



## Variable stepsize schemes for effective order methods and enhanced order composition methods

J.C. Butcher<sup>a</sup> and T.M.H. Chan<sup>b</sup>

<sup>a</sup> *Department of Mathematics, The University of Auckland, Private Bag 92019, Auckland, New Zealand*  
E-mail: butcher@math.auckland.ac.nz

<sup>b</sup> *Department of Information Management, National Taichung Institute of Technology, Taichung, Taiwan*  
E-mail: tchan@ntic.edu.tw

Received 4 August 1999

Communicated by C. Brezinski

The interest in the concept of “*effective order*” has been revived by its rediscovery in applications to symplectic problems. In this paper we revert to the original application, the construction of explicit Runge–Kutta methods. Changing stepsize is a characteristic difficulty with effective order methods and we propose a way of overcoming this difficulty. We also consider the possible cancellation of local truncation errors of two methods over two successive steps. Using the algebraic approach for deriving these results gives us further insight into these methods and compositions of methods. A particular sixth stage Runge–Kutta pair is derived in the paper and is shown to be competitive.

**Keywords:** effective order, the Picard integral, the  $C$  and  $D$  simplifying assumptions, composition methods, principal local truncation error

### 1. Introduction

The main goal of this paper is to introduce variable stepsize selection scheme for effective order methods, and to obtain enhanced order composition methods. In each case, the analysis is facilitated by use of the algebraic approach of [4].

In 1969, Butcher [2] proposed the effective order concept. Using this idea, the Butcher barrier for explicit Runge–Kutta methods (for order  $p \geq 5$ , at least  $p + 1$  stages are necessary) was broken. Six stage methods with effective order six were derived in [13]. Little further progress has been made on effective order methods, mainly because of the difficulty in changing stepsize. More recently, López-Marcos et al. have applied the idea of effective order to symplectic methods [16]. This rediscovery led to a renewed interest in effective order and this has now been extended to Singly-Implicit Runge–Kutta methods (SIRK) [1]. The effective order generalization permits a free choice of the distinct abscissae in both SIRK and in extended singly implicit Runge–Kutta methods (DESI) [5]. Variable stepsize schemes for these methods were developed in [7–9]. For these methods, with high stage order, this presented no special difficulty.

For explicit methods, however, the difficulties remain. In this paper, we point out a scheme for changing stepsize for effective order methods, especially for explicit Runge–Kutta methods.

In section 2, we discuss the concept of effective order methods, and a changing stepsize scheme for these methods. We give an example to show how to derive an effective order five method and an associated variable stepsize effective order method. In section 3, we discuss a way of cancelling out the principal local truncation error. Enhanced order composition methods can be derived by two different methods within two continuous steps. A competitive composition method, **rk66**, is derived. In section 4, we carry out the experiments of a changing stepsize scheme for an effective order method. Moreover, comparisons are made between the new enhanced order methods and the DOPRI(5,4) method, which has the same number of stages.

A Runge–Kutta method with  $s$  stages is denoted by  $(A, b, c)_s$ . The algebraic form of the Taylor series expansion of a method  $\alpha$  at  $y_0$  over stepsize  $h$  is defined by

$$\alpha(\emptyset)y_0 + \sum_{t \in T} \frac{\alpha(t)}{\sigma(t)} F(t)(y_0)h^{r(t)},$$

where  $\alpha$  is the elementary weight function,  $\sigma(t)$  is the symmetry function,  $F(t)(y_0)$  is the elementary differential corresponding to the tree  $t$ , and  $r(t)$  is order of the tree  $t$  (see [3]). We use Butcher’s normalized elementary weight function so that the composition rule is

$$(\alpha\beta)(t) = \beta(\emptyset)\alpha(t) + \beta(t) + \sum_{u < t} \beta(u)\alpha(t \setminus u), \quad \forall t \in T,$$

where  $u$  is a subtree of  $t$  sharing the same root with the tree  $t$  and  $t \setminus u$  is the remaining part of  $t$  after deleting the subtree  $u$ .

Let  $\gamma(t)$  be the density function. We define  $E : T \rightarrow \mathbb{R}$ , by  $E(t) = 1/\gamma(t)$ ,  $\forall t$ , the “exact method”. This can be represented in terms of the Picard integral equation, interpreted as a limiting Runge–Kutta method  $(A, b, c)_s$  as  $s \rightarrow \infty$  (see [11]).

Since results computed by a Runge–Kutta method can be represented as members of  $G$ , the set of mappings from trees and  $\{\emptyset\}$  to real numbers. Let  $G_1 = \{\alpha \in G \mid \alpha(\emptyset) = 1\}$  and  $H_p = \{\alpha \in G_1 \mid \alpha(t) = 0, \forall r(t) \leq p\}$ . In Butcher [3],  $H_p$  is found to be a normal subgroup of  $G_1$ , therefore,  $G_1/H_p = \{\alpha H_p \mid \alpha \in G_1\}$  forms a factor group. The coset  $EH_p \in G_1/H_p$  contains all the methods of order greater than or equal to  $p$ . The following notations are made in [3]. For any  $\alpha \in G$ ,  $\alpha^{(\rho)}$  means the method is over stepsize  $\rho h$ , that is  $\alpha^{(\rho)}(\tau) = \rho$ . But  $\alpha^n = \alpha \cdots \alpha$ , where  $\alpha$  occurs  $n$  times using the same stepsize. Note that the Picard integral  $E$  is of infinite order and it can be proved that  $E^{(\rho)} = E^\rho$ .

## 2. A changing stepsize scheme for effective order methods

Our aim is to avoid the inconvenience of separately removing the perturbation for the previous step and then introducing a new perturbation with the new stepsize. In

order to retain the perturbation introduced by  $\beta$ , but adapted to the new stepsize, we need to modify the coefficients of the first step taken with the new stepsize. Ideally, we would like the effective order method used for the stepsize changing remains the same as the original effective order method except for the weights. However, this is difficult to achieve for lower stage order effective order methods. We use an explicit effective order method, which is of lower stage order, as an example to show how to implement variable stepsize schemes.

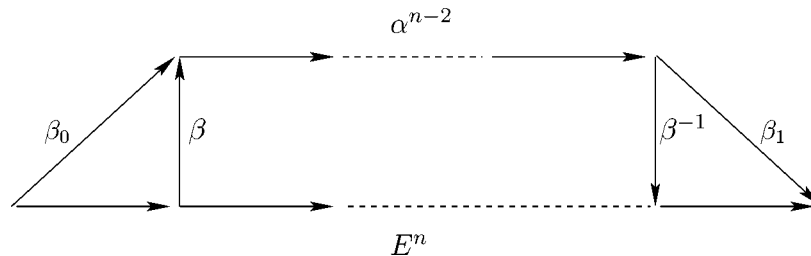
2.1. Effective order methods

In this subsection, we explain the idea of effective order and give formulas for deriving the order conditions for effective order methods on tall and bushy trees with starting method  $\beta$  satisfies  $\beta(\tau) = 0$ . These formulas simplify the derivation of effective order conditions. An example is given to show the detail derivation of a variable stepsize scheme.

**Definition 1** (Butcher [2] 1969). A method  $\alpha \in G_1$  is of effective order  $p$  if there exists  $\beta \in G_1$  such that  $\beta\alpha\beta^{-1}$  is of order  $p$ .

The effect of this definition is that we seek a method represented by  $\alpha$ , which preserves accuracy, not in the exact trajectory, but in a trajectory perturbed by the method represented by  $\beta$ . Therefore, the starting method  $\beta$  offers some freedom in the effective order conditions of  $\alpha$ . To use the method, the perturbation  $\beta$  is applied at the start of the integration; this is compensated for by applying the method  $\beta^{-1}$  at the end of the integration.

