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A method for the construction of combined 11 and 12 Runge-Kutta schemes is described here. The embedded order 11 scheme is provided with the aim of it being used for error control in the standard manner. The method of construction of these schemes is motivated by a 10(9) scheme due to Tom Baker at the University of Teeside and is similar to the method used elsewhere to construct order 11(10) schemes.

When the construction reaches the stage of requiring equations derived from the order conditions, the order conditions used at each step were selected from those that remained to be satisfied after the preceding step. Details of how this was achieved can be seen by viewing Maple worksheets which are available online.

The parameters that determine the specific schemes described here were obtained from a random search followed by a lengthy process of minimization of the principal error norm.

We first indicate how to construct a 30 stage order 12 Runge-Kutta scheme.

Step 1:

We specify the following stage-orders for stages 3 to 20.

Thus we have the following stage-order conditions involving the nodes  $c_i$  and linking coefficients  $a_{i,i}$ .

$$\sum_{j=1}^{i-1} a_{i,j} = c_i \text{ for } i = 3..20, \qquad \sum_{j=2}^{i-1} a_{i,j} c_j = \frac{c_i^2}{2} \text{ for } i = 3..20, \qquad \sum_{j=2}^{i-1} a_{i,j} c_j^2 = \frac{c_i^3}{3} \text{ for } i = 3..20,$$

$$\sum_{j=2}^{i-1} a_{i,j} c_j^3 = \frac{c_i^4}{4} \text{ for } i = 6..20, \qquad \sum_{j=2}^{i-1} a_{i,j} c_j^4 = \frac{c_i^5}{5} \text{ for } i = 9..20, \qquad \sum_{j=2}^{i-1} a_{i,j} c_j^5 = \frac{c_i^6}{6} \text{ for } i = 12..20,$$

$$\sum_{j=2}^{i-1} a_{i,j} c_j^6 = \frac{c_i^7}{7} \text{ for } i = 15..20, \qquad \sum_{j=2}^{i-1} a_{i,j} c_j^7 = \frac{c_i^8}{8} \text{ for } i = 19, 20.$$

We also have zero linking coefficients as follows.

$$a_{i,2} = 0, i = 4 ... 20,$$
  $a_{i,3} = 0, i = 6 ... 20,$   $a_{i,4} = 0, i = 7 ... 20,$   $a_{i,5} = 0, i = 9 ... 20,$   $a_{i,6} = 0, i = 11 ... 20,$   $a_{i,7} = 0, i = 11 ... 20,$   $a_{i,8} = 0, i = 12 ... 20,$   $a_{i,9} = 0, i = 15 ... 20,$   $a_{i,10} = 0, i = 15 ... 20,$   $a_{i,11} = 0, i = 19 ... 20,$   $a_{i,12} = 0, i = 19 ... 20,$   $a_{i,13} = 0, i = 19 ... 20.$ 

The following table in which the first column is omitted illustrates the zero linking coefficients.

We can use this information to obtain certain relations involving the nodes  $c_2$  to  $c_{20}$ . In the first instance these relations are given by the following integral equations.

$$\int_{0}^{c_{16}} x (x - c_{11}) (x - c_{12}) (x - c_{13}) (x - c_{14}) (x - c_{15}) dx = 0 \qquad ----- (xi)$$

$$\int_{0}^{c_{19}} x (x - c_{14}) (x - c_{15}) (x - c_{16}) (x - c_{17}) (x - c_{18}) dx = 0 \quad ----- (xii)$$

$$\int_{0}^{c_{19}} x^{2} (x - c_{14}) (x - c_{15}) (x - c_{16}) (x - c_{17}) (x - c_{18}) dx = 0 \quad ----- (xiii)$$

$$\int_{0}^{c_{20}} x (x - c_{14}) (x - c_{15}) (x - c_{16}) (x - c_{17}) (x - c_{18}) (x - c_{19}) dx = 0 \quad ----- \text{(xiv)}$$

Introducing the relation  $c_{11} = \frac{2}{3}c_{13}$  allows the equations (vi), (vii) and (viii) to produce the relations

$$c_9 = \frac{98 - \sqrt{10} + \sqrt{3694 - 212\sqrt{10}}}{156}c_{13}, \qquad c_{10} = \frac{98 - \sqrt{10} - \sqrt{3694 - 212\sqrt{10}}}{156}c_{13}$$

and

$$c_{12} = \frac{40 - 2\sqrt{10}}{39} c_{13}.$$

The equations (ix) and (x) in conjunction with the relations  $c_{11} = \frac{2}{3}c_{13}$  and  $c_{12} = \frac{40 - 2\sqrt{10}}{39}c_{13}$  give rise to the relations  $c_{13} = \eta c_{15}$ 

and

$$c_{14} = \frac{80 \left(\sqrt{10} - 20\right) \,\eta^3 + 10 \left(417 - 15\sqrt{10}\right) \,\eta^2 + 36 \left(2\sqrt{10} - 105\right) \,\eta + 1170}{1404 + 120 \left(\sqrt{10} - 20\right) \,\eta^3 + 40 \left(139 - 5\sqrt{10}\right) \,\eta^2 + 45 \left(2\sqrt{10} - 105\right) \,\eta} \,c_{15}.$$

where  $\eta$  is a real zero of the degree 6 polynomial

$$P(z) = 28000 z^{6} - (117600 + 1680 \sqrt{10}) z^{5} + (6090 \sqrt{10} + 203910) z^{4} - (188700 + 8700 \sqrt{10}) z^{3} + (99969 + 6276 \sqrt{10}) z^{2} - (29250 + 2340 \sqrt{10}) z + 3690 + 360 \sqrt{10}.$$

