1
7	4	-2.15979497620388810544292166846E2	12	5	2.59748166009870704285753056776E1
7	5	2.02287446902906568511069478446E2	12	6	-1.02295021872616869663633791656E1
7	6	-6.71643932529490873285047978155E1	13	1	-2.84608939125612693786991431373E-1
8	1	-2.14183863541985721594046947605E1	13	2	4.29888914910786433803628796472E-3
8	2	2.2543825665248598292363025894E2	13	3	5.20337256488446600050553460014E0
8	3	-8.84829314979143198157611115581E2	13	4	-1.46885666621411381932249338734E1
8	4	1.57460856803292263565777875922E3	13	5	1.54411838034484010111998278429E1
8	5	-1.29008703344712019545777930343E3	13	6	-5.63734836553123961550522315598E0
8	6	3.96188374740802854662306442791E2	14	1	2.91422009445041363278596489354E-1
9	1	3.15180535325053411373578467654E1	14	2	4.38587473682482536753098062593E-1
9	2	-2.71413850918964647969857885217E2	14	3	-8.48742089186228431556770654766E0
9	3	9.52348654179583905315594876659E2	14	4	2.37789877586610534396939312211E1
9	4	-1.59274235351047950380282579202E3	14	5	-2.63071727836903908960901174964E1
9	5	1.25795594603754462227636944346E3	14	6	1.0285596433764097871932198271E1
9	6	-3.7745901138561751061022989217E2			



## 2.6 Order 8

From Table 1 there are 200 equations associated with a process of order 8 and the value of  $C_8$  is not precisely known. This section briefly outlines a solution of the equations with  $s^* = 18$ . The solution builds upon the analysis from the previous orders and assumes the FSAL conditions (2) together with the equations (8), (10), (11), (14) and (16). A significant requirement for the continuous process to be of order 8 is either

$$a_{1110} = 0 \quad \text{or} \quad c_{12} = c_{11} \quad \text{and} \quad a_{1211} \neq 0$$

or

$$a_{1211} = 0 \quad \text{and} \quad c_{12} \neq c_{11} \tag{17}$$

The easiest way forward is to impose equation (17) and at this stage the continuous process is of order 8. There are still a large number of degrees of freedom available and it is possible using equation (12) to make the discrete formula of order 9. In fact considering the discrete formula in isolation it is possible, Hairer [8], to make it order 10 by zeroising certain of the  $\widehat{R}_{1j}$  from equation (13). Unfortunately this violates the requirement from equation (5) meaning that the continuous process cannot be of order 8. So having made the discrete process of order 9 the remaining free parameters are chosen to give small values for  $J^{(9)} (\approx 1.97 \times 10^{-6})$  and  $A^{(10)} (\approx 3.59 \times 10^{-9})$ . The resulting triple utilising a seventh order embedded process can be found in Tables 9 and 10 which contain only the non-zero entities.

Table 9: RKT9(7)8 which is continued in Table 10. Note that  $\hat{b}_i = a_{18i}$ ,  
 $i = 1, 2, \dots, 17$  and  $c_i = \sum_{j=1}^{i-1} a_{ij}$ ,  $i = 1, 2, \dots, 18$ .

$i$	$j$	$a_{ij}$	$i$	$j$	$a_{ij}$
2	1	1.03703703703703703703703703704E-1	13	11	1.11825158329569318169361499236E-4
3	1	3.88888888888888888888888888889E-2	13	12	5.9232826064386410109019245474E-2
3	2	1.1666666666666666666666666667E-1	14	1	-1.08294884409577446575423573542E1
4	1	1.5555555555555555555555555556E-1	14	3	-4.58555384056239216218818778683E1
4	2	-4.6666666666666666666666666667E-1	14	4	-1.32193447471870660838992789085E1
4	3	6.2222222222222222222222222222E-1	14	5	3.05914618343960445376558308999E1
5	1	5.18518518518518518518518518519E-2	14	6	1.90922815696523943781555810831E-1
5	3	2.0740740740740740740740740740E-1	14	7	-1.88814404888067339077866227303E0
5	4	5.18518518518518518518518518519E-2	14	8	2.120320047452681450999642799E1
6	1	1.43904006046863189720332577476E0	14	9	1.58374092516843429808128896804E0
6	2	-4.29081632653061224489795918367E0	14	10	1.01434070966925954939865647766E1
6	3	2.79697656840513983371126228269E0	14	11	-3.75623558814887119657201098616E-1
6	4	-3.79589677140697548860814166937E0	14	12	-8.5871515129714592091127087542E0
6	5	4.49514091350826044703595724004E0	14	13	1.75314464568442281881693067004E1
7	1	1.15627362055933484504913076342E-1	15	1	1.23847409176679080375217053279E0
7	3	-4.18968597540026111454682883254E-2	15	3	1.09333898278372589827844780651E0
7	4	-1.02048779829392074290033473707E0	15	4	3.31536159352838127791365049203E-1
7	5	1.48135325558794946550048590865E0	15	5	-2.09936149938613061202956506086E0
7	6	1.09848484848484848484848484849E-1	15	6	-6.32995160818675610148594925667E-3
8	1	6.01213282247765006385696040869E-2	15	7	8.53402652892084128305708186158E-2
8	3	1.16077441077441077441077441078E-1	15	8	-7.13566595489746263585587501118E-2
8	4	-4.0833333333333333333333333333E-2	15	9	-2.39880075764678496228135351925E-2
8	5	1.87962962962962962962962962963E-2	15	10	-1.65181846577159146362072750765E0
8	6	7.59713798041186071308940908624E-3	15	11	6.245576312291875410038570643E-3
8	7	-6.20331469003684620014386165793E-3	15	12	1.58274616357353025449630677489E0
9	1	7.51874092848346235045742434905E-2	15	13	1.41814358816879890444609368724E-1
9	3	3.08577739962730314518376303984E0	15	14	9.34364104078509623504023164074E-3
9	4	1.0277024339893729511937200674E0	16	1	-1.72854883427149906480834787355E1
9	5	-7.05175775924447499201004659796E-1	16	3	-8.51259795469259804679437273731E0
9	6	-2.78778538145998406742566524436E-2	16	4	-2.80551782495675369923611987322E0
9	7	2.85805153481527740360777028619E-1	16	5	3.51919004458313930717487691522E1
9	8	-2.99148657605355546429322500644E0	16	6	7.36701829077372132621075400047E-2
10	1	1.785480471498944405348346233505E-2	16	7	-1.2458454706806936083664523748E0
10	3	5.16426091974317668823733047791E-3	16	8	6.34431710970183708662917963423E-1
10	4	-3.43681317296491684696604004926E-3	16	9	-2.99382194728825930237778575253E0
10	5	2.32372133623022296941501964109E-3	16	10	2.58384480400235896878583385841E1
10	6	5.14201281710644115584844336227E-4	16	11	7.60451062344283617975442262104E-1
10	7	-4.33506924343872955710236185757E-4	16	12	-2.72531371870126046405092063507E1
10	8	-1.98666815536469802404438057068E-3	16	13	-7.66905838615669874875007702991E0
11	1	-1.18757288815909505564677978471E0	16	14	-4.30717080246156504921654666097E-2
11	3	1.13239724969350324395658487817E-1	16	15	6.242970712783360378435415972E0
11	4	4.15212324887617856117414455329E-2	17	1	2.38352607101136790911153507492E1
11	5	6.55529796136042083177053423077E-1	17	3	7.7738756188986200797865735259E0
11	6	-1.43685337376884729223927086404E-3	17	4	2.57266456224187218683628421487E0
11	7	5.0120866241769657823310092071E-3	17	5	-4.27301289332539628209504430154E1
11	8	-7.07903479324387044990828600376E-1	17	6	-6.84309506233548912384135730021E-2
11	9	2.87573843923931191319441255834E-1	17	7	1.30451149660509620846896301402E0
11	10	1.66070320338165526431028870115E0	17	8	3.34387872500134107823468680391E0
12	1	2.9326637612934925469041347559E-2	17	9	2.90875579291685107583165783656E0
12	3	2.27648379357749274981640086384E-1	17	10	-3.51867845271413839756884852364E1
12	4	6.42188982905375335427504387651E-2	17	11	-3.99562978143036844261012184204E-1
12	5	4.54015730358590118030630636463E-2	17	12	3.35175018689652853293607378584E1
12	6	-7.94683657147007110737301019097E-4	17	13	9.93231523768212904432842366324E0
12	7	2.4861235148309752048563545005E-3	17	14	8.37781070877954481643354905414E-2
12	8	-3.8188748663301078106113860815E-2	17	15	-5.98649811509162584079618360502E0
12	9	-6.35233112974332282906394142683E-4	17	16	9.88633847406948308075244574403E-2
12	10	3.05370536215106964984062651216E-2	18	1	3.07799270475412360737919532866E-2
13	1	-6.0881392683555120739135947005E-2	18	8	9.27611792928056326667152622109E-2
13	3	-4.43438802229705377088167804351E-3	18	9	1.22968704959599330688571533231E-2
13	4	4.85920262412870550959705396755E-2	18	11	1.54432519665121535509579924022E-1
13	5	-1.23883926446739678566391896451E-1	18	12	2.62981836369090817847088871306E1
13	6	-5.40541062978150844511169211286E-3	18	13	1.08761305196919820431285749084E-1
13	7	2.22380334943109355360348696484E-3	18	14	5.88466616840491098220532404464E-3
13	8	3.9784387690238541442182630348E-2	18	15	2.6027080199888572877897873278E-1
13	9	4.00102754975348157308270345129E-4	18	16	4.29012449776118791099335675107E-2
13	10	1.39498241761820581940505774544E-1	18	17	2.89296487876585055315634624318E-2