It seems natural to require the starting method to serve as a first step and to integrate the solution forward a distance  $h$  as well as applying the perturbation. If  $\beta(\tau) = 0$ , this could mean defining a starting step from  $\beta_0 = E\beta$ . Similarly, the finishing procedure could be defined from  $\beta_1 = \beta^{-1}E$ , so that  $\beta_1(\tau) = 1$ . This would mean that a further step is taken while the perturbation is being removed. Therefore, this integration for effective order methods over  $n$  steps is



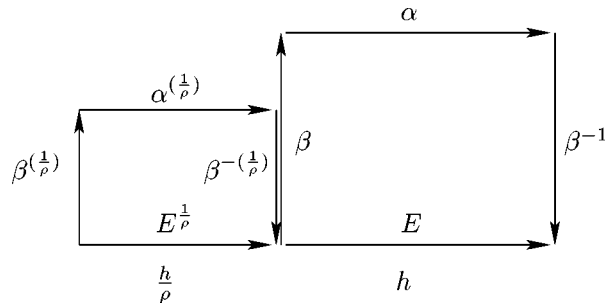
Under the assumption that  $\beta\alpha\beta^{-1} \in EH_p$  with  $\beta(\tau) = 0$ , the order conditions for the effective order method for tall and bushy trees are:

$$\alpha([\tau]_s) = \frac{1}{(s+1)!}, \quad \text{for all } s = 0, \dots, p-1, \quad (1)$$

$$\alpha([\tau^m]) = \frac{1}{m+1} + \sum_{i=1}^m \binom{m}{i} \beta([\tau^{m-i}]), \quad \text{for all } m = 1, \dots, p-1. \quad (2)$$

These two conditions, (1) and (2), were derived by expanding the composition rule of  $(\beta\alpha)(t) = (E\beta)(t)$  for a tall tree and a bushy tree respectively with the assumption that  $\beta(\tau) = 0$ . Therefore, we can derive the effective order method  $\alpha$  using the above formulas, and then find a starting method  $\beta_0 = E\beta$  and finishing method  $\beta_1 = \beta^{-1}E$  (see [4]).

Without changing the effective order method  $\alpha$ , the stepsize-changing scheme for effective order method is represented by the diagram



This means that the cancellation of the perturbed and reperturbed actions is destroyed. Because of this, it has always seemed to be difficult to use effective order with variable stepsize.

In order that the cancellations for perturbed and reperturbed actions still hold for changing stepsize scheme for effective order methods, we propose a variable stepsize scheme in figure 1. An effective order method  $\alpha_\rho$  using for changing stepsize in figure 1 is derived in example 1. An error estimation for this effective order method in stepsize-changing scheme is also obtained based on an embedded method.

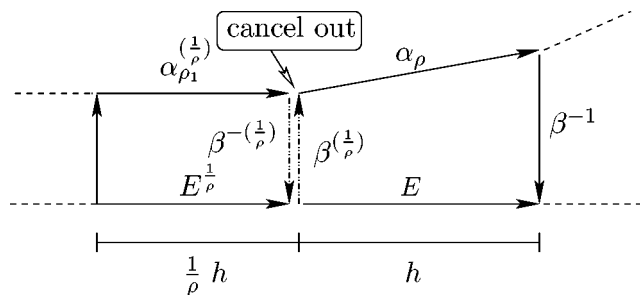


Figure 1. Variable stepsize for effective order methods.

2.2. The variable stepsize scheme

There are several key points for changing stepsize for effective order methods in figure 1.

1. It seems natural that the first method  $\beta$  for changing stepsize satisfies  $\beta(\tau) = 0$  in order to make sure that the perturbed initial values are at the same points of the original initial value and also a preparation for the design of (3) in which the perturbed and anti-perturbed action under a variable stepsize scheme could be cancelled.
2. We should find a method  $\alpha_\rho$  such that

$$\beta^{(1/\rho)}\alpha_\rho\beta^{-1} \in EH_p, \quad \text{this is equivalent to } \beta^{(1/\rho)}\alpha_\rho = E\beta, \quad \forall r(t) \leq p, \quad (3)$$

where  $\rho \in \mathbb{R}$  denotes the stepsize ratio. In particular, we choose  $\alpha_\rho(\tau) = 1$ . Note that in figure 1, we have

- (a) If  $\rho = 1$ , then  $\alpha_\rho = \alpha$ . Therefore, the first two steps taken for experiment are  $\beta_0$ , followed by  $\alpha$ .
  - (b)  $\alpha_\rho$  is the method for stepsize changing. If the current step is accepted with output value  $y_1$  and stepsize ratio  $\rho_0$ , then  $\alpha_{\rho_0}$  is the method for carry out the next integration with initial value  $y_1$  and stepsize  $\rho_0 h$ .
3. The error estimate should be based on the changing stepsize effective order solution flows rather than the original solution flows.

**Example 1.** In this example, we show a way of analysing methods of effective order five with five stages together with a starting method  $\beta_0$  and a finishing method  $\beta_1$ . The main part is to show how to find a relative effective order changing stepsize method  $\alpha_\rho$  and its error estimation for stepsize-changing scheme.

Let  $\beta$  (with  $\beta(\tau) = 0$ ),  $\beta_0$ ,  $\beta_1$  and the effective order explicit Runge–Kutta method  $(A, b, c)_s$  satisfy  $C(2)$  and  $D(1)$ . In order to satisfy  $C(2)$  up to order 5 for explicit method  $(A, b, c)_s$  (associated with the  $D(1)$  conditions), we assume

$$b_2 = 0 \quad \text{and} \quad \sum_{i=1}^5 b_i(1 - c_i)a_{i2} = 0.$$

Using the above formulas for tall trees and bushy trees, the order conditions for effective order methods up to order five are

Tall tree	Bushy tree
$\alpha(\cdot) = 1$	
$\alpha(!) = \frac{1}{2}$	
$\alpha(\uparrow) = \frac{1}{6}$	$\alpha(\vee) = \frac{1}{3} + 2\beta(!)$
$\alpha(\uparrow\uparrow) = \frac{1}{24}$	$\alpha(\vee\vee) = \frac{1}{4} + 3\beta(!) + 3\beta(\vee)$
$\alpha(\uparrow\uparrow\uparrow) = \frac{1}{120}$	$\alpha(\vee\vee\vee) = \frac{1}{5} + 4\beta(!) + 6\beta(\vee) + 4\beta(\vee\vee)$

Because of  $C(2)$ , we have  $\alpha(\uparrow\uparrow) = \frac{1}{2}\alpha(\vee)$ . Therefore,  $\beta(!) = 0$ .

The equation

$$(\beta\alpha)(\vee\vee) = (E\beta)(\vee\vee)$$

together with the conditions  $\beta(\tau) = \beta(!) = 0$  and  $C(2)$ ,  $D(1)$ , we have

$$\alpha(\vee\vee) = \frac{1}{15} + \frac{5}{2}\beta(\vee).$$

Applying the  $D(1)$  conditions on the tall tree of order five, we have  $\beta(\uparrow\uparrow\uparrow) = 0$ . By applying  $b^T(1-c)Ac(c-c_3)$  to the order condition  $\alpha(\vee\vee) = \frac{1}{15}$ , we have  $c_3 = \frac{2}{5}$ .