This polynomial has two real zeros with the approximate values 0.46400913396513 and 0.90501790944446. Equation (xi) gives rise to a relation of the form

$$c_{15} = \theta c_{16}$$

iwhere  $\theta$  is a real zero of the cubic polynomial

$$S(z) = d_3 z^3 + d_2 z^2 + d_1 z + d_0$$

with

$$d_0 = 42 \; (\; 4000 \; \eta^6 - \; 16800 \; \eta^5 - \; 240 \; \eta^5 \sqrt{10} \; + \; 870 \; \eta^4 \sqrt{10} \; + \; 29130 \; \eta^4 - \; 1500 \; \eta^3 \sqrt{10} \; - \; 32100 \; \eta^3 \; + \; 26367 \; \eta^2 + \; 1668 \; \eta^2 \sqrt{10} \; - \; 14625 \; \eta^2 + \; 1668 \; \eta^2 \sqrt{10} \; + \; 166$$

$$d_1 = 35 \left(4000 \, \eta^6 - 240 \, \eta^5 \sqrt{10} - 16800 \, \eta^5 + 48330 \, \eta^4 + 1470 \, \eta^4 \sqrt{10} - 3300 \, \eta^3 \sqrt{10} - 72300 \, \eta^3 + 3258 \, \eta^2 \sqrt{10} + 52452 \, \eta^2 - 1170 \, \eta \sqrt{10} - 14625 \, \eta\right),$$

$$d_2 = 200 \ (560 \ \eta^6 - 84 \ \eta^5 \sqrt{10} - 5880 \ \eta^5 + 12327 \ \eta^4 + 357 \ \eta^4 \sqrt{10} - 462 \ \eta^3 \sqrt{10} - 10122 \ \eta^3 + 2961 \ \eta^2 + 189 \ \eta^2 \sqrt{10} \ ),$$

$$d_3 = 4200 (80 \eta^6 - 210 \eta^5 - 3 \eta^5 \sqrt{10} + 6 \eta^4 \sqrt{10} + 192 \eta^4 - 3 \eta^3 \sqrt{10} - 60 \eta^3).$$

We take

 $\eta \simeq 0.9050179094444592302850092001266376783360386842107738556985099105305710627647138909540$  and choose the largest of the three resulting values for  $\theta$ , namely

 $\theta \sim 1.900460407318210405781574017326160583594516445668076545674045253102940120877393399745$ .

At this stage we have

$$c_{13} = \eta \ c_{15}$$
,  $c_{14} = \sigma \ c_{15}$ ,  $c_{15} = \theta \ c_{16}$ ,

where

$$\sigma = \frac{80 (\sqrt{10} - 20) \eta^3 + 10 (417 - 15 \sqrt{10}) \eta^2 + 36 (2 \sqrt{10} - 105) \eta + 1170}{1404 + 120 (\sqrt{10} - 20) \eta^3 + 40 (139 - 5 \sqrt{10}) \eta^2 + 45 (2 \sqrt{10} - 105) \eta}.$$

Suppose that

$$c_{16} = \xi c_{17}$$

where  $\,\xi\,$  is a parameter whose value we can choose later.

Then we can use equations (xii) and (xiii) to find  $\tau$  such that  $c_{17} = \tau c_{19}$ , where  $\tau$  is a zero of a degree 8 polynomial

$$H(z) = h_8 z^8 + h_7 z^7 + h_6 z^6 + h_5 z^5 + h_4 z^4 + h_3 z^3 + h_2 z^2 + h_1 z + h_0,$$

where

$$h_0 = 150$$
,

$$h_1 = -420 ((\xi + \sigma \xi) \theta + 1 + \xi),$$

$$h_2 = 35 ((8 \sigma^2 \xi^2 + 35 \xi^2 \sigma + 8 \xi^2) \theta^2 + ((35 \xi + 35 \xi^2) \sigma + 35 \xi + 35 \xi^2) \theta + 8 \xi^2 + 8 + 35 \xi),$$

$$h_3 = -420$$

$$((2 \xi^3 \sigma + 2 \sigma^2 \xi^3) \theta^3 + ((2 \xi^3 + 2 \xi^2) \sigma^2 + (9 \xi^3 + 9 \xi^2) \sigma + 2 \xi^3 + 2 \xi^2) \theta^2 + ((2 \xi^3 + 9 \xi^2 + 2 \xi) \sigma + 2 \xi^3 + 9 \xi^2 + 2 \xi) \theta + 2 \xi^2 + 2 \xi),$$

$$h_4 = 42 \left(14 \sigma^2 \theta^4 \xi^4 + \left((64 \xi^3 + 64 \xi^4) \sigma^2 + (64 \xi^3 + 64 \xi^4) \sigma\right) \theta^3 + \left((14 \xi^2 + 14 \xi^4 + 64 \xi^3) \sigma^2 + (64 \xi^4 + 303 \xi^3 + 64 \xi^2) \sigma + 14 \xi^2 + 14 \xi^4 + 64 \xi^3\right) \theta^2 + \left((64 \xi^2 + 64 \xi^3) \sigma + 64 \xi^2 + 64 \xi^3\right) \theta + 14 \xi^2\right),$$

$$h_5 = -280 ((7 \xi^4 + 7 \xi^5) \sigma^2 \theta^4 + ((7 \xi^3 + 7 \xi^5 + 34 \xi^4) \sigma^2 + (7 \xi^3 + 7 \xi^5 + 34 \xi^4) \sigma) \theta^3 + ((7 \xi^4 + 7 \xi^3) \sigma^2 + (34 \xi^4 + 34 \xi^3) \sigma + 7 \xi^4 + 7 \xi^3) \theta^2 + (7 \xi^3 + 7 \xi^3) \theta),$$

$$h_6 = 1470 \left( (\xi^4 + 5 \, \xi^5 + \xi^6) \, \sigma^2 \, \theta^4 + ((5 \, \xi^4 + 5 \, \xi^5) \, \sigma^2 + (5 \, \xi^4 + 5 \, \xi^5) \, \sigma \right) \, \theta^3 + (5 \, \xi^4 \, \sigma + \xi^4 + \sigma^2 \, \xi^4) \, \theta^2 \right),$$