Table 10: Continuation of the RKT9(7)8 from Table 9. Note that  $b_i^*(\sigma) = \sum_{k=0}^7 B_{ik}\sigma^k$ ,  $i = 1, 2, \dots, 18$ .

$i$	$b_i$	$i$	$b_i$
1	-1.27690537577646353299981537083E-1	12	1.18421357803228938463464105438E0
5	-9.5E-1	13	-1.52346033048153512791475335877E-1
7	2.5E-2	14	2.79212408462991738161601055159E-2
8	4.20967933030044959322296039676E-1	15	-2.13862748653591616107674163303E-1
9	4.73337930270267175222242790533E-1	16	5.43489879984277053495778555136E-2
10	2.5E-1	17	5.12952095724889595292725269046E-2
11	-4.31855604704258756750593362625E-2		

$i$	$k$	$B_{ik}$	$i$	$k$	$B_{ik}$
1	0	1.0E0	12	1	1.15334997254946792039603096315E1
1	1	-2.77735116893550678899410577323E1	12	2	-1.18814083869203384405600072643E2
1	2	2.5165978861779362829892054496E2	12	3	3.08134567500691900387880121103E2
1	3	-1.08626391924281399602886402221E3	12	4	2.33436352026189303075135007582E1
1	4	2.53356539924885542940296045855E3	12	5	-9.66772385163294883072158319407E2
1	5	-3.24230250171399947308061311167E3	12	6	1.15794887039996694701727086852E3
1	6	2.13055284911623123780143489376E3	12	7	-4.15111121959905098621019319093E2
1	7	-5.60407324409664217267823913703E2	13	1	2.15636542120343295525422617798E0
5	1	-1.18697364879199052960842505705E1	13	2	2.23094376381637869726414340883E1
5	2	1.02459915482709922665427835603E2	13	3	-2.14860691636078809627896996708E2
5	3	-1.16095838290346893556824162957E2	13	4	6.77621572331989459966523793888E2
5	4	-6.70639976556572401329871695175E2	13	5	-1.0140266973350173253494403702E3
5	5	1.94483721571669034924983554886E3	13	6	7.31016153941917335279615104043E2
5	6	-1.85445230708830610183339303496E3	13	7	-2.04107379056980960376265905544E2
5	7	6.057607272237450301009097592E2	14	1	5.08899586642482571660412314383E-2
7	1	2.65383553931689365018564794762E-1	14	2	-7.42202087910459104358965739767E-1
7	2	-3.84957223533893082531676747188E0	14	3	4.42595830228471928946003912407E0
7	3	1.98583488086398818369789716893E1	14	4	-1.24465247279828531500574820871E1
7	4	-4.89425851614840465067296601841E1	14	5	1.80205784909925668387118635985E1
7	5	6.25680078034413170103241113952E1	14	6	-1.29526679902614061184352135296E1
7	6	-4.00860955038855039119026804046E1	14	7	3.64985272038158889849592272644E0
7	7	1.01865127346955930316274601813E1	15	1	-4.43001472145292266932794194954E0
8	1	4.10881688594931446561283260961E-1	15	2	6.21578560270965455283632655849E1
8	2	3.12020001032662815102399649694E1	15	3	-3.07676880364428105577295947394E2
8	3	-2.49707701312674989659598434886E2	15	4	7.15128713595346851864396276583E2
8	4	7.78195589210511825395485214743E2	15	5	-8.41901562801894856570402038232E2
8	5	-1.17201077920519207960027474654E3	15	6	4.86997480884687474061182189924E2
8	6	8.50532394815990090483253786076E2	15	7	-1.10015321817356100908136825784E2
8	7	-2.38529624121203253943000352364E2	16	1	6.39746391350199829505667086882E-1
9	1	4.14906689983933914089354123183E0	16	2	-8.92447331136320993314728274381E0
9	2	-6.0201083012212029122532262984E1	16	3	4.39375977273632452580211911017E1
9	3	3.1340256450693611124013315901E2	16	4	-1.00055397522875981592003636938E2
9	4	-7.81911886672181247720231054571E2	16	5	1.13223500868691469540904428159E2
9	5	1.01249775080717639184821281449E3	16	6	-6.09041019096722296163008301721E1
9	6	-6.56660710999561695264414176554E2	16	7	1.21260290014841183921303970742E1
9	7	1.6873659534049908981100683653E2	17	1	-3.42936518565914843445423340005E-2
10	1	2.70087958974258880514796095306E1	17	2	1.02263992789510082522682584494E0
10	2	-3.08300187466966862891517091984E2	17	3	-7.67553082732108617644153808883E0
10	3	1.4465177948042279851428814073E3	17	4	2.8768270773488980917298956223E1
10	4	-3.51700174110387571456172732356E3	17	5	-5.45304700130068082381237392245E1
10	5	4.60841657049002751224578802649E3	17	6	4.87822504767962797310095764161E1
10	6	-3.07258687363984008871483884247E3	17	7	-1.63039370372082342435249147736E1
10	7	8.15911656342806467356527481271E2	18	1	4.5079310103374101284304267947E-2
11	1	-2.15215229602329501142575462752E0	18	2	-1.39971037232777581505134835254E0
11	2	3.14196745583973862967039208679E1	18	3	1.12995963892492747523307993272E1
11	3	-1.6532985104192405065217131984E2	18	4	-4.40393736681488335868754595851E1
11	4	4.18414305050309583418887171955E2	18	5	8.56383538309449928529333409909E1
11	5	-5.53657581775559173675697808708E2	18	6	-7.86288962134219494870125843802E1
11	6	3.70441653709359610572530943729E2	18	7	2.70849507236009171823909477318E1
11	7	-9.89816156848949394133175734526E1			

## 2.7 Order 9

From Table 1 there are 486 equations associated with a process of order 9 and the value of  $C_9$  is not precisely known. This section briefly outlines a solution of the equations with  $s^* = 22$ . The solution builds upon the analysis from the previous orders and assumes the FSAL conditions (2) together with the equations (8), (10), (11), (14), (16), (17) and the following additional requirements

$$b_5^* = b_7^* = b_{10}^* = Q_{i4} = 0, \quad i = 8, 9, 11, \dots, s^*, \quad (18)$$

which imply  $c_6 = 7c_3/15$ ,  $c_9 = 7c_3/3$  and  $c_{10}$  is restricted as follows

$$c_{10} = \frac{8pc_3(329c_3^2 - 175sc_3 + 109p)}{4557c_3^4 - 3878sc_3^3 + (553s^2 + 3034p)c_3^2 - 790spc_3 + 237p^2}$$

$$\text{where } s = c_{11} + c_{12} \quad \text{and} \quad p = c_{11}c_{12}.$$

It is now possible by imposing equation (12) to make the discrete formula of order 10 but not of order 11 without violating equation (5). The remaining degrees of freedom ( $c_3, c_i, i = 11, 12, \dots, 20$ ) can now be chosen to give small values for  $J^{(10)} (\approx 2.86 \times 10^{-7})$  and  $A^{(11)} (\approx 7.32 \times 10^{-9})$ . The resulting triple utilising an eighth order embedded process can be found in Tables 11, 12 and 13 which contain only the non-zero entities.