The linear combination  $b^Tc(c-c_3)(c-c_4)(c-1)$  and the order conditions of  $\alpha$  on bushy trees give

$$0 = \frac{1}{5} + 4w - \frac{c_3 + c_4 + 1}{4} + \frac{c_3 + c_4 + c_3c_4}{3} - \frac{c_3c_4}{2}, \quad \text{where } w = \beta(\vee).$$

Therefore, we have

$$w = \frac{1 - c_4}{240}.$$

For starting and finishing methods, we have to evaluate  $\beta_0(t)$  and  $\beta_1(t)$  for all  $r(t) \leq 4$ . Since all these methods satisfy  $C(2)$  and  $D(1)$ ,  $\beta_0 = E\beta$ ,  $\beta_1 = \beta^{-1}E$ , and  $\beta(t) = 0$ , for  $r(t) \leq 3$ , we have

$$\beta_0(\cdot) = \beta_1(\cdot) = 1, \quad \beta_0(!) = \beta_1(!) = \frac{1}{2}, \quad \beta_0(\vee) = \beta_1(\vee) = \frac{1}{3}.$$

Since  $\beta^{-1}$  is the inverse of  $\beta$ , by the formula  $\beta\beta^{-1} = \mathbb{1}$ , we have  $\beta^{-1}(t) = 0$  for all  $r(t) \leq 3$ , and

$$0 = (\beta\beta^{-1})(\vee\vee) = \beta(\vee\vee) + \beta^{-1}(\vee\vee) = w + \beta^{-1}(\vee\vee) \Rightarrow \beta^{-1}(\vee\vee) = -w.$$

Therefore, we obtain

$$\beta_0(\vee\vee) = E(\vee\vee) + \beta(\vee\vee) = \frac{1}{4} + w,$$

$$\beta_1(\vee\vee) = (\beta^{-1}E)(\vee\vee) = \beta^{-1}(\vee\vee) + E(\vee\vee) = -w + \frac{1}{4}.$$

The order conditions for an effective order 5 method  $\alpha$  satisfying  $C(2)$  and  $D(1)$  up to order 5 with a starting method  $\beta_0$  and finishing method  $\beta_1$  up to order 4 are

	.	!	∨	∇	∇	∇
$\alpha$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{15}$	$\frac{1}{5} + 4w$
$\beta_0$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4} + w$		
$\beta_1$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4} - w$		

where  $w = \beta(\nabla)$ .

Solving the quadrature formulas up to order 4 for  $\alpha$ ,  $\beta_0$  and  $\beta_1$ , we have

$$(b_3, b_4, b_5) = \left(\frac{1}{2}, \frac{1}{3}, \frac{1}{4} + \tilde{w}\right) \begin{pmatrix} c_3 & c_3^2 & c_3^3 \\ c_4 & c_4^2 & c_4^3 \\ 1 & 1 & 1 \end{pmatrix}^{-1},$$

where for  $\alpha$ ,  $\tilde{w} = 0$ ; for  $\beta_0$ ,  $\tilde{w} = w$ , and for  $\beta_1$ ,  $\tilde{w} = -w$ . And  $b_1 = 1 - b_3 - b_4 - b_5$ .

By the  $C(2)$  conditions up to order 5 for these methods, we have

$$a_{32} = \frac{c_3^2}{2c_2}, \quad a_{31} = c_3 - a_{32}, \quad a_{42} = -\frac{b_3(1 - c_3)}{b_4(1 - c_4)},$$

$$a_{43} = \frac{c_4^2 - 2a_{42}c_2}{2c_3}, \quad a_{41} = c_4 - a_{42} - a_{43}.$$

The value  $c_3 = \frac{2}{5}$  follows from the order condition  $\alpha(\nabla) = \frac{1}{4}$  and the order condition of  $\alpha$  on bushy tree of order five gives  $w = (1 - c_4)/240$ .

By choosing the abscissae of  $\beta_0$ ,  $\alpha$  and  $\beta_1$ , we derive an effective order method with starting and finishing methods as follows.

A first method  $(\bar{A}, \bar{b}, \bar{c})_5$  ( $\beta_0$ , with  $\beta_0(\tau) = 1$ )

0	0	0	0	0	0
$\frac{1}{5}$	$\frac{1}{5}$	0	0	0	0
$\frac{2}{5}$	0	$\frac{2}{5}$	0	0	0
$\frac{3}{4}$	$\frac{75}{64}$	$-\frac{9}{4}$	$\frac{117}{64}$	0	0
1	$-\frac{37}{36}$	$\frac{7}{3}$	$-\frac{3}{4}$	$\frac{4}{9}$	0
1	$\frac{19}{144}$	0	$\frac{25}{48}$	$\frac{2}{9}$	$\frac{1}{8}$

the effective order method  $(A, b, c)_5 (\alpha)$

$$\begin{array}{c|cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & 0 & 0 & 0 & 0 \\ \frac{2}{5} & 0 & \frac{2}{5} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{3}{16} & 0 & \frac{5}{16} & 0 & 0 \\ 1 & \frac{1}{4} & 0 & -\frac{5}{4} & 2 & 0 \\ \hline 1 & \frac{1}{6} & 0 & 0 & \frac{2}{3} & \frac{1}{6} \end{array}$$

and a finishing method  $(\hat{A}, \hat{b}, \hat{c})_5 (\beta_1, \text{ with } \beta_1(\tau) = 1)$

$$\begin{array}{c|cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & 0 & 0 & 0 & 0 \\ \frac{2}{5} & 0 & \frac{2}{5} & 0 & 0 & 0 \\ \frac{3}{4} & \frac{161}{192} & -\frac{19}{12} & \frac{287}{192} & 0 & 0 \\ 1 & -\frac{27}{28} & \frac{19}{7} & -\frac{291}{196} & \frac{36}{49} & 0 \\ \hline 1 & \frac{7}{48} & 0 & \frac{475}{1008} & \frac{2}{7} & \frac{7}{72} \end{array}$$

The three tableaux were derived in [4].

We use the following three steps to show a way of deriving an effective order method for stepsize-changing scheme.

**Step 1.** Find the starting method  $\beta$  with  $\beta(\tau) = 0$ . Since the effective order method  $(A, b, c)_5$  is of order 4, we have

$$\beta(\cdot) = \beta(1) = \beta\left(\begin{array}{c} 1 \\ \vdots \\ 1 \end{array}\right) = \beta(\nabla) = 0,$$

and by the composition rule for  $E\beta$  and the fact that  $\beta_0 = E\beta$ , the order conditions for  $\beta$  on trees of order 4 and 5 are

$$\begin{aligned} \beta(\nabla) &= \beta_0(\nabla) - \frac{1}{4} = \bar{b}^T \bar{c}^3 - \frac{1}{4} = \frac{1}{480}, \\ \beta(\Psi) &= \beta_0(\Psi) - \frac{1}{5} - 4\beta(\nabla) = \bar{b}^T \bar{c}^4 - \frac{1}{5} - 4\beta(\nabla) = \frac{1}{3200}, \\ \beta(\check{\Psi}) &= \beta_0(\check{\Psi}) - \frac{1}{15} = \bar{b}^T \bar{c} \bar{A} \bar{c}^2 - \frac{1}{15} = -\frac{1}{600}. \end{aligned}$$



**Step 2.** Find the effective order method  $(A(\rho), b(\rho), c(\rho))_5$  ( $\alpha_\rho$ ) for changing stepsize, the order conditions are

$$(\beta^{(1/\rho)}\alpha_\rho)(t) = (E\beta)(t), \quad \text{for all } t: r(t) \leq 5. \quad (4)$$

