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Eighth Order/sixth Order Methods for Second Order Initial Value Problems

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Abstract: A family of eighth order and sixth order P-stable methods for solving second order initial value problems is considered. The nonlinear algebraic system, which results on applying one of the methods in this family to a nonlinear differential system, may be solved by using a modified Newton method. The present study, introduces a local error estimation technique based on the derivation of suitable formula pairs. Thus, to obtain the local error estimate, we compute two approximations of the solution, one with a sixth order method and the other with an eighth order method. The error estimate is then obtained by subtracting our two approximations. The methods in each pair are chosen to have certain features in common. They have the same iteration matrix and some of the function evaluations are common to both methods. Finally numerical results are presented to illustrate our local error estimation technique.

Key words: Second order initial value problems, oscillation problems, combination of 8th and 6th order P-stable methods

INTRODUCTION

We consider an extension of the class of direct hybrid methods proposed by Cash (1981) for solving the second order initial value problem

$$\ddot{y} = f(t,y), y(0), y'(0), given$$
 (1)

The basic method has the form:

$$\begin{array}{ll} y_{n+1}\text{--}2y_{n}+y_{n-1} = & h^{2}\left\{\beta_{0}(\ddot{y}_{n+1}+\ddot{y}_{n-1})+\gamma\ddot{y}_{n}+\beta_{1}\left(\ddot{y}_{n+\alpha 1}+\ddot{y}_{n-\alpha 1}\right)\right\} \\ & + h^{2}\left\{\beta_{2}(\ddot{y}_{n+\alpha 2}+\ddot{y}_{n-\alpha 2})+\beta_{3}(\ddot{y}_{n+\alpha 3}+\ddot{y}_{n-\alpha 3})\right\} \end{array} \tag{2}$$

$$y_{n\pm\alpha 1} = A_{\pm}y_{n+1} + B_{\pm}y_n + C_{\pm}y_{n-1} + h^2\{s_{\pm}\ddot{y}_{n+1} + q_{\pm}\ddot{y}_n + u_{\pm}\ddot{y}_{n-1}\}, \qquad (3)$$

$$\begin{array}{ll} y_{_{n\pm\alpha2}}=&R_{_{\pm}}y_{_{n+1}}+L_{_{\pm}}y_{_{n}}+T_{_{\pm}}y_{_{n-1}}+h^{2}\{Y_{_{\pm}}\ddot{y}_{_{n+1}}+\\ &V_{_{\pm}}\ddot{y}_{_{n}}+W_{_{\pm}}\ddot{y}_{_{n-1}}\}+h^{2}\{Z_{_{\pm}}\ddot{y}_{_{n+\alpha}}+X_{_{\pm}}\ddot{y}_{_{n-\alpha}}\}, \end{array} \eqno(4)$$

$$\begin{array}{ll} y_{n\pm\alpha3} = & D_{\pm}y_{n+1} + E_{\pm}y_{n} + G_{\pm}y_{n-1} + h^{2}\{H_{\pm}\ddot{y}_{n+1} + K_{\pm}\ddot{y}_{n} + M_{\pm}\ddot{y}_{n-1}\} \\ & + h^{2}\{P_{\pm}\ddot{y}_{n+\alpha1} + N_{\pm}\ddot{y}_{n-\alpha1} + S_{\pm}\ddot{y}_{n+\alpha2} + Q_{\pm}\ddot{y}_{n-\alpha2}\} \end{array} \tag{5}$$

and

$$\begin{split} \ddot{y}_n &= f(t_n, y_n), \ \ddot{y}_{n \pm 1} = f(t_n \pm h, y_{n \pm 1}), \ \ddot{y}_{n \pm \alpha} = f(t_n \pm \alpha, h, y_{n \pm \alpha 1}), \\ \ddot{y}_{n \pm \alpha 2} &= f(t_n \pm \alpha_2 h, y_{n \pm \alpha 2}), \ \ddot{y}_{n \pm \alpha 3} = f(t_n \pm \alpha_3 h, y_{n \pm \alpha 3}). \end{split}$$