Table 11: RKT10(8)9 which is continued in Table 12. Note that  $\hat{b}_i = a_{22i}$ ,

$i = 1, 2, \dots, 21$  and  $c_i = \sum_{j=1}^{i-1} a_{ij}$ ,  $i = 1, 2, \dots, 22$ .

$i$	$j$	$a_{ij}$	$i$	$j$	$a_{ij}$
2	1	1.71428571428571428571428571429E-1	14	4	7.61153218749380388515161951786E-3
3	1	6.42857142857142857142857142857E-2	14	5	-1.41394031054949048041621789167E-2
3	2	1.92857142857142857142857142857E-1	14	6	-1.7095555323508155354294620146E-1
4	1	2.57142857142857142857142857143E-1	14	7	5.30514733461304180522911933357E-1
4	2	-7.71428571428571428571428571429E-1	14	8	-5.11031289248798174898569773741E-2
4	3	1.02857142857142857142857142857E0	14	9	9.400854146796907519751117567394E-3
5	1	8.57142857142857142857142857143E-2	14	10	-4.52042349903216396534832819473E-2
5	3	3.42857142857142857142857142857E-1	14	11	-9.9578622937639938106967691848E-3
5	4	8.57142857142857142857142857143E-2	14	12	-2.21770771247996610673849359841E-1
6	1	6.80444444444444444444444445E-2	14	13	6.09529832932070843559292477197E-3
6	2	6.44E-2	15	1	2.71722196517267073721919988737E-2
6	3	-9.955555555555555555555555555E-3	15	3	3.36111714500765050195471053533E-3
6	4	-1.393777777777777777777777777E-2	15	4	2.92271056087621782778670481333E-4
6	5	1.144888888888888888888888889E-2	15	5	-9.10415966436935539116562416401E-4
7	1	4.708888888888888888888888889E-2	15	6	-6.56442866656426475295926935115E-3
7	3	-1.442777777777777777777777777E-2	15	7	3.30757277239804600985460593148E-2
7	4	3.593333333333333333333333333E-3	15	8	7.24437088394392664852811821195E-2
7	5	-2.5044444444444444444444444E-3	15	9	-9.5131112062075069280861431775E-4
7	6	8.625E-2	15	10	-1.02426896941633891961563238252E-1
8	1	3.82653061224489795918367346939E-2	15	11	1.60643797941239012292483444089E-3
8	3	5.08928571428571428571428571429E-2	15	12	-5.51368718332946785146311721738E-3
8	4	4.42546583850931677018633540373E-3	15	13	-9.96109320699920624283449061858E-4
8	5	-4.89130434782608695652173913044E-3	15	14	1.94113668036311350585167948512E-2
8	6	-9.93962768742387584253253016032E-2	16	1	2.53806341201199324666315214607E-2
8	7	2.67846809261106549019823970636E-1	16	3	3.7531000076108783558977100526E-1
9	1	5.277777777777777777777777777E-2	16	4	3.26356522400945943991105221965E-2
9	3	7.77139450056116722783389450056E-1	16	5	5.26325269986361373786615121734E-2
9	4	6.75773434831405845898599521788E-2	16	6	-7.32999065951547844478691298224E-1
9	5	1.39548260381593714927048260382E-1	16	7	9.67678996523823578769532202087E-1
9	6	-1.51779193160336827633614023028E0	16	8	2.15791589050093115948614702104E-1
9	7	1.6196941055164117545970097955E0	16	9	3.67553527064403441681259310579E-2
9	8	-5.38945005611672278338945005612E-1	16	10	-1.81530947002862058971722916931E-1
10	1	3.88353461879046773963440614956E-2	16	11	-4.09922890594496687340524305813E-2
10	3	4.79464320723202865567932468526E-2	16	12	2.15236785669238150386436039164E-1
10	4	4.5769292181296043927159035332E-3	16	13	2.2953702084828654883891671399E-2
10	5	-4.88880091474728780149720288497E-3	16	14	-4.55519604807169438472975127833E-1
10	6	-8.87583529719000069454414466987E-2	17	1	1.51078938700081213900635874424E-3
10	7	2.54437297141552907740401224724E-1	17	3	7.53566292007116950326864746808E-1
10	8	-1.83774831423237984479567378777E-2	17	4	6.55275036527927782892925866789E-2
11	1	-6.66675065650641000724509489908E-2	17	5	8.46747951362504290540732821269E-2
11	3	-1.05367308433973749664957424838E0	17	6	-1.47175238350604897998910257348E0
11	4	-9.16237464643249997086586302935E-2	17	7	2.1544076679551517246754174083E0
11	5	-2.43751186211772783274461089616E-1	17	8	-2.95817130713649583710180908561E-1
11	6	2.05787584949265887766230841109E0	17	9	1.4110855729595437212721604452E-1
11	7	-1.1231886312992026938265345702E0	17	10	9.93363998637091884807695896669E-4
11	8	6.08712534525018370495459105367E0	17	11	-9.49402391923509994190801602882E-2
11	9	4.3459596156342027900897900295E-1	17	12	-4.09994248367412059381729023618E-1
11	10	-5.27847077920393856587197675801E0	17	13	5.17440541722880221140981310637E-2
12	1	3.87942523461117041377971875372E-2	17	14	-3.62816777296553733507007891428E-1
12	3	2.62854887215373583030498361145E-2	17	15	6.5360732511345784837404560211E-2
12	4	2.28569467143803115678694227083E-3	17	16	-1.83572977040522609441080256973E-1
12	5	-5.22163450008847739571621732795E-3	18	1	5.33868129054430002753837028879E-3
12	6	-5.13368645703417601208247348983E-2	18	3	1.47470382943225743303202666729E-1
12	7	1.85631908317522880760632258473E-1	18	4	1.28235115602804994176697971069E-2
12	8	1.20451382273352635107082214494E-1	18	5	-1.01268353155170256618697863596E-2
12	9	9.09566403893770608709777784378E-4	18	6	-2.88016979919787170816119555695E-1
12	10	-1.92799793663426142557517264448E-1	18	7	6.9824510039379039160059721042E-1
13	1	-6.12172589287871747048472015259E-3	18	8	-3.37974521430012528505134988237E-1
13	3	-2.35054787000214690914783867723E-1	18	9	2.86414411975806736110165973921E-1
13	4	-2.04395466956708426882420754542E-2	18	10	3.7131816347799479039918797965E-1
13	5	-4.82769557359166681354132197148E-2	18	11	-2.44811592512287236385020747211E-2
13	6	4.5907369684266375817327005265E-1	18	12	-3.4196135976548130845457690019E-1
13	7	-1.92474861837713007220976018487E-1	18	13	1.42807674655094881558598522546E-2
13	8	2.91535209036744365879418079661E0	18	14	-5.331526505770455656362956804E-2
13	9	2.53783494031343851135063073233E-1	18	15	7.7569789608923353488598800183E-2
13	10	-2.70463757085476242661593215442E0	18	16	-1.56043051859614787897656163996E-2
13	11	5.73922969626822774434055704329E-2	18	17	-6.42963423431277070352269767695E-3
13	12	2.71403896971420189855855610407E-1	19	1	2.14923549969032701447324062889E-1
14	1	3.86425821831108415990101575487E-2	19	3	-3.31284355637506491687356054727E-2
14	3	8.75326201561787446792436244553E-2	19	4	-2.88073352728266514510744395414E-3