Therefore, by expanding the composition rule of (4), the order conditions for  $\alpha_\rho$  up to order 5, which satisfies the  $C(2)$  simplifying assumption up to order 5, are

$$b(\rho)_2 = 0, \quad \sum_{i=1}^5 b(\rho)_i(1 - c(\rho)_i)a(\rho)_{i2} = 0,$$

and

$$\begin{aligned} \alpha_\rho(\cdot) &= 1, & \alpha_\rho(1) &= \frac{1}{2}, \\ \alpha_\rho(\nabla) &= \frac{1}{3}, & \alpha_\rho(\nabla) &= \frac{1}{4} + \left(1 - \frac{1}{\rho^4}\right)\beta(\nabla), \\ \alpha_\rho(\Psi) &= \frac{1}{5} + \left(1 - \frac{1}{\rho^5}\right)\beta(\Psi) + 4\beta(\nabla), \\ \alpha_\rho(\check{\nabla}) &= \frac{1}{5} + \left(1 - \frac{1}{\rho^5}\right)\beta(\check{\nabla}). \end{aligned}$$

By solving for the above order conditions and the  $D(1)$  and  $C(2)$  conditions (up to order 5), we find the effective order method  $\alpha_\rho$  for changing stepsize to be

$$\begin{aligned} a_{32}(\rho) &= \frac{2w_1^2}{5\rho w_2^2}, & a_{31}(\rho) &= c_3(\rho) - a_{32}(\rho), \\ a_{42}(\rho) &= \frac{(-1 + \rho)w_2^2 w_3 w_1 w_4}{4\rho^2 w_5^3}, & a_{43}(\rho) &= \frac{w_2^3 w_3 w_6}{64\rho w_1 w_5^3}, \\ a_{41}(\rho) &= c_4(\rho) - a_{42}(\rho) - a_{43}(\rho), & a_{52}(\rho) &= \frac{(1 - \rho)w_1 w_2 w_4}{\rho w_7}, \\ a_{53}(\rho) &= \frac{w_2^2 w_8 w_9}{4w_1 w_6 w_7}, & a_{54}(\rho) &= \frac{4(-w_8)w_5^3 w_{10}}{w_2 w_3 w_6 w_7}, \\ a_{51}(\rho) &= 1 - a_{52}(\rho) - a_{53}(\rho) - a_{54}(\rho), & b_3(\rho) &= \frac{25(-1 + \rho)w_2^4(-w_4)}{48\rho w_1(-w_8)w_6}, \\ b_4(\rho) &= \frac{2w_5}{3\rho w_2 w_3 w_{10} w_6}, & b_5(\rho) &= \frac{w_7}{24\rho^2(-w_8)w_{10}}, \\ b_1(\rho) &= 1 - b_3(\rho) - b_4(\rho) - b_5(\rho), \end{aligned}$$

where

$$\begin{aligned} w_1 &= -4 + 5\rho + 39\rho^5, \\ w_2 &= 1 + 39\rho^4, \\ w_3 &= 7 - 12\rho + 21\rho^5, \end{aligned}$$

$$\begin{aligned}
w_4 &= -1 - \rho - \rho^2 + 11\rho^3 - 147\rho^4 - 147\rho^5 - 147\rho^6 - 147\rho^7, \\
w_5 &= 1 + 128\rho^3 - 82\rho^4 + 273\rho^8, \\
w_6 &= 67 - 100\rho + 4096\rho^3 - 5014\rho^4 - 1607\rho^5 + 22035\rho^8 - 68406\rho^9 + 74529\rho^{13}, \\
w_7 &= -1 - 672\rho^2 + 1840\rho^3 - 1116\rho^4 + 6560\rho^6 + 8928\rho^7 - 6806\rho^8 \\
&\quad + 105456\rho^{11} + 97188\rho^{12} + 95823\rho^{16}, \\
w_8 &= -8 + 5\rho - 117\rho^5, \\
w_9 &= -3 + 60\rho + 13512\rho^3 - 36628\rho^4 + 39303\rho^5 + 524288\rho^6 \\
&\quad - 973584\rho^7 + 206398\rho^8 + 1235628\rho^9 + 2820168\rho^{11} + 2255820\rho^{12} \\
&\quad + 12023490\rho^{13} + 575757\rho^{16} - 15187536\rho^{17} + 4695327\rho^{21}, \\
w_{10} &= -7 + 16\rho + 239\rho^4 + 119\rho^5 + 273\rho^9, \\
c(\rho) &= \left(0, \frac{1}{5}, \frac{2(1+39\rho^4)}{1+199\rho^4}, \frac{12-187\rho^4-51305\rho^8}{-4+3049\rho^4+253155\rho^8}, 1\right).
\end{aligned}$$

**Step 3.** Find an error estimate on the solution flow of the effective order method  $(A(\rho), b(\rho), c(\rho))_5$ . Let  $(\tilde{A}, \tilde{b}, \tilde{c})_6$  ( $\tilde{\beta}$ ) be an embedded method for  $(A(\rho), b(\rho), c(\rho))_5$  ( $\alpha_\rho$ ). That is,

$$\tilde{c} = \left(0, \frac{1}{5}, c_3(\rho), c_4(\rho), 1, 1\right), \quad \tilde{b}^T = (\tilde{b}_1(\rho), 0, \tilde{b}_3(\rho), \tilde{b}_4(\rho), \tilde{b}_5(\rho), \tilde{b}_6(\rho)),$$

and the order conditions for the embedded method are

$$\begin{aligned}
s_1 &= \tilde{b}^T e - 1, & s_2 &= \tilde{b}^T \tilde{c} - \frac{1}{2}, \\
s_3 &= \tilde{b}^T \tilde{c}^2 - \frac{1}{3}, & s_4 &= \tilde{b}^T \tilde{c}^3 - \left(\frac{1}{4} + \left(1 - \frac{1}{\rho^4}\right)\beta(\nabla)\right).
\end{aligned} \tag{5}$$

Note that the conditions in (5) are derived by expanding the composition rule of  $(\beta^{(1/\rho)}\alpha_\rho)(t) - (E\beta)(t)$  on the relative trees. Solving system (5) equal zero, there is a free parameter  $\tilde{b}_6$  left. For effective order methods, it is quite difficult to have a random choice of  $\tilde{b}_6$  such that the choice of  $\tilde{b}_6$  involves the stepsize ratio  $\rho$  and also control the stepsize properly.

We choose the condition

$$s_5 = b^T(\rho)A^3(\rho)c(\rho) - \tilde{b}^T\tilde{A}^2\tilde{c} = 0$$

in order that this error estimation has better performance for a two-step zero approximation (see [6]). Solve  $s_5 = 0$  for  $\tilde{b}_6$ , and we have

$$\tilde{b}_6 = -\frac{(-4 + 5\rho + 39\rho^5)u}{8\rho^3v},$$

where  $u = -1 - 672\rho^2 + 1840\rho^3 - 1116\rho^4 + 6560\rho^6 + 8928\rho^7 - 6806\rho^8 + 105456\rho^{11} +$

$97188\rho^{12} + 95823\rho^{16}$ ,  $v = 456 - 1773\rho + 860\rho^2 - 49152\rho^3 + 61104\rho^4 - 4913\rho^5 - 42387\rho^6 - 784504\rho^8 + 1688553\rho^9 - 1573823\rho^{10} - 536523\rho^{13} + 1151943\rho^{14} + 3162159\rho^{18}$ .

The error estimate is  $\tilde{b}^T - \tilde{A}[6] = (0, 0, 0, 0, -\tilde{b}_6, \tilde{b}_6)$ , where  $\tilde{A}[6]$  is the sixth row of  $\tilde{A}$ . See [11] for details.

The method  $(A(\rho), b(\rho), c(\rho))_5$  for stepsize-changing scheme for effective order involves the stepsize ratio  $\rho$ . For solving a simple system, this stepsize-changing scheme seems not to be very efficient because of the extra work for caring out the method  $\alpha_\rho$  using for the next step. However, for solving large problems, this extra work does not affect the result too much. See the result on integrating the DETEST problem C5 (see [15]) in the experiments.