The methods proposed by Cash (1981) are given by Eq. 2 with $\beta_3 = 0$, (3) and (4). Khiyal (1991), Khiyal and

Thomas (1997a) and Thomas and Khiyal (1992) have derived eighth order, P-stable (Lambert and Watson, 1976) methods of the form (2-5)

When the method (2-5) is applied to a nonlinear deferential system (1), a nonlinear algebraic system must be solved at each step. This may be solved by using a modified Newton iteration scheme. The resulting iteration matrix involves J, J², J³ and J⁴, where Jis an approximation for the Jacobian matrix of f with respect to y. Since matrix products are expensive, especially for large systems and any sparsity in J will be weakened in J2, J3 and J4 and any ill-conditioning in J will be magnified in its powers, we wish to avoid the calculation of J², J³ and J⁴. Khiyal (1991), Khiyal and Thomas (1997a) and Thomas and Khiyal (1992) have derived eighth order P-stable methods of the form (2-5) for which the iteration matrix is a true perfect quartic. This implies that at most one real matrix must be factorised at each step and the formation of J², J³ and J⁴ is avoided. In general, these eighth order methods require seven function evaluations per iteration. Khiyal (1991), Khiyal and Thomas (1997a) and Thomas and Khiyal (1992) have derived methods which require only four function evaluations per iteration.

Notation A method which requires m function evaluations per iteration will be called an m-evaluation method.

By taking $\beta_3 = 0$ in (2) and choosing the remaining parameters appropriately, several authors (Cash, 1981,

Chawla and Rao, 1985) have derived sixth order methods of the form (2-5) which are P-stable. The methods proposed by Cash (1981) require five function evaluations per iteration, in general. Cash (1984), Voss and Serbin (1988) show how the number of function evaluations may be reduced to four per iteration. The method proposed by Cash (1981) is obtained by taking $\alpha_2 = 0$ and requiring the points $(t_{n\pm\alpha2},y_{n\pm\alpha2})$ to be coincident. Voss and Serbin (1988) have modified this method in an attempt to obtain a fourevaluation method with a true perfect cube iteration matrix. (There is a typographical error in their paper and the method which they derive is not sixth order accurate. The correct version is given by Khiyal (1991).) For the method proposed by Chawla and Rao (1985), the number of function evaluations per iteration is reduced to three by requiring that $y_{n-\alpha 1}$ and $y_{n-\alpha 2}$ are independent of y_{n+1} . This implies that $f(t_{n \cdot \alpha 1}, y_{n \cdot \alpha 1})$ and $f(t_{n \cdot \alpha 2}, y_{n \cdot \alpha 2})$ must be computed once per step rather than once per iteration. However, the particular methods proposed by Chawla and Rao (1985) do not have a perfect cube iteration matrix. Finally, Thomas (1988) and Khiyal (1991) have derived sixth order, P-stable, three-evaluation methods (of the form (2-5) with $\beta_3 = 0$) for which the iteration matrix is a true perfect cube.

The present consider the sixth order methods of Thomas (1988) and the eighth order methods of Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992). We give necessary and sufficient conditions for there to exist

- Sixth order, P-stable, three evaluation, two-step methods with iteration matrix (I-rh²J)³,
- Eighth order, P-stable, four evaluation, two-step methods with iteration matrix (I-rh²J)⁴.

The important point to note is that the methods may be chosen so that the value of r is the same for both the sixth and eighth order methods. This means that a saving can be made in the amount of computational effort involved when they are combined together. We derive some particular formula pairs and discuss a local error estimation technique. We present some numerical results to illustrate the performance of the formula pairs.