Table 12: Continuation of the RKT10(8)9 from Table 11

$i$	$j$	$a_{ij}$	$i$	$j$	$a_{ij}$
19	5	-1.24468160743674116046379662049E-2	20	19	2.39771105500080177790811432148E0
19	6	6.47014795113952630750063665388E-2	21	1	4.13666331788568646314671459781E-2
19	7	5.14370598499741879276769473802E-3	21	3	-4.6085087722059010473154473953E-1
19	8	-1.43046105116307215521975907197E0	21	4	-4.00739893235295743244821512635E-2
19	9	2.8721437377474197463041334418E-2	21	5	-1.87482210748488705850730209348E-1
19	10	8.78687940562103891093510434214E-3	21	6	9.00064644855228349679196498542E-1
19	11	-1.57537511615043694291339630709E-1	21	7	6.00984146321174224002305454373E-1
19	12	1.58483196482085928507966531199E0	21	8	1.684608594095337611555270728E0
19	13	2.4923172103039147318147293828E-1	21	9	5.30003044813386314235741018963E0
19	14	-1.30642815150584000544713644415E0	21	10	-4.2080611537944712705604048092E0
19	15	-5.28959072870432651573430444804E-1	21	11	4.32979699798406374581760208508E0
19	16	1.00741207592023609430941633181E0	21	12	1.95388343086605943251642605032E0
19	17	-8.775590457123529971261338772E-1	21	13	-7.74274861680373310963503498563E0
19	18	1.99675911512324586842776245057E0	21	14	-3.13510062968838311211920910556E0
20	1	-2.97166149971555334413883837806E-2	21	15	-4.78663380485811935550439247685E-1
20	3	-3.93561746825012462479575933126E-1	21	16	-6.03141603406035774837148626753E0
20	4	-3.42227605934793445634413854892E-2	21	17	1.35672452470896311806863413262E0
20	5	-1.58696967693592826136419752921E-1	21	18	4.36880260572859992367639746079E0
20	6	7.68645632229322013542244960244E-1	21	19	2.75280494424400909789700873245E0
20	7	4.96090687123684429260132170967E-1	21	20	-4.67007799087175905838696203928E-3
20	8	1.92649797393520230726050104946E0	22	1	3.92740785119914854000268988182E-2
20	9	4.46513079425448299443002782977E0	22	12	4.68444158055361823794214145044E-1
20	10	-3.58323257191568143688861876877E0	22	13	-2.3636350361826723946475816494E-2
20	11	3.7003765504475496211886812753E0	22	14	-4.1001974032294058576898297272E-1
20	12	1.24038802088878265649236798944E0	22	15	-2.97256966740860193040952924122E-2
20	13	-6.61304590135240072826990058323E0	22	16	5.76476584209117916904648266301E-1
20	14	-2.32192461516956715430435503205E0	22	17	-3.20051029759055386286764973125E-1
20	15	-2.08786912217290485002957585106E-1	22	18	3.73265122088390393431398983892E-1
20	16	-5.1100351397439630950486041015E0	22	19	2.46074190640257467948091174643E-1
20	17	1.25420454344261812247625210394E0	22	20	4.88504071988586166889784770355E-1
20	18	3.20027172318569914357693982537E0	22	21	-4.08605388375796539061845184294E-1

$i$	$b_i$	$i$	$b_i$
1	1.6923713048071774678167962342E-1	15	-4.11056665125909373103182261953E-1
8	-5.5E-1	16	4.20137072018899352803788919616E-1
9	2.0E-1	17	-4.07267073390825120527856167596E-1
11	1.0E-1	18	1.14415870529411131962321567601E0
12	1.49788508979634065630064615597E0	19	3.00298070359876651423408830867E-1
13	-2.12348185097986841873295284576E-1	20	4.99331001586965891752992972611E-1
14	-1.33059869039202370169631358297E0	21	-4.197764555301665814850848814E-1

Table 13: Continuation of the RKT10(8)9 from Tables 11 and 12. Note that

$$b_i^*(\sigma) = \sum_{k=0}^8 B_{ik} \sigma^k, \quad i = 1, 2, \dots, 22.$$

$i$	$k$	$B_{ik}$	$i$	$k$	$B_{ik}$
1	0	1.0E0	15	5	7.16249850677466769812869812474E3
1	1	-2.06297782812448935889003344791E1	15	6	-6.09824643516338291055945318713E3
1	2	1.99970176048388561019274681466E2	15	7	2.81520634280299703935993919373E3
1	3	-9.22654837092107700126634271173E2	15	8	-5.4824113126420653773851264253E2
1	4	2.31222312792268813253542444857E3	16	1	-3.01648978960918371803963335019E0
1	5	-3.36805982998121579505655492833E3	16	2	5.87536701899315845616874210878E1
1	6	2.86779930979446876870346996672E3	16	3	-5.55607498535208412476473482541E2
1	7	-1.33009659749051336937054709224E3	16	4	2.39215015269716575399237428541E3
1	8	2.60487703158048287369867556359E2	16	5	-5.1369584299446201649980782042E3
8	1	-4.5861545909972734840606542538E0	16	6	5.82660273225751977620329263459E3
8	2	-3.43246388036553518122971208411E1	16	7	-3.35911159614824317109118564421E3
8	3	3.09486850078952618787463125081E2	16	8	7.77763935857272935443327217475E2
8	4	-6.14802040674386044371724189846E2	17	1	-1.56065665159331057732607100341E0
8	5	1.7310803832386438983509630622E2	17	2	1.39173777524727035508035241556E1
8	6	6.59677271084104987273220731019E2	17	3	-1.33437194028282508797164633795E2
8	7	-6.88853829878109035239941941896E2	17	4	6.73365409739643774512539517957E2
8	8	2.00294504460225709012243744517E2	17	5	-1.67196796583630511285236447147E3
9	1	3.47732466883096028887251751081E0	17	6	2.11584335238948234994960839082E3
9	2	-5.92490712105459256032488058304E1	17	7	-1.31751860530872646114657780275E3
9	3	5.68658548319989900493945781598E2	17	8	3.21038230913549509974194781111E2
9	4	-2.56306468722100318797831395987E3	18	1	9.34193888791873862812244205862E0
9	5	5.80470372175372051326344179587E3	18	2	-3.87753944045788759746877558967E1
9	6	-6.91311865221701067191638950388E3	18	3	3.33501822703837688986890042108E2
9	7	4.15224530103838188508336576403E3	18	4	-1.89106977539173495698057758062E3
9	8	-9.93652485132363473631673589432E2	18	5	4.82013028954164025673410278997E3
11	1	1.34663686046235080290387565235E0	18	6	-6.02334485547518422386023637806E3
11	2	-2.58804873304224303664083918462E1	18	7	3.65368701068403665949817652999E3
11	3	2.48212680978950604447262596116E2	18	8	-8.63097771423846896638358690559E2
11	4	-1.11476732055076869932396566606E3	19	1	-1.91132340938196948061289881587E-1
11	5	2.54147893462516058275681867833E3	19	2	1.94583814910815996810661656457E0
11	6	-3.06590343710225795141536267335E3	19	3	-1.91764522790416307850488506448E1
11	7	1.8712324135966540561979422169E3	19	4	8.24223992823041297141088673633E1
11	8	-4.5571942107778513099190635734E2	19	5	-1.73932819187320347159046403168E2
12	1	-1.09848345718521052705684043776E-1	19	6	1.95129106419493159569653996863E2
12	2	2.37545383059934117890189125521E2	19	7	-1.10389525803352906554037850095E2
12	3	-1.48031852859346556766872317475E3	19	8	2.44386599503878896622730041735E1
12	4	3.73732991166234759962890853683E3	20	1	2.83986897250454500650248073256E0
12	5	-4.84230983703745358888134561558E3	20	2	-4.91430010822156343410779466753E1
12	6	3.38228426572331858440361176138E3	20	3	4.85603254086018436823082501704E2
12	7	-1.20565338653341576589325198712E3	20	4	-2.27195016307781611626194920667E3
12	8	1.71700484222508503397111251905E2	20	5	5.4589650068104898255990085068E3
13	1	-1.70630269533425952944445664144E0	20	6	-7.02973017700117520597832555491E3
13	2	3.34627541102967460124100531515E1	20	7	4.6217251757857124825948112538E3
13	3	-3.23243454145416293380601322224E2	20	8	-1.21782146042152974727521459389E3
13	4	1.47881306032917864920140996938E3	21	1	-2.5831753725099044992882722222E0
13	5	-3.44623375671007767107644058027E3	21	2	4.50229147599410572355643033391E1
13	6	4.24829425145108678784311765986E3	21	3	-4.42245832045825204341093428442E2
13	7	-2.64596733630927079224341425009E3	21	4	2.05450590783890414371356509087E3
13	8	6.56557147619175006449016451009E2	21	5	-4.90444245053620048359003799753E3
14	1	-7.78853771367157794303769750711E0	21	6	6.27850727502860920633477140288E3
14	2	-2.270812790575367409073485668E1	21	7	-4.1062143790225666958181465556E3
14	3	8.0907933972872291769019776807E1	21	8	1.07704113396127208442560361151E3
14	4	4.9470615417990074607218275683E2	22	1	-9.50046718078759926599527956E-2
14	5	-2.16269478733290895408424222346E3	22	2	1.36456304182752713536970146404E0
14	6	3.18669482783876005542919399735E3	22	3	-1.62187843007174977273779256203E1
14	7	-2.08159122651751575390515006417E3	22	4	9.12757176743336247657360025741E1
14	8	5.12063743733578988759117126981E2	22	5	-2.54284621263441148619108121807E2
15	1	2.52613110637084026071227727079E1	22	6	3.69511164972167288019826755834E2
15	2	-3.6190195637472856518495054898E2	22	7	-2.68699760896068171471981770269E2
15	3	1.8665314908750283365875710649E3	22	8	7.71467254437062538901953531036E1
15	4	-4.86113785441075754921971887272E3			