$$h_7 = 5880 ((\xi^6 + \xi^5) \sigma^2 \theta^4 + (\xi^5 \sigma + \sigma^2 \xi^5) \theta^3),$$

$$h_8 = 4900 \,\sigma^2 \,\theta^4 \,\xi^6.$$

Equations (xii) and (xiii) also give rise to the relation  $c_{18} = \omega c_{19}$ , where

$$\omega = \frac{7 \, \xi^2 \, \sigma \, \tau^2 \, (20 \, \tau^2 \, \xi - 15 \, \xi \, \tau - 15 \, \tau + 12) \, \theta^2 - 7 \, \xi \, \tau \, (10 - 12 \, \xi \, \tau - 12 \, \tau + 15 \, \tau^2 \, \xi) \, (\sigma + 1) \, \theta + 60 + 84 \, \tau^2 \, \xi - 70 \, (1 + \xi) \, \tau}{35 \, \xi^2 \, \sigma \, \tau^2 \, (3 - 4 \, \tau - 4 \, \xi \, \tau + 6 \, \tau^2 \, \xi) \, \theta^2 - 7 \, \xi \, \tau \, (20 \, \tau^2 \, \xi - 15 \, \xi \, \tau - 15 \, \tau + 12) \, (\sigma + 1) \, \theta + 70 + 105 \, \tau^2 \, \xi - 84 \, (1 + \xi) \, \tau}$$

Equation (xiv) then gives rise to a relation  $c_{19} = \zeta c_{20}$ , where  $\zeta$  is a real zero of a degree 6 polynomial

$$K(z) = k_6 z^6 + k_5 z^5 + k_4 z^4 + k_3 z^3 + k_2 z^2 + k_1 z + k_0$$

where

$$k_0 = 105$$
,

$$k_1 = -120 ((1 + \sigma) \tau \xi \theta + \omega + 1 + \tau + \xi \tau),$$

$$k_2 = (\theta^2 \xi^2 \tau^2 + (\xi^2 \tau^2 + (\tau^2 + (1 + \omega)\tau)\xi)\theta)\sigma + (\xi^2 \tau^2 + (\tau^2 + (1 + \omega)\tau)\xi)\theta + (\tau^2 + (1 + \omega)\tau)\xi + (1 + \omega)\tau + \omega,$$

$$\begin{split} k_3 = & -168 \left( \left( \left( \xi^3 \, \tau^3 + \left( \tau^3 + \left( 1 + \omega \right) \tau^2 \right) \xi^2 \right) \theta^2 + \left( \left( \tau^3 + \left( 1 + \omega \right) \tau^2 \right) \xi^2 + \left( \left( 1 + \omega \right) \tau^2 + \omega \tau \right) \xi \right) \theta \right) \sigma \\ & + \left( \left( \tau^3 + \left( 1 + \omega \right) \tau^2 \right) \xi^2 + \left( \left( 1 + \omega \right) \tau^2 + \omega \tau \right) \xi \right) \theta + \left( \left( 1 + \omega \right) \tau^2 + \omega \tau \right) \xi + \omega \tau \right), \end{split}$$

$$k_{4} = 210 \ ( (((\tau^{4} + (1 + \omega)\tau^{3})\xi^{3} + ((1 + \omega)\tau^{3} + \omega\tau^{2})\xi^{2})\theta^{2} + (((1 + \omega)\tau^{3} + \omega\tau^{2})\xi^{2} + \omega\tau^{2}\xi)\theta) \sigma + (((1 + \omega)\tau^{3} + \omega\tau^{2})\xi^{2} + \omega\tau^{2}\xi)\theta + \omega\tau^{2}\xi)$$

$$k_5 = 280 \left( \left( \left( \left( \left( \left( \left( 1 + \omega \right) \tau^4 + \tau^3 \omega \right) \xi^3 + \xi^2 \tau^3 \omega \right) \theta^2 + \theta \xi^2 \tau^3 \omega \right) \sigma + \theta \xi^2 \tau^3 \omega \right),$$

$$k_6 = 420 \, \sigma \, \theta^2 \, \xi^3 \, \tau^4 \, \omega.$$

This polynomial is obtained by making the substitutions

$$c_{14} = \sigma \theta \xi \tau c_{19}, \quad c_{15} = \theta \xi \tau c_{19}, \quad c_{16} = \xi \tau c_{19}, \quad c_{17} = \tau c_{19}, \quad c_{18} = \omega c_{19},$$

in equation (xiv). The coefficients depend on  $\sigma$ ,  $\theta$ ,  $\xi$ ,  $\tau$  and  $\omega$ .

Specifying the nodes  $c_7$  anc<sub>13</sub> together with the linking coefficient  $a_{18,17}$  allows all the nodes and linking coefficients in stages 2 to 20 to be calculated. This can be done in 3 stages. The nodes and linking coefficients in stages 2 to 13 can be obtained from the relations between the nodes in conjunction with suitable stage-order conditions. Some of the stage-order conditions must be omitted to avoid obtaining an over-determined system of equations. Additional relations between the nodes can be used in conjunction with suitable stage order conditions to calculate the nodes and linking coefficients in stages 14, 15 and 16.

The nodes and linking coefficients in stages 18, 19 and 20 can be obtained in a similar way.

#### Step 2

We specify the remaining nodes  $c_{21}$ ,  $c_{22}$ ,  $c_{23}$ ,  $c_{24}$ ,  $c_{25}$ ,  $c_{26}$ ,  $c_{27}$ ,  $c_{28}$ ,  $c_{29}$ ,  $c_{30} = 1$  and the weight  $b_{30}$ .