In order not to carry out  $\alpha_\rho$  every step, we use the effective order methods corresponding to the stepsize ratio

$$\rho = 0.5, 0.6, 0.65, 0.7, 0.75, 0.85, 1, 1.3, 1.5, 1.65, 1.7, 1.75, 1.8, 1.9, 2.$$

The above coefficients of  $\rho$  are chosen according to our stepsize control. In the experiment, if the stepsize ratio  $\rho$  for the next step is chosen between any of above interval, then the stepsize ratio is chosen to be the left-hand-side end point.

### 3. Enhanced order composition methods

In this section, we propose a way of getting one order higher composition method by analysing the principal local truncation error over two successive methods. By cancelling the principal term of two methods integrating one followed by another, we derive a formula of one order higher composition methods. Especially, we give techniques in solving the order conditions for a sixth order composition methods where the original order of each method is five.

In figure 2, the principal local truncation errors for these two methods are

$$d_1 = \sum_{r(t)=p+1} \frac{1}{\gamma(t)} \left( \alpha(t) - \frac{\theta_1^{p+1}}{\sigma(t)} \right) F(t)(y_0)h^{p+1},$$

$$d_2 = \sum_{r(t)=p+1} \frac{1}{\gamma(t)} \left( \alpha(t) - \frac{\theta_2^{p+1}}{\sigma(t)} \right) F(t)(y_1)h^{p+1}.$$

If we let principal local truncation error  $(d_1 + d_2)$  over two steps equal zero, then we have

$$0 = \alpha(t) - \frac{\theta_1^{p+1}}{\beta_1(t)} + \beta(t) - \frac{\theta_2^{p+1}}{\beta_1(t)} = \alpha(t) + \beta(t) - \frac{\theta_1^{p+1} + \theta_2^{p+1}}{\gamma(t)}.$$

By letting  $\theta_1 = \theta_2 = 1$ , we derive the following theorem.

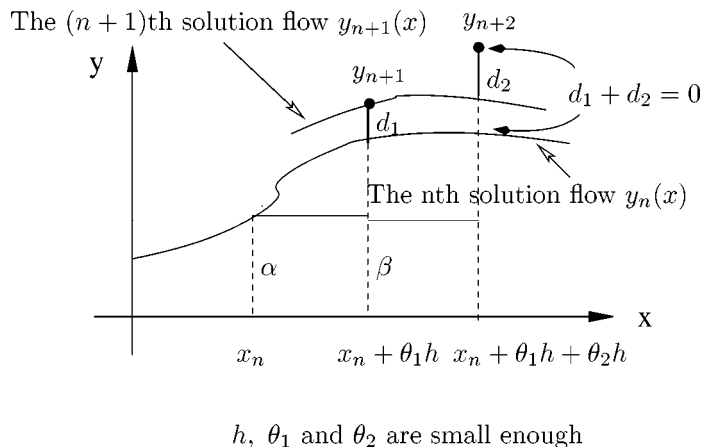


Figure 2. The principal local truncation error of a composite method.

**Theorem 1.** Let  $\alpha$  and  $\beta$  be of order  $p$  over stepsize  $h$ , then  $\alpha\beta$  is of order  $p + 1$  over stepsize  $2h$  if and only if

$$\alpha(t) + \beta(t) = \frac{2}{\gamma(t)}, \quad \text{for any } t: r(t) = p + 1.$$

**Example 2.** We discuss a derivation of a sixth order composite pair. A pair of methods,  $(A, b, c)_6$  and  $(\bar{A}, \bar{b}, \bar{c})_6$  satisfying  $D(1)$  are

$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$c_2$	$c_2$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$c_3$	$a_{31}$	$a_{32}$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$c_4$	$a_{41}$	$a_{42}$	$a_{43}$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$c_5$	$a_{51}$	$a_{52}$	$a_{53}$	$a_{54}$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$1$	$a_{61}$	$a_{62}$	$a_{63}$	$a_{64}$	$a_{65}$	$0$	$0$	$0$	$0$	$0$	$0$
	$b_1$	$0$	$0$	$b_4$	$b_5$	$b_6$	$0$	$0$	$0$	$0$	$0$

and

$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$\bar{c}_2$	$\bar{c}_2$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$\bar{c}_3$	$\bar{a}_{31}$	$\bar{a}_{32}$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$\bar{c}_4$	$\bar{a}_{41}$	$\bar{a}_{42}$	$\bar{a}_{43}$	$0$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$\bar{c}_5$	$\bar{a}_{51}$	$\bar{a}_{52}$	$\bar{a}_{53}$	$\bar{a}_{54}$	$0$	$0$	$0$	$0$	$0$	$0$	$0$
$1$	$\bar{a}_{61}$	$\bar{a}_{62}$	$\bar{a}_{63}$	$\bar{a}_{64}$	$\bar{a}_{65}$	$0$	$0$	$0$	$0$	$0$	$0$
	$\bar{b}_1$	$0$	$\bar{b}_3$	$\bar{b}_4$	$\bar{b}_5$	$\bar{b}_6$	$0$	$0$	$0$	$0$	$0$

In order that the order conditions for these methods could be used as  $C(2)$  up to order six (associated with the  $D(1)$  conditions), we need the conditions.

$$0 = b_2 = \bar{b}_2, \tag{6}$$

$$0 = \sum_{i=1}^6 b_i(1 - c_i)a_{i2} = \sum_{i=1}^6 \bar{b}_i(1 - \bar{c}_i)\bar{a}_{i2}, \tag{7}$$

$$0 = \sum_{i,j=1}^6 b_i(1 - c_i)a_{ij}a_{j2} = \sum_{i,j=1}^6 \bar{b}_i(1 - \bar{c}_i)\bar{a}_{ij}\bar{a}_{j2}, \tag{8}$$

$$0 = \sum_{i=1}^6 b_i(1 - c_i)(c_i - c_5)a_{i2} = \sum_{i=1}^6 \bar{b}_i(1 - \bar{c}_i)(\bar{c}_i - \bar{c}_5)\bar{a}_{i2}. \tag{9}$$

However, even though we could reduce the calculation work using equations (6)–(9), it seems not very economic using two extra conditions to eliminate just one order condition for the composite method. Therefore, we use only (6) and (7) because each of them could reduce more than two order conditions. Without using (8) and (9), two extra order conditions on trees  $\downarrow$  and  $\downarrow$  for the composite method should be also taken into account in addition to the order conditions on

$$., I, \vee, \vee, \vee, \vee, \vee, \vee, \vee, \vee, \vee, \vee, \vee.$$

For the quadrature formulas for these two method up to order 4 for  $(A, b, c)_6$ , we have

$$(b_4, b_5, b_6) = \left(\frac{1}{2}, \frac{1}{3}, \frac{1}{4}\right) \begin{pmatrix} c_4 & c_4^2 & c_4^3 \\ c_5 & c_5^2 & c_5^3 \\ 1 & 1 & 1 \end{pmatrix}^{-1},$$

with  $b_1 = 1 - b_4 - b_5 - b_6$ . Note that we choose  $b_3 = 0$  so that the calculation work could be reduced. And for the quadrature formulas up to order 5 for  $(\bar{A}, \bar{b}, \bar{c})_6$ , we have

$$(\bar{b}_3, \bar{b}_4, \bar{b}_5, \bar{b}_6) = \left(\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}\right) \begin{pmatrix} \bar{c}_3 & \bar{c}_3^2 & \bar{c}_3^3 & \bar{c}_3^4 \\ \bar{c}_4 & \bar{c}_4^2 & \bar{c}_4^3 & \bar{c}_4^4 \\ \bar{c}_5 & \bar{c}_5^2 & \bar{c}_5^3 & \bar{c}_5^4 \\ 1 & 1 & 1 & 1 \end{pmatrix}^{-1},$$

with  $\bar{b}_1 = 1 - \bar{b}_3 - \bar{b}_4 - \bar{b}_5 - \bar{b}_6$ .