THE METHODS

The Newton iteration scheme for eighth order methods of the form (2-5) is given by

$$F'(y^{(p-1)}_{n+1})(y^{(p)}_{n+1}-y^{(p-1)}_{n+1}) = -F(y^{(p-1)}_{n+1}), p = 1, 2,$$
 (6)

Where

$$\begin{split} F(y) &= y - 2y_n + y_{n-1} - h^2 \left\{ \beta_0 f(t_{n+1}, y) + \beta_0 f(t_{n-1}, y_{n-1}) + \right. \\ &\left. \gamma f(t_n, y_n) \right\} - h^2 \left\{ \beta_1 f(t_{n+\alpha}, y_{n+\alpha 1}) + \beta_1 f(t_{n-\alpha 1}, y_{n-\alpha 1}) \right. \\ &\left. + \beta_2 f(t_{n+\alpha 2}, y_{n+\alpha 2}) + \beta_2 f(t_{n-\alpha 2}, y_{n-\alpha 2}) + \right. \\ &\left. \beta_3 f(t_{n+\alpha 3}, y_{n+\alpha 3}) + \beta_3 f(t_{n-\alpha 3}, y_{n-\alpha 3}) \right\} \end{split} \tag{7}$$

$$\begin{split} y_{\mathtt{n}\pm\alpha1} &\equiv & A_{\pm}y + B_{\pm}y_{\mathtt{n}} + C_{\pm}y_{\mathtt{n}\cdot\mathtt{l}} + h^2 \{ s_{\pm}f(t_{\mathtt{n}+\mathtt{l}},y) + \\ & q_{\pm}f(t_{\mathtt{n}},y_{\mathtt{n}}) + u_{\pm}f(t_{\mathtt{n}\cdot\mathtt{l}},y_{\mathtt{n}\cdot\mathtt{l}}) \}, \\ y_{\mathtt{n}\pm\alpha2} &\equiv & R_{\pm}y + L_{\pm}y_{\mathtt{n}} + T_{\pm}y_{\mathtt{n}\cdot\mathtt{l}} + h^2 \{ Y_{\pm}f(t_{\mathtt{n}+\mathtt{l}},y) + V_{\pm}f(t_{\mathtt{n}},y_{\mathtt{n}}) \} \end{split}$$

$$\begin{array}{ll} \forall_{n\pm\alpha2} \equiv & R_{\pm}y + L_{\pm}y_n + 1_{\pm}y_{n-1} + n^* \left\{ Y_{\pm}I(t_{n+1}, y) + V_{\pm}I(t_{n}, y_n) + W_{\pm}I(t_{n-1}, y_{n-1}) + Z_{\pm}I(t_{n+\alpha_1}, y_{n+\alpha_1}) + X_{\pm}I(t_{n-\alpha_1}, y_{n-\alpha_1}) \right\}, \\ \forall x_{n+\alpha} \equiv & D_{n}y + P_{n}y + G_{n}y_{n+\alpha_1} + h^2 \left\{ H_{n}f(t_{n+\alpha_1}, y_{n+\alpha_1}) + K_{n}f(t_{n+\alpha_1}, y_{n+\alpha_1}) \right\}, \end{array}$$

$$\begin{split} y_{n\pm\alpha\beta} &\equiv D_{\pm}y + E_{\pm}y_n + G_{\pm}y_{n-1} + h^2 \left\{ H_{\pm}f(t_{n+1},y) + K_{\pm}f(t_n,y_n) \right. \\ &+ M_{\pm}f(t_{n-1},y_{n-1}) + P_{\pm}f(t_{n+\alpha_1},y_{n+\alpha_1}) + N_{\pm}f(t_{n-\alpha_1},y_{n-\alpha_1}) \\ &+ S_{\pm}f(t_{n+\alpha_2},y_{n+\alpha_2}) + Q_{\pm}f(t_{n-\alpha_2},y_{n-\alpha_2}) \right\}, \end{split}$$

and

$$\begin{split} F'\left(y\right) &= I - \left\{\beta_0 + \beta_1(A_+ + A_-) + \beta_2(R_+ + R_-) + \beta_3(D_+ + D_-)\right\} \\ &\quad h^2 J - \left\{\beta_1(s_+ + s_-) + \beta_2[Y_+ + Y_- + A_-(X_+ + X_-) + A_+(Z_+ + Z_-)] + \beta_3[H_+ + H_-) + \beta_3[A_-(N_+ + N_-) + A_+(P_+ + P_-) + R_-(Q_+ + Q_-) + R_+(S_+ + S_-)]\right\} h^4 J^2 - \\ &\quad \left\{\beta_2[s_-(X_+ + X_-) + s_+(Z_+ + Z_-)] + \beta_3[s_-(N_+ + N_-) + s_+(P_+ + P_-)] + \beta_3[(Q_+ + Q_-)(Y_- + X_- A_- + Z_- A_+) + (S_+ + S_-)(Y_+ + X_- A_- + Z_+ A_+)]\right\} h^6 J^3 - \beta_3[(Q_+ + Q_-)(X_- s_- + Z_- s_+) + (S_+ + S_-)(X_+ s_- + Z_+ s_+)]h^3 J^4 \end{split} \tag{8}$$