We also require that  $b_i = 0$ , i = 2 ... 18. Then we can obtain all the remaining weights by using the order 12 quadrature conditions:

$$\sum_{i=1}^{30} b_i = 1, \quad \sum_{i=1}^{30} b_i c_i^k = \frac{1}{k+1}, \quad k = 1 \dots 11.$$

Step 3:

We specify the linking coefficients:  $a_{22,21}$ ,  $a_{23,21}$ ,  $a_{23,22}$ ,  $a_{24,19}$ ,  $a_{24,22}$ ,  $a_{26,20}$ .

We also specify the zero linking coefficients in rows 21 to 31.

$$a_{i,j} = 0$$
,  $j = 2 ... 13$ ,  $i = 21 ... 30$ .

The stage-orders of stages 3 to 30 are given as follows.

The stages 21 to 30 have stage-order 8. Thus the following conditions hold.

$$\sum_{j=1}^{i-1} a_{i,j} = c_i, \text{ for } i = 21..30, \qquad \sum_{j=2}^{i-1} a_{i,j} c_j^k = \frac{c_i^{(k+1)}}{k+1}, \text{ for } i = 21..30, k = 1..7.$$

After specifying the zero linking coefficients  $a_{i,j} = 0$  for j = 2 ... 13, i = 21 ... 30, these equations provide linear relations among the linking coefficients in stages 21 to 30.

We can obtain linear expressions for 80 of the linking coefficients with the following 39 linking coefficients remaining as parameters.

$$a_{24,\,18},\quad a_{25,\,i},\ i=18,\,19,\,22,\,24 \quad a_{26,\,i},\,i=18,\,19,\,22,\,24, \quad a_{27,\,i},\,i=1,\,14,\,16,\,22,\,23,\,24, \quad a_{28,\,i},\,i=17,\,18,\,19,\,20,\,21,\,22,\,24,\\ a_{29,\,i},\,i=17,\,18,\,19,\,20,\,21,\,22,\,24,\,28, \quad a_{30,\,i},\,i=17,\,18,\,19,\,20,\,22,\,23,\,24,\,27,\,29.$$

### Step 4:

A system of equations arising from the 7 column simplifying conditions

$$\sum_{i=j+1}^{30} b_i a_{i,j} = b_j (1 - c_j), \quad j = 19, 20, 22, 24, 27, 28, 29,.$$

can be solved to give linear expressions for  $a_{25,24}$ ,  $a_{27,22}$ ,  $a_{27,23}$ ,  $a_{30,19}$ ,  $a_{30,20}$ ,  $a_{30,27}$ ,  $a_{30,29}$ .

By means of substitution we obtain linear expressions for 87 linking coefficients with the following 32 linking coefficients remaining as parameters.

$$a_{24,\,18},\quad a_{25,\,i},\ i=18,\,19,\,22\quad a_{26,\,i},\,i=18,\,19,\,22,\,24,\quad a_{27,\,i},\,i=1,\,14,\,16,\,24,\quad a_{28,\,i},\,i=17,\,18,\,19,\,20,\,21,\,22,\,24,\\ a_{29,\,i},\,i=17,\,18,\,19,\,20,\,21,\,22,\,24,\,28,\quad a_{30,\,i},\,i=17,\,18,\,22,\,23,\,24.$$

A system of equations arising from the following pair of column simplifying conditions.

$$\sum_{i=j+1}^{30} b_i a_{i,j} = b_j (1 - c_j), \quad j = 23, 25,$$

can be solved to give linear expressions for  $a_{26, 18}$  and  $a_{27, 1}$ .

By means of substitution we obtain linear expressions for 89 linking coefficients with the following 30 linking coefficients remaining as parameters.

$$a_{24,\,18},\quad a_{25,\,i},\ i=18,\,19,\,22 \quad a_{26,\,i},\,i=19,\,22,\,24,\quad a_{27,\,i},\,i=14,\,16,\,24,\quad a_{28,\,i},\,i=17,\,18,\,19,\,20,\,21,\,22,\,24,\\ a_{29,\,i},\,i=17,\,18,\,19,\,20,\,21,\,22,\,24,\,28,\quad a_{30,\,i},\,i=17,\,18,\,22,\,23,\,24.$$

It turns out that the following two additional column simplifying conditions are also satisfied at this stage.

$$\sum_{i=j+1}^{30} b_i a_{i,j} = b_j (1 - c_j), \quad j = 21, 26.$$

# Step 5:

A system of equations arising from the 6 order conditions

$$\begin{split} \sum_{i=3}^{30} b_i \, c_i \left( \sum_{j=2}^{i-1} a_{i,j} \, c_j^{\, 9} \right) &= \frac{1}{120}, \quad \sum_{i=3}^{30} b_i \, c_i^{\, 2} \left( \sum_{j=2}^{i-1} a_{i,j} \, c_j^{\, 8} \right) = \frac{1}{108}, \\ \sum_{i=4}^{30} b_i \, c_i^{\, 2} \left( \sum_{j=3}^{i-1} a_{i,j} \left( \sum_{k=2}^{j-1} a_{j,k} \, c_k^{\, 7} \right) \right) &= \frac{1}{864}, \quad \sum_{i=4}^{30} b_i \, c_i \left( \sum_{j=3}^{i-1} a_{i,j} \, c_j \left( \sum_{k=2}^{j-1} a_{j,k} \, c_k^{\, 7} \right) \right) = \frac{1}{960}, \\ \sum_{i=4}^{30} b_i \, c_i^{\, 2} \left( \sum_{j=3}^{i-1} a_{i,j} \, c_j \left( \sum_{k=2}^{j-1} a_{j,k} \, c_k^{\, 6} \right) \right) &= \frac{1}{756}, \quad \sum_{i=4}^{30} b_i \, c_i \left( \sum_{j=3}^{i-1} a_{i,j} \, c_j^{\, 2} \left( \sum_{k=2}^{j-1} a_{j,k} \, c_k^{\, 6} \right) \right) = \frac{1}{840}, \end{split}$$

can be solved to give linear expressions for  $a_{25, 18}$ ,  $a_{26, 19}$ ,  $a_{27, 16}$ ,  $a_{30, 17}$ ,  $a_{30, 18}$  and  $a_{30, 23}$ .