Let  $a_{42} = u$ , and  $\bar{a}_{42} = v$ . In order that the simplifying effects of  $C(2)$  conditions holds for these methods, we have to let

$$\begin{aligned} a_{32} &= \frac{c_3^2}{2c_2}, & a_{31} &= c_3 - a_{32}, & \bar{a}_{32} &= \frac{\bar{c}_3^2}{2\bar{c}_2}, \\ \bar{a}_{31} &= \bar{c}_3 - \bar{a}_{32}, & a_{43} &= \frac{c_4^2 - 2uc_2}{2c_3}, & \bar{a}_{43} &= \frac{\bar{c}_4^2 - 2v\bar{c}_2}{2\bar{c}_3}, \\ a_{41} &= c_4 - a_{43} - u, & \bar{a}_{41} &= \bar{c}_4 - \bar{a}_{43} - v, \\ a_{51} &= c_5 - a_{52} - a_{53} - a_{54}, & \bar{a}_{51} &= \bar{c}_5 - \bar{a}_{52} - \bar{a}_{53} - \bar{a}_{54}, \\ \bar{a}_{53} &= \frac{\bar{c}_5^2 - 2\bar{a}_{52}\bar{c}_2 - 2\bar{a}_{54}\bar{c}_4}{2\bar{c}_3}, & a_{53} &= \frac{c_5^2 - 2a_{52}c_2 - 2a_{54}c_4}{2c_3}. \end{aligned}$$

We solve the following order conditions by linear combinations of order conditions. This involve the Picard integral  $E$  in terms of integral (see [4,11]).

For the order condition on the tree  $\vee$ , we can solve the order conditions

$$b^T(1 - c)Ac(c - c_3) = \frac{1}{60} - \frac{c_3}{24}, \quad \bar{b}^T(1 - \bar{c})\bar{A}\bar{c}(\bar{c} - \bar{c}_3) = \frac{1}{60} - \frac{\bar{c}_3}{24}$$

for  $a_{54}$  and  $\bar{a}_{54}$ . Therefore, we have

$$a_{54} = \frac{1/60 - c_3/24}{b_5(1 - c_5)c_4(c_4 - c_3)}, \quad \bar{a}_{54} = \frac{1/60 - \bar{c}_3/24}{\bar{b}_5(1 - \bar{c}_5)\bar{c}_4(\bar{c}_4 - \bar{c}_3)}.$$

The conditions

$$a_{52} = -\frac{b_3(1 - c_3)a_{32} + b_4(1 - c_4)u}{b_5(1 - c_5)},$$

$$\bar{a}_{52} = -\frac{\bar{b}_3(1 - \bar{c}_3)\bar{a}_{32} + \bar{b}_4(1 - \bar{c}_4)v}{\bar{b}_5(1 - \bar{c}_5)}$$

enable these methods to be used in place of  $C(2)$  up to order 5.

For  $D(1)$ , we have

$$(a_{61}, a_{62}, a_{63}, a_{64}, a_{65}, 0) = \frac{b^T(1 - c) - b_4A[4] - b_5A[5]}{b_6},$$

$$(\bar{a}_{61}, \bar{a}_{62}, \bar{a}_{63}, \bar{a}_{64}, \bar{a}_{65}, 0) = \frac{\bar{b}^T(1 - \bar{c}) - \bar{b}_3\bar{A}[3] - \bar{b}_4\bar{A}[4] - \bar{b}_5\bar{A}[5]}{\bar{b}_6},$$

where  $A[i]$  and  $\bar{A}[i]$  are the  $i$ th row of matrix  $A$  and  $\bar{A}$ , respectively.

For the tree  $\begin{array}{c} \vee \\ \vee \end{array}$ , the order condition

$$\begin{array}{c} c \quad c - c_2 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ c - c_5 \quad 1 - c \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ b^T \end{array} \quad + \quad \begin{array}{c} \bar{c} \quad \bar{c} - \bar{c}_2 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ \bar{c} - \bar{c}_5 \quad 1 - \bar{c} \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ \bar{b}^T \end{array}$$

leads to an equivalent order condition.

$$w_1 = \left( \frac{1}{15} - \frac{c_2}{40} - \frac{c_5}{60} + \frac{c_2c_5}{24} \right) - (b_4(1 - c_4)(c_4 - c_5))a_{43}(c_3(c_3 - c_2))$$

$$+ \left( \frac{1}{15} - \frac{\bar{c}_2}{40} - \frac{\bar{c}_5}{60} + \frac{\bar{c}_2\bar{c}_5}{24} \right) - (\bar{b}_4(1 - \bar{c}_4)(\bar{c}_4 - \bar{c}_5))\bar{a}_{43}(\bar{c}_3(\bar{c}_3 - \bar{c}_2)) - \frac{1}{9}$$

$$= 0.$$

The order condition  $b^T c^2 A^2 c + \bar{b}^T \bar{c}^2 \bar{A}^2 \bar{c} = \frac{1}{18}$  is equivalent to

$$0 = w_2 = b_4(1 - c_4)(c_4 - c_5)a_{43}a_{32}c_2 + \bar{b}_4(1 - \bar{c}_4)(\bar{c}_4 - \bar{c}_5)\bar{a}_{43}\bar{a}_{32}\bar{c}_2$$

$$- \int_0^1 (1 - x_2)(x_2 - c_5) \int_0^{x_2} \int_0^{x_1} \xi \, d\xi \, dx_1 \, dx_2$$

$$- \int_0^1 (1 - x_2)(x_2 - \bar{c}_5) \int_0^{x_2} \int_0^{x_1} \xi \, d\xi \, dx_1 \, dx_2,$$

$$= b_4(1 - c_4)(c_4 - c_5)a_{43}a_{32}c_2 + \bar{b}_4(1 - \bar{c}_4)(\bar{c}_4 - \bar{c}_5)\bar{a}_{43}\bar{a}_{32}\bar{c}_2 - \left( \frac{2}{180} - \frac{c_5}{5!} - \frac{\bar{c}_5}{5!} \right).$$

We can solve  $w_1 = 0$ ,  $w_2 = 0$  for  $u$ ,  $v$ . For the order condition  $b^T c A^3 c + \bar{b}^T \bar{c} \bar{A}^3 \bar{c} = \frac{2}{144}$ , we have

$$w_3 = \frac{1}{360} + \frac{(2 - 5c_3)c_3(-c_4^2 + 2c_2u)}{480c_4(-c_3 + c_4)} + \frac{(2 - 5\bar{c}_3)\bar{c}_3(-\bar{c}_4^2 + 2\bar{c}_2v)}{480\bar{c}_4(-\bar{c}_3 + \bar{c}_4)} = 0.$$

Solving  $w_3 = 0$ , we can find  $c_2$ .