To avoid the calculation of J², J³ and J⁴ in (5), Khiyal and Thomas (1997a) choose the free parameters of the method so that the iteration matrix may be factorised as a true perfect quartic

$${I-rh^2J}^4$$

where

$$r = 0.25[\beta_0 + \beta_1(A_+ + A_-) + \beta_2(R_+ + R_-) + \beta_3(D_+ + D_-)].$$

The necessary and sufficient conditions for this are

$$\begin{split} \beta_{1}(s_{+}+s_{-}) + \beta_{2}[Y_{+}+Y_{-}+(Z_{+}+Z_{-})(A_{+}+A_{-})] + \beta_{3}[H_{+}+H_{-}+(P_{+}+P_{-})(A_{+}+A_{-}) + (S_{+}+S_{-})(R_{+}+R_{-})] &= -6r^{2}, \beta_{2}(Z_{+}+Z_{-})\\ (s_{+}+s_{-}) + \beta_{3}(s_{+}+s_{-})(P_{+}+P_{-}) + \beta_{3}(S_{+}+S_{-})[Y_{+}+Y_{-}+(Z_{+}+Z_{-})(A_{+}+A_{-})] &= 4r^{3}, \beta_{3}(s_{+}+s_{-})(Z_{+}+Z_{-})(S_{+}+S_{-}) &= -r^{4}. \end{split}$$

The resulting methods are P-stable if and only if

$$\begin{split} 1 + & [4r-1/4]H^2 + [6r^2 - r + 1/48]H^4 + [4r^3 - 1.5r^2 \\ & + r/12 - 1/1440]H^6 + [r^4 - r^3 + r^2/8 - r/360 + \\ & 1/80640]H^8 \ge 0, 1 + [4r - 1/12]H^2 + [6r^2 - r/3 \\ & + 1/360]H^4 + [4r^3 - r^2/2 + r/90 - 1/20160]H^6 \ge 0 \end{split} \tag{10}$$

hold for all H. These conditions are satisfied provided r is greater than or equal to the largest root (R^*) of the polynomial equation

$$r^4-r^3+r^2/8-r/360+1/80640=0,$$
 (11)

because in this case the coefficients of the powers of H in the inequalities (10) are all non-negative. (Note that R* = 0.8581 to four significant figures.)

The Newton iteration scheme for sixth order methods of the form (2-5) with $\beta_3 = 0$ is given by (3)

$$F'(y^{(p-1)}_{n+1})(y^{(p)}_{n+1}-y^{(p-1)}_{n+1}) = -F(y^{(p-1)}_{n+1}), \quad p=1,2,\ldots$$

Where

$$\begin{split} F(y) &= y - 2y_n + y_{n-1} - h^2 \left\{ \beta_0 f(t_{n+1}, y) + \beta_0 f(t_{n-1}, y_{n-1}) \right. \\ &+ \gamma f(t_n, y_n) + \beta_1 f(t_{n+\alpha_1}, y_{n+\alpha_1}) + \beta_1 f(t_{n-\alpha_1}, y_{n-\alpha_1}) \\ &+ \beta_2 f(t_{n+\alpha_2}, y_{n+\alpha_2}) + \beta_2 f(t_{n-\alpha_2}, y_{n-\alpha_2}) \right\} \end{split} \tag{12}$$