### 3 Numerical Testing and Comparisons

A representative sample of problem equations taken from the DETEST suite [10] and from those used by Hairer et al. [9] was used for the testing of the various triples. Standard parameters were used for all the triples involved and relative error per step was monitored for a range of tolerances between  $10^{-3}$  and  $10^{-14}$ . For those problems where the true solution was known  $M$ ,  $M^*$  and  $M_E$  were computed where  $M$  is the maximum absolute value of  $\epsilon_n$  over all equation components and all integration steps,  $M^*$  is the maximum absolute value of  $\epsilon_{n+\sigma}$  over all equation components and over 100 equally spaced points within each step interval  $[x_n, x_{n+1}]$  and  $M_E$  is the maximum absolute value of the discrete global error,  $\epsilon(x = x_{end})$ , over all equation components at the integration end point. Efficiency plots of  $\log_{10}M/M^*/M_E$  against function evaluations could then be considered. If the true solution was not available approximate values of the global errors were obtained by solving the equation system with a higher order RK process with suitable tolerance and quadruple precision arithmetic.

For the triples of order 3 the practical tests over a wide range of problems confirm, as expected from the sizes of the  $A^{(4)}$  values, that there is little to choose between the RKT3(2)3 and the corresponding triple of Owren and Zennaro (RK3(2)OZ) except where the absence of the endpoint evaluation in the error estimation process is significant. To demonstrate this situation consideration is given to the EULR problem of [9] with a modified exterior function of  $(1/4)\cos^2x\sin x$  instead of  $(1/4)\sin^2x$ . Figure 1 shows the plots of  $\log_{10}M_E$  ( $x_{end} = 20$ ) against function evaluations.

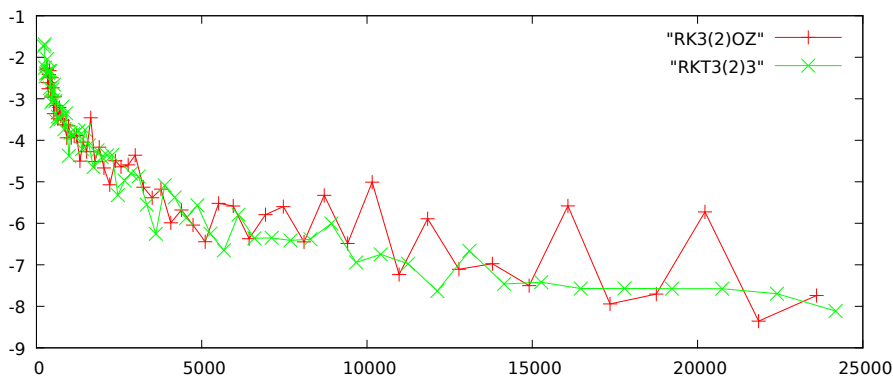


Figure 1: Modified EULR problem -  $\log_{10}M_E$  against Function Evaluations.



For the triples of order 4 the practical tests show that, as expected from the sizes of the  $A^{(5)}$  values, the RKT4(3)4 generally gives significantly better results when considering  $M$ ,  $M^*$  or  $M_E$  than the corresponding Owren and Zennaro triple (RK4(3)OZ). Typical situations are the solution of DETEST problems D3 and A4 [10] and the AREN and BRUS problems of [9] as seen in Figures 2 to 5. Problem A4 was chosen since this does show significant differences between plots using  $M$  and  $M^*$  for each of the two triples. On many problems there is no significant difference between the  $M$  and  $M^*$  plots for the same triple. As expected the RK4(3)OZ gives similar poor results to the RK3(2)OZ on the modified EULR problem because of the absence of the endpoint evaluation in the error estimation process.

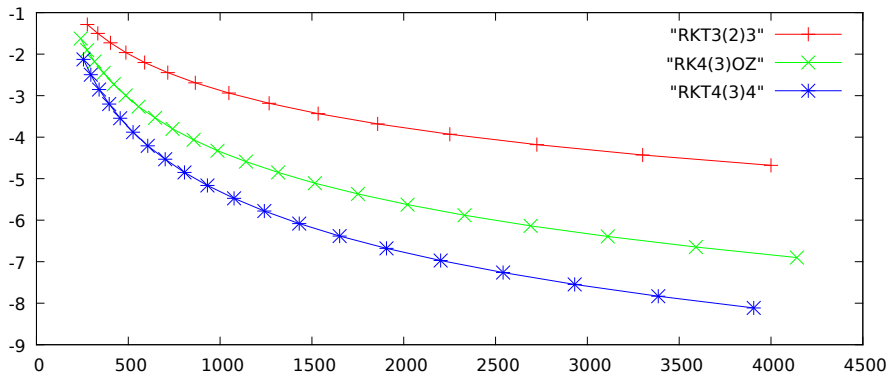


Figure 2: DETEST Problem D3 -  $\log_{10}M$  against Function Evaluations.

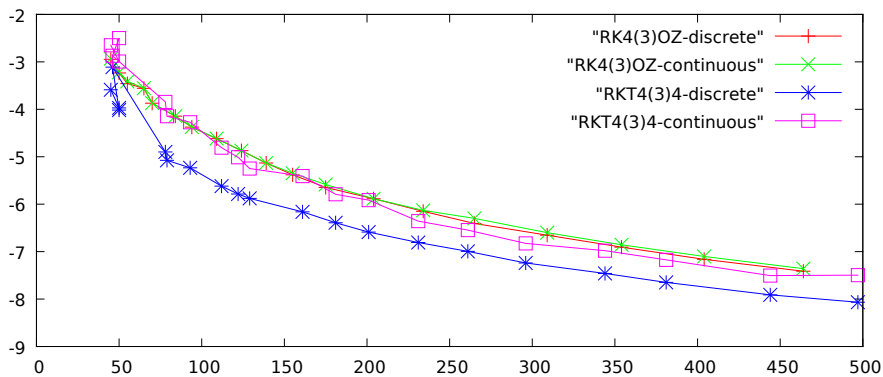


Figure 3: DETEST Problem A4 -  $\log_{10}M/M^*$  against Function Evaluations.