The order condition  $b^T c^5 + \bar{b}^T \bar{c}^5 = \frac{1}{3}$  can be reduced to

$$w_4 = \frac{1 + c_3 + c_4 + c_5}{5} - \frac{c_3 + c_4 + c_5 + c_3c_4 + c_4c_5 + c_3c_5}{4} + \frac{c_3c_4 + c_4c_5 + c_3c_5 + c_3c_4c_5}{3} - \frac{c_3c_4c_5}{2} + \frac{1 + \bar{c}_3 + \bar{c}_4 + \bar{c}_5}{5} - \frac{\bar{c}_3 + \bar{c}_4 + \bar{c}_5 + \bar{c}_3\bar{c}_4 + \bar{c}_4\bar{c}_5 + \bar{c}_3\bar{c}_5}{4} + \frac{\bar{c}_3\bar{c}_4 + \bar{c}_4\bar{c}_5 + \bar{c}_3\bar{c}_5 + \bar{c}_3\bar{c}_4\bar{c}_5}{3} - \frac{\bar{c}_3\bar{c}_4\bar{c}_5}{2} - \frac{1}{3}.$$

For the order condition  $b^T c A c^3 + \bar{b}^T \bar{c} \bar{A} \bar{c}^3 = \frac{1}{12}$ , the equation

$$w_5 = \frac{1}{20} - \frac{c_3 + c_4}{60} + \frac{c_3c_4}{24} + \frac{1}{20} - \frac{\bar{c}_3 + \bar{c}_4}{60} + \frac{\bar{c}_3\bar{c}_4}{24} - \frac{1}{12} = 0$$

is a simplified equation.

The order condition for the bushy tree of order 5 for  $(A, b, c)_6$  could be simplified to

$$w_6 = \frac{1}{5} - \frac{1 + c_4 + c_5}{4} + \frac{c_4 + c_5 + c_4c_5}{3} - \frac{c_4c_5}{2}.$$

We can obtain  $c_4$ ,  $\bar{c}_4$ ,  $\bar{c}_5$  by solving  $w_4 = w_5 = w_6 = 0$ .

For the tree  $\mathcal{Y}$ , we have

$$w_7 = b_5(1 - c_5)a_{54}a_{43}c_3(c_3 - c_2) + e_5(1 - \bar{c}_5)\bar{a}_{54}\bar{a}_{43}\bar{c}_3(\bar{c}_3 - \bar{c}_2) - \int_0^1 (1 - x_2) \int_0^{x_2} \int_0^{x_1} \xi(\xi - c_2) d\xi dx_1 dx_2 - \int_0^1 (1 - x_2) \int_0^{x_2} \int_0^{x_1} \xi(\xi - \bar{c}_2) d\xi dx_1 dx_2$$

$$= b_5(1 - c_5)a_{54}a_{43}c_3(c_3 - c_2) + \bar{b}_5(1 - \bar{c}_5)\bar{a}_{54}\bar{a}_{43}\bar{c}_3(\bar{c}_3 - \bar{c}_2) - \left( \frac{1}{180} - \frac{c_2}{120} - \frac{\bar{c}_2}{120} \right).$$

Solving for  $w_7 = 0$ , we can get  $c_5 = 1$ , or  $\frac{21}{26}$ . The case  $c_5 = 1$  is not possible. Therefore, a sixth order composite method, say  $(L, m, n)_{12}$ , is derived.

The following error estimation is a zero approximation of method  $(L, m, n)_{12}$  based on embedded technique [6]. Let  $e = (1, \dots, 1)^T \in \mathbb{R}^{13}$  and

$$\hat{\delta}^T = (\hat{\delta}_1, 0, \hat{\delta}_3, \hat{\delta}_4, \hat{\delta}_5, \hat{\delta}_6, \hat{\delta}_7, 0, \hat{\delta}_9, \hat{\delta}_{10}, \hat{\delta}_{11}, \hat{\delta}_{12}, \hat{\delta}_{13})$$

be the weights of the error estimation for the composition method  $(L, m, n)_{12}$ . The conditions up to 4 and some trees of order 5 are

$$\begin{aligned} q_1 &= \hat{\delta}^T e, & q_2 &= \hat{\delta}^T \tilde{c}, & q_3 &= \hat{\delta}^T \tilde{c}^2, & q_4 &= \hat{\delta}^T \tilde{c}^3, \\ q_5 &= \hat{\delta}^T \tilde{A} \tilde{c}^2, & q_6 &= \hat{\delta}^T \tilde{A}^2 \tilde{c}, & q_7 &= \hat{\delta}^T \tilde{c}^4, & q_8 &= \hat{\delta}^T \tilde{A}^3 \tilde{c}, \\ q_9 &= \hat{\delta}^T \tilde{A}^2 \tilde{c}^2, & q_{10} &= \hat{\delta}^T \tilde{A} \tilde{c}^3. \end{aligned}$$

Solving  $q_1 = q_2 = \dots = q_{10} = 0$ , we obtain  $\hat{\delta}_1, \hat{\delta}_3, \hat{\delta}_4, \hat{\delta}_5, \hat{\delta}_6, \hat{\delta}_7, \hat{\delta}_9, \hat{\delta}_{10}, \hat{\delta}_{11}, \hat{\delta}_{12}$ .

We choose the following equation so that this error estimation performs better using multi-step zero approximation.

$$q_{11} = \hat{\delta}^T \tilde{c}^5 - \left( m^T n^6 - \frac{2^7}{7} \right).$$

Solving  $q_{11} = 0$  for  $\hat{\delta}_{13}$ , have  $\hat{\delta}_{13} = \frac{75641011}{2866090115}$ .

Therefore, the **rk66** methods are

0	0	0	0	0	0	0
$\frac{29}{60}$	$\frac{29}{60}$	0	0	0	0	0
$\frac{1}{4}$	$\frac{43}{232}$	$\frac{15}{232}$	0	0	0	0
$\frac{27}{80}$	$\frac{59589}{464000}$	$\frac{1863}{92800}$	$\frac{189}{1000}$	0	0	0
$\frac{21}{26}$	$\frac{145502}{318565}$	$-\frac{5796}{63713}$	$-\frac{55491}{21970}$	$\frac{6520}{2197}$	0	0
1	$-\frac{16535641}{4686255}$	$\frac{368}{551}$	$\frac{46994}{1995}$	$-\frac{6012320}{277263}$	$\frac{1164410}{585333}$	0
	$\frac{359}{3402}$	0	0	$\frac{1024000}{2099277}$	$\frac{57122}{154035}$	$\frac{19}{530}$



and

0	0	0	0	0	0	0
$-\frac{1}{20}$	$-\frac{1}{20}$	0	0	0	0	0
$\frac{1}{8}$	$\frac{9}{32}$	$-\frac{5}{32}$	0	0	0	0
$\frac{29}{40}$	$-\frac{80011}{4000}$	$\frac{10643}{800}$	$\frac{928}{125}$	0	0	0
$\frac{141}{286}$	$\frac{10067339323}{848020030}$	$-\frac{23857153}{2924207}$	$-\frac{399281873}{116968280}$	$\frac{131286745}{678416024}$	0	0
1	$\frac{1380889809}{44168015}$	$-\frac{394252}{19443}$	$-\frac{62235743}{81855030}$	$\frac{540628165}{1496449938}$	$\frac{718272965410}{510521636607}$	0
	$-\frac{379}{24534}$	0	$\frac{8864}{26523}$	$\frac{1204000}{3809817}$	$\frac{9199555222}{34265840445}$	$\frac{6481}{66990}$

with the weights of error estimation  $\hat{\delta}^T = (\hat{\delta}_1, 0, 0, \hat{\delta}_4, \dots, \hat{\delta}_{13})$ , where

$$\begin{aligned} \hat{\delta}_1 &= -\frac{9606408397}{1392919795890}, & \hat{\delta}_4 &= \frac{30014353164800}{1203343411669371}, & \hat{\delta}_5 &= -\frac{3157482722173}{63068312980575}, \\ \hat{\delta}_6 &= -\frac{5748716836}{759513880475}, & \hat{\delta}_7 &= -\frac{114671772676}{35158327440705}, & \hat{\delta}_8 &= 0, \\ \hat{\delta}_9 &= \frac{83810240188}{551373635105}, & \hat{\delta}_{10} &= -\frac{7480895987900}{311979395533113}, \\ \hat{\delta}_{11} &= \frac{420924520242786131}{98208986581581701175}, & \hat{\delta}_{12} &= -\frac{490229392291}{27428482400550}, & \hat{\delta}_{13} &= \frac{75641011}{2866090115}. \end{aligned}$$

*Note.* The error estimation  $\hat{\delta}^T$  is of order four and is derived by the embedded method of the composition method **rk66**.