By means of substitution we obtain linear expressions for 95 linking coefficients with the following 24 linking coefficients remaining as parameters.

$$a_{24, 18}, \quad a_{25, i}, \quad i = 19, 22 \quad a_{26, i}, \quad i = 22, 24, \quad a_{27, i}, \quad i = 14, 24, \quad a_{28, i}, \quad i = 17, 18, 19, 20, 21, 22, 24, \\ a_{29, i}, \quad i = 17, 18, 19, 20, 21, 22, 24, 28, \quad a_{30, i}, \quad i = 22, 24.$$

# Step 6:

A system of equations arising from the 3 order conditions

$$\sum_{i=4}^{30} b_i \left( \sum_{j=3}^{i-1} a_{i,j} c_j \left( \sum_{k=2}^{j-1} a_{j,k} c_k^8 \right) \right) = \frac{1}{1188}, \quad \sum_{i=4}^{30} b_i c_i^3 \left( \sum_{j=3}^{i-1} a_{i,j} \left( \sum_{k=2}^{j-1} a_{j,k} c_k^6 \right) \right) = \frac{1}{672},$$

$$\sum_{i=5}^{30} b_i \left( \sum_{i=4}^{i-1} a_{i,j} c_j \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} c_l^{7} \right) \right) \right) = \frac{1}{9504}$$

can be solved to give linear expressions for  $a_{24,18}$ ,  $a_{25,22}$  and  $a_{27,14}$ .

By means of substitution we obtain linear expressions for 98 linking coefficients in terms of the 21 linking coefficients

$$a_{25, 19}, \ a_{26, i}, \ i = 22, 24, \ a_{27, 24}, \ a_{28, i}, \ i = 17, 18, 19, 20, 21, 22, 24, \\ a_{29, i}, \ i = 17, 18, 19, 20, 21, 22, 24, 28, \ a_{30, i}, \ i = 22, 24.$$

# Step 7:

A system of equations arising from the 3 order conditions

$$\sum_{i=5}^{30} b_i c_i^3 \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} c_l^5 \right) \right) \right) = \frac{1}{4032}, \quad \sum_{i=5}^{30} b_i c_i^2 \left( \sum_{j=4}^{i-1} a_{i,j} c_j \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} c_l^5 \right) \right) \right) = \frac{1}{4536},$$

$$\sum_{i=5}^{30} b_i c_i \left( \sum_{j=4}^{i-1} a_{i,j} c_j^2 \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} c_l^5 \right) \right) \right) = \frac{1}{5040}$$

can be solved to give a linear expressions for  $\,a_{25,\,19},\,\,a_{26,\,24}\,$  and  $\,a_{29,\,17}.$ 

By means of substitution we obtain linear expressions for 101 linking coefficients in terms of the 18 linking coefficients

$$a_{26, 22}$$
,  $a_{27, 24}$ ,  $a_{28, i}$ ,  $i = 17, 18, 19, 20, 21, 22, 24, 
 $a_{29, i}$ ,  $i = 18, 19, 20, 21, 22, 24, 28,  $a_{30, i}$ ,  $i = 22, 24$ .$$ 

### Step 8:

A system of equations arising from the 2 order conditions

$$\sum_{i=5}^{30} b_i c_i^2 \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{j-1} a_{j,k} c_k \left( \sum_{l=2}^{k-1} a_{k,l} c_l^5 \right) \right) \right) = \frac{1}{5184}, \quad \sum_{i=5}^{30} b_i c_i \left( \sum_{j=4}^{i-1} a_{i,j} c_j \left( \sum_{k=3}^{j-1} a_{j,k} c_k \left( \sum_{l=2}^{k-1} a_{k,l} c_l^5 \right) \right) \right) = \frac{1}{5760}$$

can be solved to give a linear expressions for  $a_{26,22}$  and  $a_{27,24}$ .

By means of substitution we obtain linear expressions for 103 linking coefficients in terms of the 16 linking coefficients

$$a_{28,i}, i=17, 18, 19, 20, 21, 22, 24, \\ a_{29,i}, i=18, 19, 20, 21, 22, 24, 28, \quad a_{30,i}, i=22, 24.$$

#### Step 9

We now specify values for 5 of the linking coefficients in rows 28 and 30, namely  $a_{28,17}$ ,  $a_{28,18}$ ,  $a_{28,19}$ ,  $a_{30,22}$  and  $a_{30,24}$ .

By means of substitution we obtain linear expressions for 64 linking coefficients in terms of the 11 linking coefficients  $a_{28}$ , i = 20, 21, 22, 24,  $a_{29}$ , i = 18, 19, 20, 21, 22, 24, 28.

A system of equations in the 11 variable linking coefficients can be constructed from the 11 order conditions