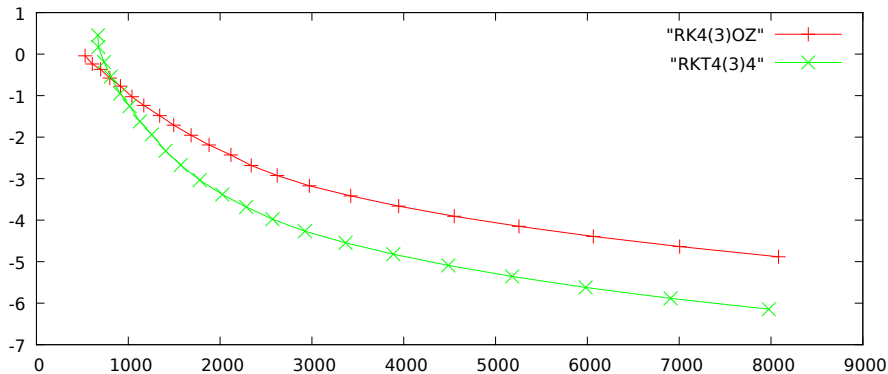


Figure 4: AREN Problem -  $\log_{10}M$  against Function Evaluations.

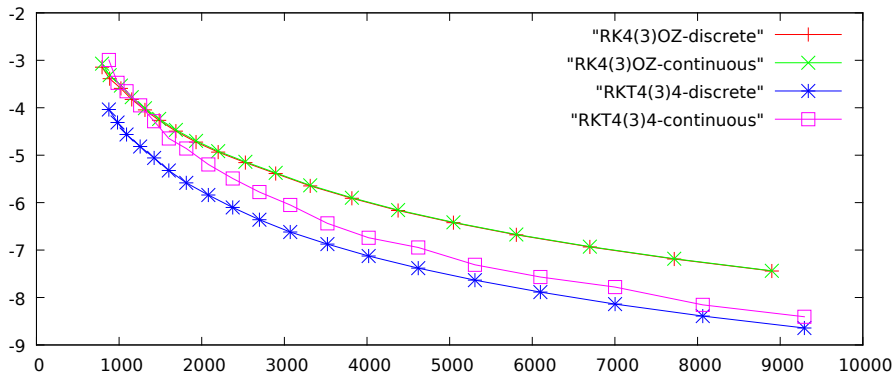


Figure 5: BRUS Problem -  $\log_{10}M/M^*$  against Function Evaluations.

For order 5 the practical tests show that the RKT5(4)5 is preferable to the triple of Owren and Zennaro (RK5(4)OZ) but neither is as efficient as the RK5(4)7FM with the fourth order dense formula on the problems tested. For  $\log_{10}M$  against function evaluations the RK5(4)7FM was only bettered by the RKT5(4)5 on two of the problems out of the dozen or so tested and was never bettered by the RK5(4)OZ which gave extremely poor results on the modified EULR problem and yet surprisingly good results on the BRUS problem. For  $\log_{10}M^*$  against function evaluations the RK5(4)7FM with the fourth order dense formula was still generally more efficient than the other two triples. Use of the fifth order continuous formula with the RK5(4)7FM was rarely worth the extra cost of two evaluations per step. Figures 6 to 10 illustrate the situation.

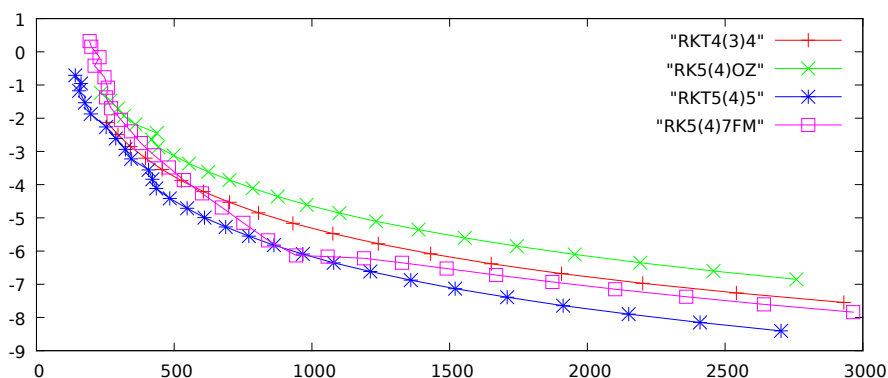


Figure 6: DETEST Problem D3 -  $\log_{10}M$  against Function Evaluations.

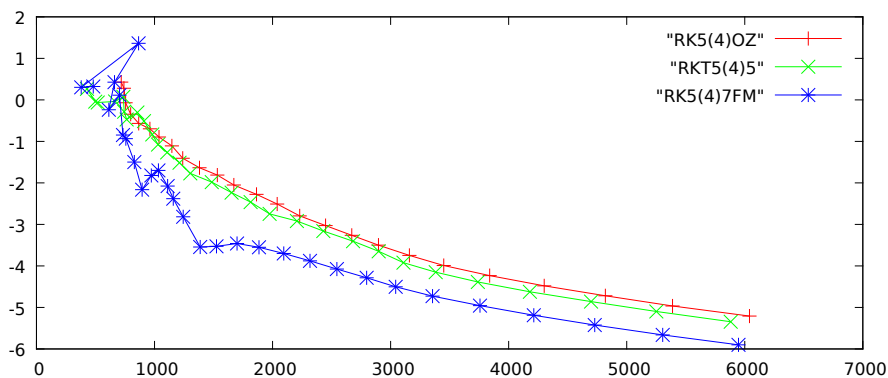


Figure 7: AREN Problem -  $\log_{10}M$  against Function Evaluations.

For order 6 the practical tests confirm that there is a preference for the RKT7(5)6 against the RK6(5)9FM with the fifth order continuous formula particularly at the more stringent tolerances. The use of the sixth order continuous process with the RK6(5)9FM did not appear to be worth the extra cost. Figures 11 to 13 illustrate the position.

For orders 7 and above the practical tests indicate that the RKT8(6)7, the RK8(6)12M or the RK8(7)13M are not as efficient as either the RKT9(7)8 or the RKT10(8)9. Figures 14 to 19 compare these with the RK5(4)7FM and the RKT7(5)6. It should be noted that the size of some of the RK coefficients in the higher order triples means that it is advisable to use high precision arithmetic when using stringent tolerances.

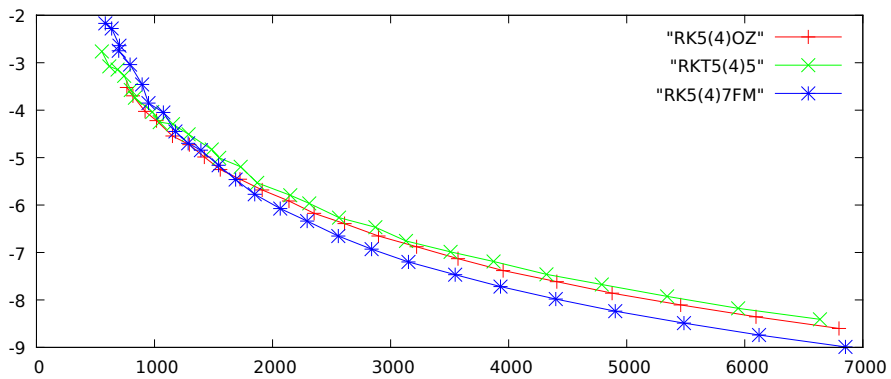


Figure 8: BRUS Problem -  $\log_{10}M$  against Function Evaluations.

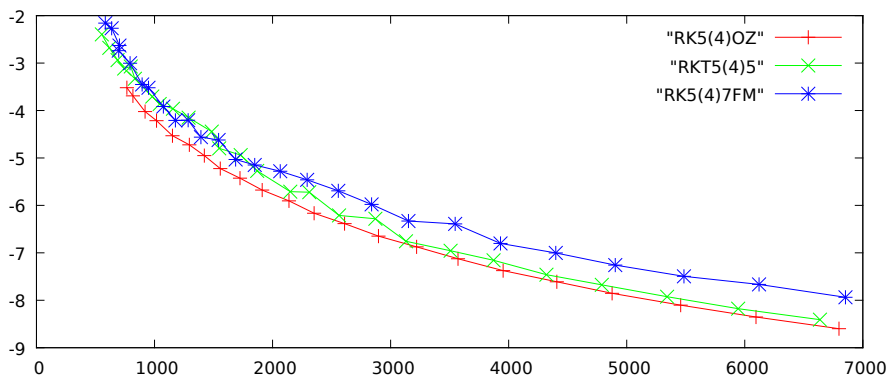


Figure 9: BRUS Problem -  $\log_{10}M^*$  against Function Evaluations.