#### 4. Experiments

In this section, we present some numerical results for the new methods. In order to investigate how well the scheme in section 2 controls stepsize, we choose the C5 problem in the DETEST set. We compare this effective order changing stepsize scheme **eff5ran**, **eff5fix** with the **England**, **rkf45**, and **Merson** methods in table 1. Note that, in this table, **eff5ran** denotes the effective order method  $\alpha_\rho$ , where  $\rho$  is the stepsize ratio for stepsize changing. **eff5fix** denotes a set of effective order methods calculated in advance for some special stepsize ratios shown in example 1. The tolerances are chosen near  $10^{-6}$  so that the global error produced by each method are almost the same. Furthermore, the global errors (GE) are found at the end point, and “step” means the number of steps taken, “rejstep” means the number of rejections, the total work is measured in the “flops” row.

Table 1  
Results of eff5ran, eff5fix, England, rkf45, and Merson on C5.

		eff5ran	eff5fix	England	rkf45	Merson
C5	Step	54	57	156	59	107
	Rejstep	0	0	0	0	0
	GE	$9.3232 \times 10^{-8}$	$7.2285 \times 10^{-8}$	$7.2905 \times 10^{-8}$	$6.7794 \times 10^{-8}$	$6.3027 \times 10^{-8}$
	Flops	476095	454466	1497520	583223	864221

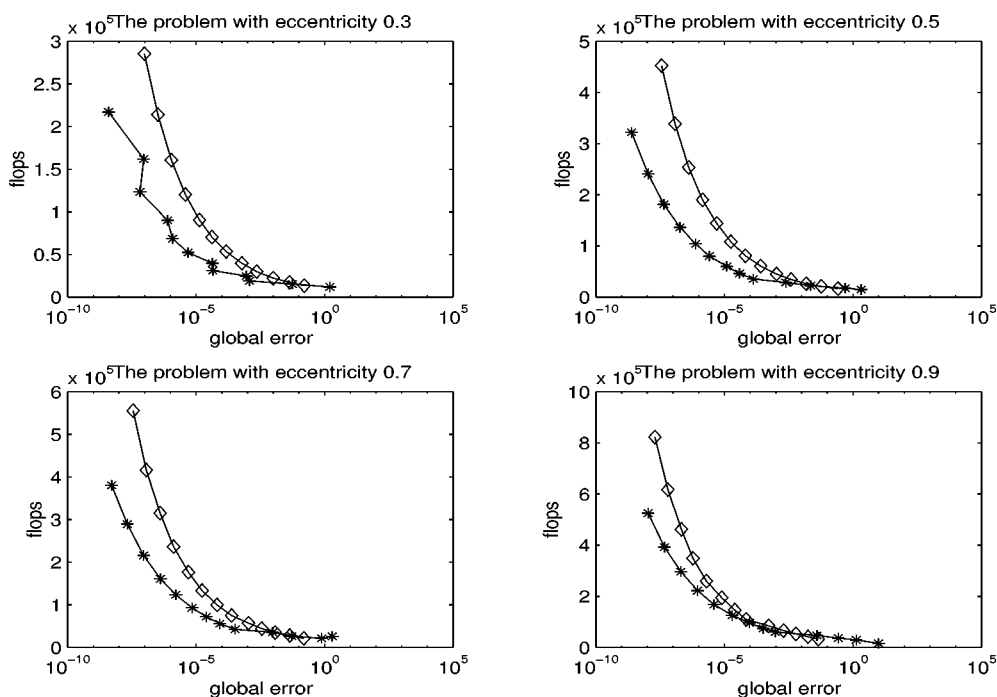


Figure 3. The Kepler orbit problems for eccentricities 0.3, 0.5, 0.7 and 0.9. eff5s5: \*, Merson:  $\diamond$ . Tolerances:  $10^{-n/2}$ ,  $n = 6-18$ .

The following experiments are based on solving the Kepler orbit problem

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

with eccentricity 0.3, 0.5, 0.7, 0.9. The integration interval is  $x \in [0, 20]$ . The global errors are found at the final point.

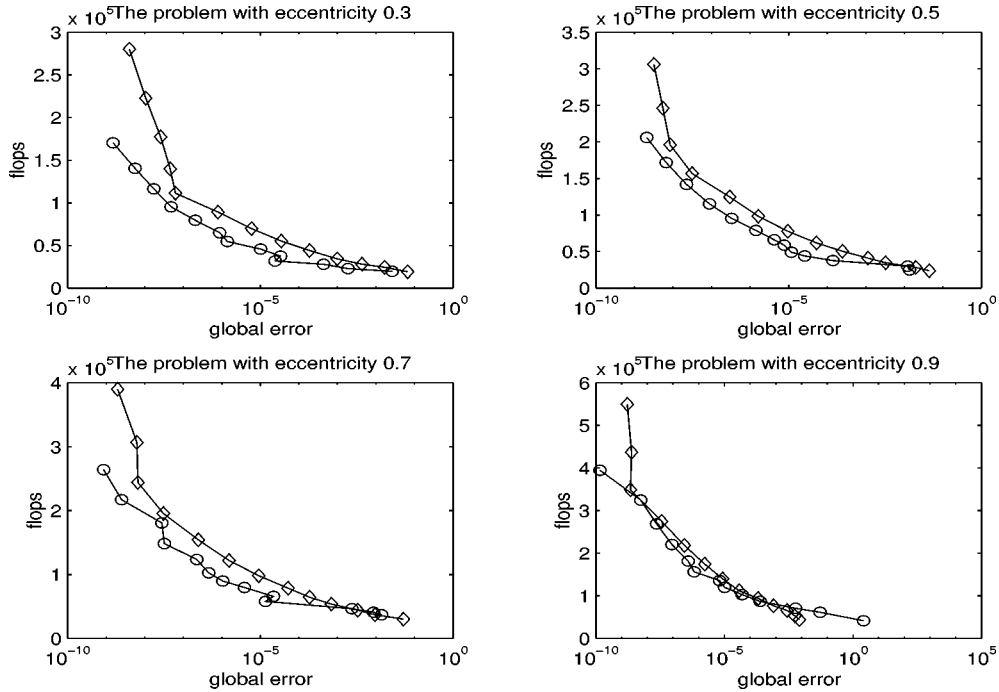


Figure 4. The results of the Kepler orbit problems with eccentricities 0.3, 0.5, 0.7 and 0.9, rk66:  $\circ$  DOPRI(5,4);  $\diamond$ . Tolerances:  $10^{-n/2}$ ,  $n = 8-20$ .

In figure 4, we have found that the **rk66** pair performs better than the DOPRI(5,4) pair.

### 5. Conclusion

Several applications of the idea of “*effective order*” have shown the potential of this type of methods. We believe that the changing stepsize scheme for effective order methods is encouraging and justifies further research of these methods.

The composition of methods with the same order is worth exploring for enhancing order, minimize the error constant, deriving better error estimation, or other purposes. There are still several ways to design composition methods. For instance, triple composition methods, experiments on a pair of composition methods without using one followed by the another. The enhanced order composition method **rk66** is found to be competitive amongst explicit Runge–Kutta methods.

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