$$\begin{split} \sum_{i=4}^{30} b_i \, c_i \left( \sum_{j=3}^{i-1} a_{i,j} \left( \sum_{k=2}^{j-1} a_{j,k} \, c_k^{\, 8} \right) \right) &= \frac{1}{1080}, \quad \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} \, c_l^{\, 7} \right) \right) \right) &= \frac{1}{8640}, \\ \sum_{i=5}^{30} b_i \, c_i^{\, 2} \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{6048}, \quad \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \, c_j \left( \sum_{k=3}^{j-1} a_{j,k} \left( \sum_{l=2}^{k-1} a_{k,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{6720}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{j-1} a_{j,k} \, c_k \left( \sum_{l=2}^{k-1} a_{k,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{j-1} a_{j,k} \, c_k \left( \sum_{l=2}^{k-1} a_{k,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{i-1} a_{j,k} \, c_k \left( \sum_{l=2}^{i-1} a_{k,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{i-1} a_{j,k} \, c_k \left( \sum_{l=2}^{i-1} a_{k,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{i-1} a_{j,k} \, c_k \left( \sum_{l=2}^{i-1} a_{k,l} \, c_l^{\, 6} \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{i-1} a_{i,k} \, c_k \left( \sum_{l=2}^{i-1} a_{k,l} \, c_l^{\, 6} \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{j=4}^{i-1} a_{i,j} \left( \sum_{k=3}^{i-1} a_{i,k} \, c_k \left( \sum_{k=3}^{i-1} a_{i,k} \, c_k \left( \sum_{l=2}^{i-1} a_{i,l} \, c_l^{\, 6} \right) \right) \right) &= \frac{1}{60480}, \\ \sum_{i=5}^{30} b_i \, c_i \left( \sum_{k=3}^{i-1} a_{i,k} \, c_k \right) \right) \right) \right) \\ \sum_{i=5}^{30} b_i \, c_i \, c_$$

$$\sum_{i=6}^{30} b_{i} c_{i}^{2} \left( \sum_{j=5}^{i-1} a_{i,j} \left( \sum_{k=4}^{j-1} a_{j,k} \left( \sum_{l=3}^{k-1} a_{k,l} \left( \sum_{m=2}^{l-1} a_{l,m} c_{m}^{5} \right) \right) \right) \right) = \frac{1}{36288},$$

$$\sum_{i=6}^{30} b_{i} c_{i} \left( \sum_{j=5}^{i-1} a_{i,j} c_{j} \left( \sum_{k=4}^{j-1} a_{j,k} \left( \sum_{l=3}^{k-1} a_{k,l} \left( \sum_{m=2}^{l-1} a_{l,m} c_{m}^{5} \right) \right) \right) \right) = \frac{1}{40320},$$

$$\sum_{i=6}^{30} b_{i} c_{i} \left( \sum_{j=5}^{i-1} a_{i,j} \left( \sum_{k=4}^{j-1} a_{j,k} c_{k} \left( \sum_{l=3}^{k-1} a_{k,l} \left( \sum_{m=2}^{l-1} a_{l,m} c_{m}^{5} \right) \right) \right) \right) = \frac{1}{45360},$$

$$\sum_{i=7}^{30} b_{i} c_{i} \left( \sum_{j=6}^{i-1} a_{i,j} \left( \sum_{k=5}^{j-1} a_{j,k} \left( \sum_{l=4}^{k-1} a_{k,l} \left( \sum_{m=3}^{l-1} a_{l,m} \left( \sum_{m=2}^{m-1} a_{m,n} c_{m}^{5} \right) \right) \right) \right) \right) = \frac{1}{362880},$$

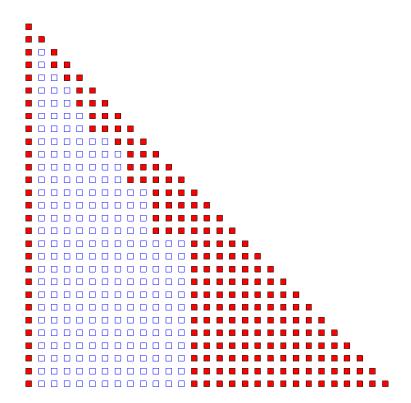
$$\sum_{i=6}^{30} b_{i} c_{i} \left( \sum_{j=5}^{i-1} a_{i,j} \left( \sum_{k=5}^{j-1} a_{j,k} \left( \sum_{k=4}^{k-1} a_{k,l} \left( \sum_{m=3}^{l-1} a_{l,m} c_{m}^{5} \right) \right) \right) \right) \right) = \frac{1}{33264}.$$

The resulting equations have respective degrees 2, 2, 2, 2, 2, 3, 2, 2, 3, 2 in the 11 variables and so would be extremely difficult to solve analytically. However, the system can be solved by using the multidimensional version of Newton's method if initial values are provided.

A given order 12 scheme is determined by specifying values for the 24 coefficients

$$c_7,\ c_{13},\ c_{21},\ c_{22},\ c_{23},\ c_{24},\ c_{25},\ c_{26},\ c_{27},\ c_{28},\ c_{29},\ b_{30},$$
 
$$a_{18,\,17},\ a_{22,\,21},\ a_{23,\,21},\ a_{23,\,22},\ a_{24,\,19},\ a_{24,\,22},\ a_{26,\,20},\ a_{28,\,17},\ a_{28,\,18},\ a_{28,\,19},\ a_{30,\,22} \ \text{and}\ a_{30,\,24}$$
 together with the constant  $\xi$  in the relation  $c_{16}=\xi\,c_{17}.$ 

A schematic picture of the linking coefficients as they appear in the Butcher tableau is given below. The red squares indicate nonzero linking coefficients while the open blue squares indicate zero coefficients.



In searching for order 12 schemes with reasonable characteristics one may change the values of these 25 parameters incrementally and use the values obtained at a given stage for the 11 coefficients which occur as the variables in the system of non-linear equations to be solved in the last step of the construction of the scheme as starting values for Newton's method in the determination of the coefficients for the next scheme.

Once an order 12 scheme has been constructed, an embedded scheme order 11 scheme can be obtained by adding a 31st row of linking coefficients. We specify that  $c_{31} = 1$ ,  $a_{31, i} = 0$  for i = 2 ... 13,  $b_{i}^{*} = 0$  for i = 2 ... 18. We set  $b_{30}^{*} = 0$  and give a value for  $b_{31}^{*}$  which means that the scheme is essentially a 30 stage scheme.