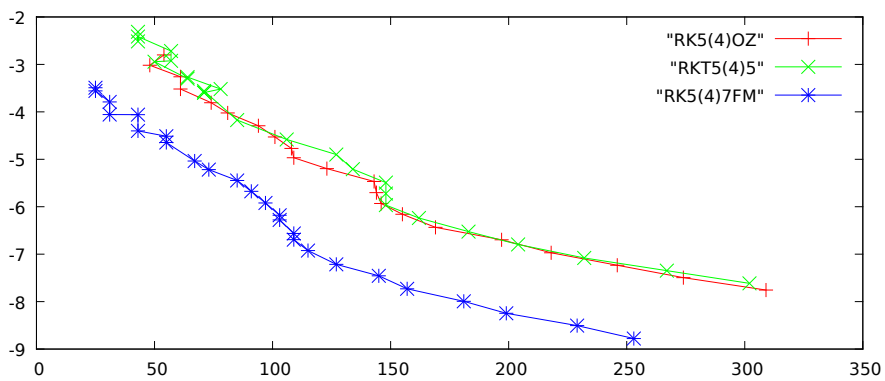


Figure 10: DETEST Problem E5 -  $\log_{10}M$  against Function Evaluations.

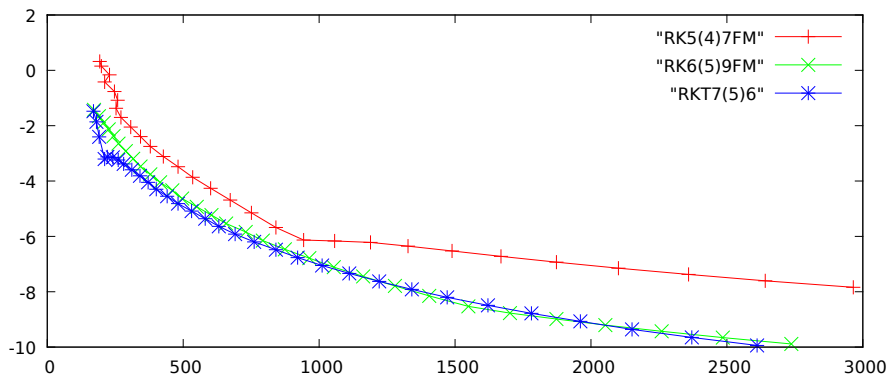


Figure 11: DETEST Problem D3 -  $\log_{10}M$  against Function Evaluations.

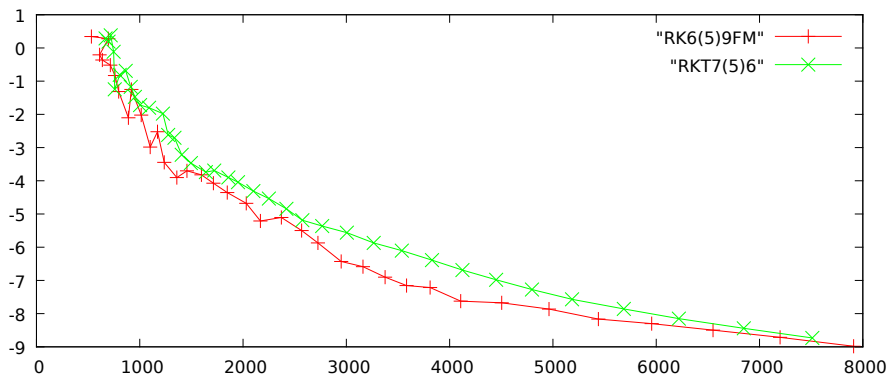


Figure 12: AREN Problem -  $\log_{10}M$  against Function Evaluations.

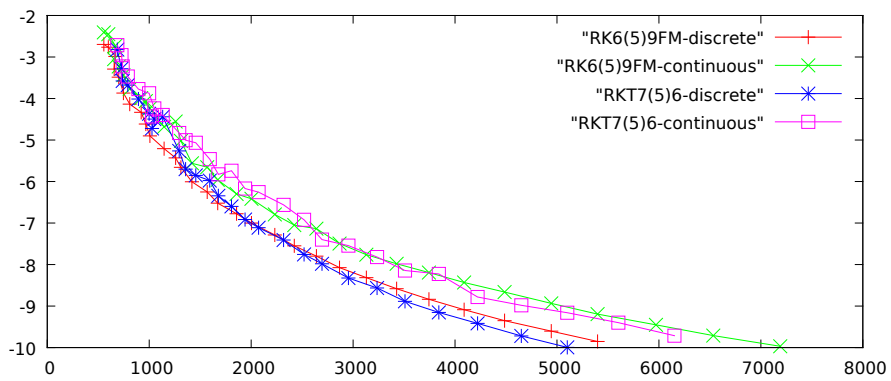


Figure 13: BRUS Problem -  $\log_{10}M/M^*$  against Function Evaluations.

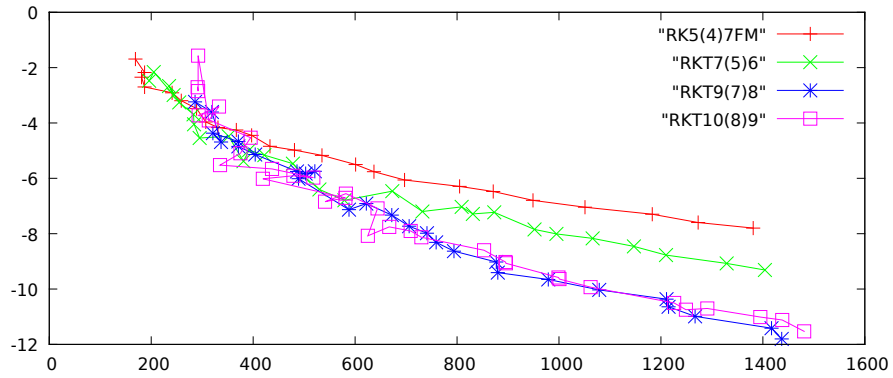


Figure 14: DETEST Problem A3 -  $\log_{10}M$  against Function Evaluations.

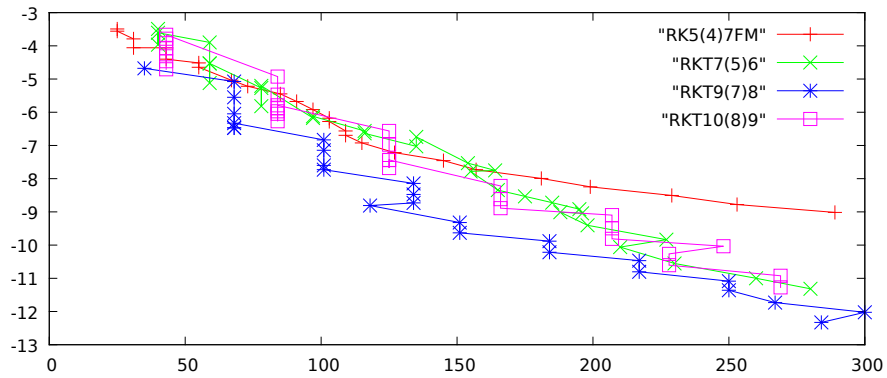


Figure 15: DETEST Problem E5 -  $\log_{10}M$  against Function Evaluations.