A system of equations can be constructed using the order 11 quadrature conditions together with the row-sum condition for the additional 31st stage and the stage-order conditions that ensure that this stage has stage-order 8, that is,

$$\sum_{i=1}^{31} b_i^* = 1, \quad \sum_{i=1}^{31} b_i^* c_i^k = \frac{1}{k+1} \text{ for } k = 1..10,$$

$$\sum_{j=1}^{30} a_{31,j} = c_{31}, \qquad \sum_{j=2}^{30} a_{31,j} c_j^k = \frac{1}{k+1} c_{26}^{(k+1)} \text{ for } k = 1..7.$$

In choosing a value for  $b_{31}^*$  we try to ensure that the stability region of the embedded order 11 scheme is compatible with that of the order 12 scheme. We make the order 12 scheme into a 31 stage scheme by specifying that  $b_{31} = 0$ .

The system of 19 equations can be solved to express the weights  $b_1^*$  and  $b_i^*$  for i = 19 to 28 in terms of  $b_{29}^*$ .

Additionally, the linking coefficients  $a_{31, i}$  and  $a_{31, i}$ , i = 14 to 20 can be expressed as linear combinations of the linking coefficients  $a_{31, i}$ , i = 21 to 30.

The column simplifying conditions

$$\sum_{i=j+1}^{31} b_i^* a_{i,j} = b_j^* (1 - c_j), \ j = 21 \dots 30,$$

can now be used to determine the linking coefficients  $a_{31,j}$  for j = 21...30 in terms of  $b^*_{29}$ .

This enables all the linking in stage 31 to be expressed in tems of  $b^*_{29}$ .

Finally,  $b^*_{29}$  can be determined by using the single order condition

$$\sum_{i=3}^{31} b_i^* c_i \left( \sum_{j=2}^{i-1} a_{i,j} c_j^8 \right) = \frac{1}{99}.$$

The stage-orders of stages 3 to 31 of the combined scheme are as follows.

The principal error norm of an order 12 scheme constructed in the manner described can be calculated using 71 of the 12486 principal error terms. These error terms are given in an abreviated form as follows.

For example, 
$$\frac{1}{1440} \left( b \ c^2 \ (a \ c \ (a \ (a \ c^6))) - \frac{1}{7280} \right)$$
 is an abreviation for 
$$\frac{1}{1440} \left( \left( \sum_{i=2}^{30} b_i \ c_i^2 \left( \sum_{j=3}^{i-1} a_{i,j} \ c_j \left( \sum_{k=4}^{j-1} a_{j,k} \left( \sum_{l=5}^{k-1} a_{k,l} \ c_l^6 \right) \right) \right) \right) - \frac{1}{7280} \right).$$

The principal error norm can be calculated as  $\sqrt{\sum_{i=1}^{71} d_i e_i^2}$ , where  $e_i$  is the value of the ith error term above and  $d_i$  is the ith member of

the sequence 2, 2, 2, 6, 4, 6, 22, 30, 22, 22, 22, 66, 30, 156, 282, 12, 22, 66, 44, 66, 330, 156, 156, 156, 468, 2052, 521/256, 330, 156, 468, 312, 468, 2340, 3102, 2052, 2052, 2052, 6156, 39432, 2340, 21996, 2052, 6156, 4104, 6156, 30780, 39432, 39432, 118296, 950112, 30780, 289332, 78864, 118296, 591480, 950112, 2850336, 28905348, 5559912, 14251680, 28905348, 86716044, 1111178724, 433580220,

$$3333536172, 49928059752, \frac{272483743562603}{144}, 1.$$

The following sets of parameter values determine schemes with the given characteristics. The coefficients for the three schemes considered here are given in separate documents.

# 1. First scheme with a small principal error norm.

$$c_7 = \frac{3}{29}$$
,  $c_{13} = \frac{44}{175}$ ,  $c_{21} = \frac{3878}{6133}$ ,  $c_{22} = \frac{6305}{47146}$ ,  $c_{23} = \frac{1515}{2149}$ ,  $c_{24} = \frac{2048}{8765}$ ,  $c_{25} = \frac{3427}{31813}$ ,

$$c_{26} = \frac{20905}{22918}, \quad c_{27} = \frac{4409}{5020}, \quad c_{28} = \frac{15391}{15693}, \quad c_{29} = \frac{6787}{7838}, \quad c_{30} = 1, \quad b_{30} = \frac{401}{23674},$$
 
$$a_{18,17} = \frac{111}{305}, \quad a_{22,21} = -\frac{181}{2892}, \quad a_{23,21} = \frac{4949}{60976}, \quad a_{23,22} = \frac{4037}{1404}, \quad a_{24,19} = \frac{491}{4721}, \quad a_{24,22} = -\frac{198}{4823}, \quad a_{26,20} = \frac{27379}{2738},$$
 
$$a_{28,17} = -\frac{88358}{691}, \quad a_{28,18} = -\frac{668762}{991}, \quad a_{28,19} = \frac{210288}{347}, \quad a_{30,22} = -\frac{362497}{582}, \quad a_{30,24} = \frac{259829}{252}.$$

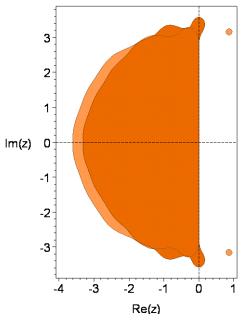
The constant  $\xi$  in the relation  $c_{16} = \xi c_{17}$  has the value  $\xi = \frac{74}{217}$ .

The order 12 scheme has principal error norm  $0.1949742902 \times 10^{(-7)}$  and the real stability interval is [-3.61216, 0].

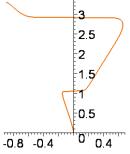
The weight that determines the order 11 embedded scheme is  $b*_{31} = \frac{1}{25}$ .

The order 11 scheme has principal error norm  $0.6755351914 \times 10^{(-7)}$  and the real stability interval is [-3.32116, 0].

The stability regions of the two schemes are shown in the following picture in which the stability region of the order 11 scheme is given the darker shade.



The following picture shows the result of distorting the boundary curve of the stability region of the order 12 scheme horizontally by taking the 11th root of the real part of points along the curve.



The stability region intersects the nonnegative imaginary axis at the origin and in the interval [1.06088 i, 2.90991 i].

The maximum magnitude of the linking coefficients is 1804.19.

# 2. Second scheme with a small principal error norm.

$$c_7 = \frac{872}{8651}, \quad c_{13} = \frac{2647}{10528}, \quad c_{21} = \frac{8455}{13323}, \quad c_{22} = \frac{5591}{41830}, \quad c_{23} = \frac{5981}{8504}, \quad c_{24} = \frac{887}{3794}, \quad c_{25} = \frac{6694}{62127},$$
 
$$c_{26} = \frac{8464}{9277}, \quad c_{27} = \frac{8455}{9627}, \quad c_{28} = \frac{3917}{3993}, \quad c_{29} = \frac{21955}{25352}, \quad c_{30} = 1, \quad b_{30} = \frac{337}{19760},$$
 
$$a_{18, 17} = \frac{4401}{12092}, \quad a_{22, 21} = -\frac{8525}{82417}, \quad a_{23, 21} = \frac{9205}{78471}, \quad a_{23, 22} = \frac{7151}{4758}, \quad a_{24, 19} = \frac{3830}{10117}, \quad a_{24, 22} = -\frac{7477}{45559}, \quad a_{26, 20} = \frac{30601}{2004},$$
 
$$a_{28, 17} = -\frac{28591}{216}, \quad a_{28, 18} = -\frac{627453}{959}, \quad a_{28, 19} = \frac{93413}{145}, \quad a_{30, 22} = -\frac{631366}{931}, \quad a_{30, 24} = \frac{321041}{323}.$$

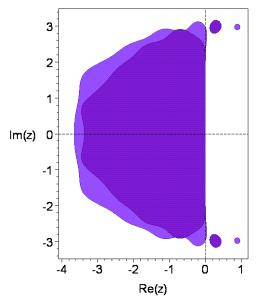
The constant  $\xi$  in the relation  $c_{16} = \xi c_{17}$ . has the value  $\xi = \frac{2669}{7827}$ .

The order 12 scheme has principal error norm  $0.1842009865 \times 10^{(-7)}$  and the real stability interval is [-3.65031, 0].

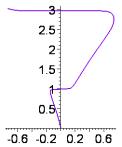
The weight that determines the order 11 embedded scheme is  $b_{31}^* = \frac{1}{29}$ 

The order 11 scheme has principal error norm  $0.5457560603 \times 10^{(-7)}$  and the real stability interval is [-3.36901, 0].

The stability regions of the two schemes are shown in the following picture in which the stability region of the order 11 scheme is given the darker shade.



The following picture shows the result of distorting the boundary curve of the stability region of the order 12 scheme horizontally by taking the 11th root of the real part of points along the curve.



The stability region intersects the nonnegative imaginary axis at the origin and in the interval  $[0.99968 \ i, 2.97170 \ i]$ . The maximum magnitude of the linking coefficients is 1938.87.

# 3. Scheme with a large stability region.

$$c_7 = \frac{873}{9193}, \quad c_{13} = \frac{44}{175}, \quad c_{21} = \frac{8076}{12775}, \quad c_{22} = \frac{2887}{21592}, \quad c_{23} = \frac{8642}{12251}, \quad c_{24} = \frac{1373}{5877}, \quad c_{25} = \frac{2557}{23733},$$
 
$$c_{26} = \frac{7859}{8616}, \quad c_{27} = \frac{6905}{7862}, \quad c_{28} = \frac{3721}{3794}, \quad c_{29} = \frac{2531}{2923}, \quad c_{30} = 1, \quad b_{30} = \frac{471}{27868},$$
 
$$a_{18, 17} = \frac{111}{305}, \quad a_{22, 21} = -\frac{368}{14025}, \quad a_{23, 21} = \frac{6158}{75321}, \quad a_{23, 22} = \frac{6731}{6876}, \quad a_{24, 19} = \frac{2409}{1961}, \quad a_{24, 22} = \frac{3439}{35333}, \quad a_{26, 20} = \frac{87787}{8804},$$
 
$$a_{28, 17} = -\frac{221987}{1736}, \quad a_{28, 18} = -\frac{50125}{73}, \quad a_{28, 19} = \frac{160219}{270}, \quad a_{30, 22} = -\frac{188701}{337}, \quad a_{30, 24} = \frac{451735}{429}.$$

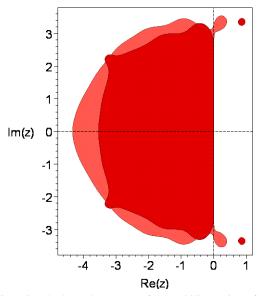
The constant  $\xi$  in the relation  $c_{16} = \xi c_{17}$ . has the value  $\xi = \frac{19741}{57889}$ .

The order 12 scheme has principal error norm  $0.2266066306 \times 10^{(-7)}$  and the real stability interval is [-4.20598, 0].

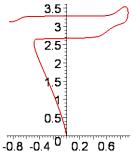
The weight that determines the order 11 embedded scheme is  $b*_{31} = \frac{1}{25}$ .

The order 11 scheme has principal error norm  $0.8868898221 \times 10^{(-7)}$  and the real stability interval is [-3.53662, 0].

The stability regions of the two schemes are shown in the following picture in which the stability region of the order 11 scheme is given the darker shade.



The following picture shows the result of distorting the boundary curve of the stability region of the order 12 scheme horizontally by taking the 11th root of the real part of points along the curve.



The stability region intersects the nonnegative imaginary axis at the origin and in the interval [2.68704 i, 3.28354 i]. The maximum magnitude of the linking coefficients is 1772.92.