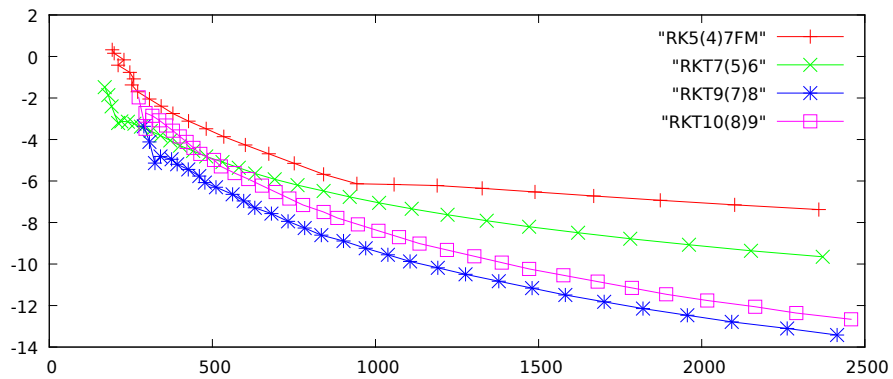


Figure 16: DETEST Problem D3 -  $\log_{10}M$  against Function Evaluations.

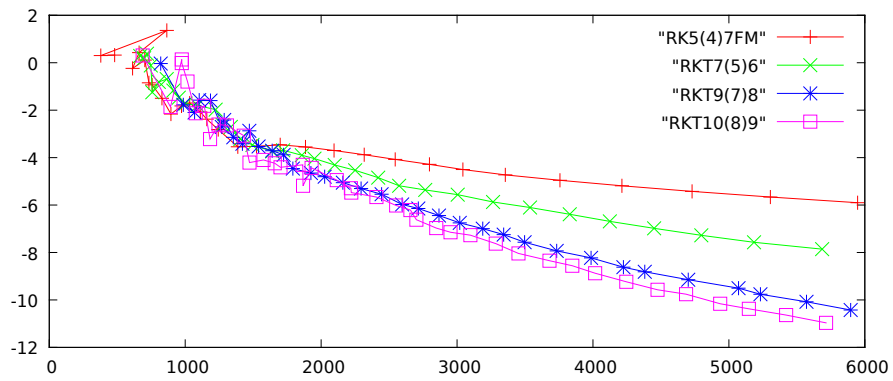


Figure 17: AREN Problem -  $\log_{10}M$  against Function Evaluations.

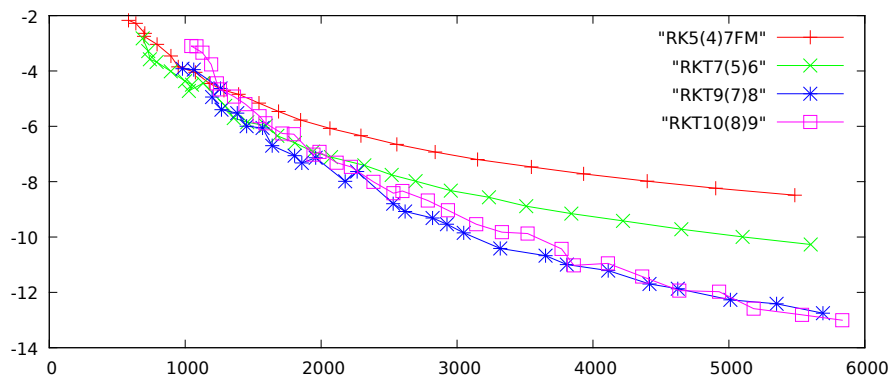


Figure 18: BRUS Problem -  $\log_{10}M$  against Function Evaluations.

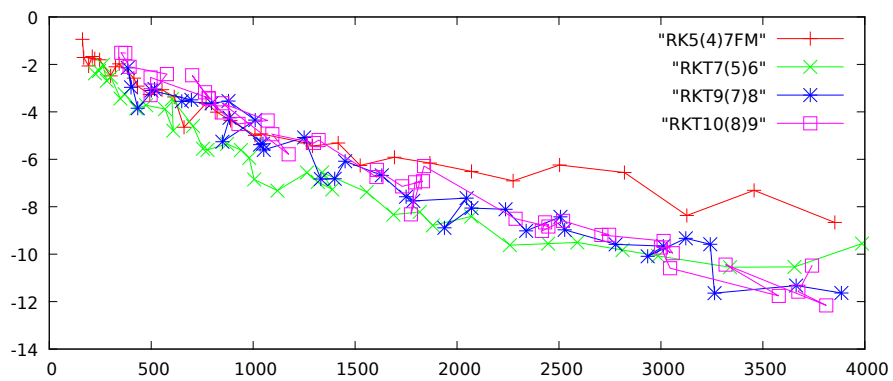


Figure 19: Modified EULR problem -  $\log_{10}M$  against Function Evaluations.

## 4 Summary and Discussion

This work advances the knowledge relating to the minimum number of stages necessary for an explicit Runge-Kutta process to be of a particular order in both the discrete and continuous cases (see Table 1). The suggestion made in [9] that new methods be developed which use all function evaluations at each stage to obtain both discrete and continuous approximations has been investigated for processes of order  $q$ ,  $q^* = 3, 4, \dots, 9$ . For each order,  $q^*$ , this development uses a strategy of first solving the RK continuous equations of condition, then obtaining a discrete process of order  $q^*$  by enforcing the  $C^1$  continuity conditions and then choosing any remaining free parameters to satisfy an efficiency condition relating global error to cost. Notice that for the higher orders this allows the discrete formula to be made order  $q = q^* + 1$ . Finally an embedded discrete formula of order  $p$  ( $= q - 1$  or  $q - 2$ ) is obtained which can be used for step size control.

The new triples have been extensively tested against currently available processes using standard test problems. As expected the new triples of orders 3 and 4 are generally not as efficient as those of higher order. The new triple of order 5 is found to be less efficient than the RK5(4)7FM (plus fourth order continuous process) which is therefore highly recommended when low accuracy is required. If high accuracy is required the new triples RKT9(7)8 and RKT10(8)9 are strongly recommended.

## 5 Acknowledgements

The author is grateful to his long time friend and colleague, Dr. John R. Dormand, for the many significant discussions held over the period of the development of this work. Thanks is also attributed for the use of the software packages g95, gfortran, gnuplot, latex and Maxima without which much of the work would not have been possible.



## References

- [1] T.S.Baker, J.R.Dormand, J.P.Gilmore and P.J.Prince, Continuous approximation with embedded Runge-Kutta methods, *Appl. Numer. Math.*, **22** (1996), 51-62.
- [2] M.Calvo, J.I.Montijano and L.Randez, A fifth-order interpolant for the Dormand and Prince Runge-Kutta method, *J. Comput. Appl. Math.*, **29** (1990), 91–100.
- [3] J.R.Dormand and P.J.Prince, A family of embedded Runge-Kutta formulae, *J. Comput. Appl. Math.* **6** (1980), 19–26.
- [4] J.R.Dormand, and P.J.Prince, Runge-Kutta triples, *Computers Math. Applic.*, **12A** (1986), 1007–1017.
- [5] J.R.Dormand and P.J.Prince, Practical Runge-Kutta processes, *SIAM J. Sci. Stat. Comput.*, **10** (1989), 977–989.
- [6] J.R.Dormand, M.A.Lockyer, N.E.McGorrigan and P.J.Prince, Global error estimation with Runge-Kutta triples, *Computers Math. Applic.*, **18** (1989), 835–846.
- [7] W.H.Enright, D.J.Higham, B.Owren and P.Sharp, A survey of the Explicit Runge-Kutta Method, *University of Toronto Technical Report*, **291** (1994).
- [8] E.Hairer, A Runge-Kutta Method of Order 10, *J. Inst. Maths Applics.* **21** (1978), 47–59.
- [9] E.Hairer, S.P.Nørsett and G.Wanner, Solving ordinary differential equations I, Second Edition, *Springer-Verlag*, (1993).
- [10] T.E.Hull, W.H.Enright, W.H.Fellen and A.E.Sedgwick, Comparing numerical methods for ordinary differential equations, *SIAM J. Numer. Anal.*, **9** (1972), 603–637.
- [11] B.Owren and M.Zennaro, Order barriers for continuous explicit Runge-Kutta methods, *Math. Comp.*, **56** (1991), 645–661.
- [12] B.Owren and M.Zennaro, Derivation of efficient continuous explicit Runge-Kutta methods, *SIAM J. Sci. Statist. Comput.*, **13** (1992), 1488–1501.
- [13] P.J.Prince and J.R.Dormand, High order embedded Runge-Kutta formulae, *J. Comput. Appl. Math.* **7** (1981), 67–75.