$$\begin{split} y_{\mathtt{n} \pm \alpha 1} &\equiv A_{\pm} y + B_{\pm} y_{\mathtt{n}} + C_{\pm} y_{\mathtt{n} - 1} + h^2 \left\{ s_{\pm} f(t_{\mathtt{n} + 1}, y) \right. \\ &+ q_{\pm} f(t_{\mathtt{n}}, y_{\mathtt{n}}) + u_{\pm} f(t_{\mathtt{n} - 1}, y_{\mathtt{n} - 1}) \right\}, \\ y_{\mathtt{n} \pm \alpha 2} &\equiv R_{\pm} y + L_{\pm} y_{\mathtt{n}} + T_{\pm} y_{\mathtt{n} - 1} + h^2 \left\{ Y_{\pm} f(t_{\mathtt{n} + 1}, y) + V_{\pm} f(t_{\mathtt{n}}, y_{\mathtt{n}}) \right. \\ &+ W_{\pm} f(t_{\mathtt{n} - 1}, y_{\mathtt{n} - 1}) + Z_{\pm} f(t_{\mathtt{n} + \alpha_{\mathtt{n}}}, y_{\mathtt{n} + \alpha_{\mathtt{n}}}) + X_{\pm} f(t_{\mathtt{n} - \alpha_{\mathtt{n}}}, y_{\mathtt{n} - \alpha_{\mathtt{n}}}) \right\}, \end{split}$$

and

$$\begin{split} F'(y) &= I - \{\beta_0 + \beta_1(A_+ + A_-) + \beta_2(R_+ + R_-)\} h^2 J - \{\beta_1(s_+ + s_-) \\ &+ \beta_2 [Y_+ + Y_- + A_-(X_+ + X_-) + A_+(Z_+ + Z_-)]\} h^4 J^2 - \\ &\{\beta_2 [s_-(X_+ + X_-) + s_+(Z_+ + Z_-)]\} h^6 J^3 \end{split} \tag{13}$$

To avoid the calculation of J² and J³, Thomas (1988) chooses the free parameters of the method so that the iteration matrix may be factorised as a true perfect cube

$${I-rh^2J}^3$$

where

$$r = (1/3) [\beta_0 + \beta_1(A_+ + A_-) + \beta_2(R_+ + R_-)].$$

The necessary and sufficient conditions for this are

$$\begin{split} \beta_1(s_+ + s_-) + \beta_2(Y_+ + Y_-) + \beta_2 A_-(X_+ + X_-) + \beta_2 A_+(Z_+ + Z_-) &= -3r^2, \\ \beta_2\{s_+(Z_+ + Z_-) + s_-(X_+ + X_-)\} &= r^3. \end{split} \tag{14}$$

The resulting methods are P-stable if and only if

$$\begin{split} 1 + & [3r - 1/4]H^2 + [3r^2 - 3r/4 + 1/48]H^4 + \\ & [r^3 - 3r^2/4 + r/16 - 1/1440]H^6 \ge 0, \\ 1 + & [3r - 1/12]H^2 + [3r^2 - r/4 + 1/360]H^4 \ge 0 \end{split} \tag{15}$$

hold for all H. These conditions are satisfied provided r is greater than or equal to the largest root (R^*) of the polynomial equation

$$r^3-3r^2/4+r/16-1/1440=0,$$
 (16)

because in this case the coefficients of the powers of H in the inequalities (15) are all non-negative. (Note that $R^+=0.6564$ to four significant figures.)

DERIVATION OF THE FORMULA PAIRS.

The four-evaluation, P-stable, eighth order methods of the type derived by Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992) may be combined in a variable step code with appropriate three-evaluation, P-stable, sixth order methods of the type derived by Thomas (1988) and Khiyal (1991). In each formula pair, the iteration matrix for the eighth order method is (I-rh²J)⁴ while for the sixth order method, the iteration matrix is (I-rh²J)³ and the value of r is the same for both. The local error estimate is given by

$$Le_{n+1} = y^{[8]}_{n+1} - y^{[6]}_{n+1}$$
 (17)

where $y^{[2m]}_{n+1}$ is the approximation for $y(t_{n+1})$ obtained by the method of order 2m, m = 3 and 4. Although this means performing the integration with two methods on each step, this can usually be achieved reasonably cheaply since most of the work comes in solving linear systems of the form $(I-rh^2I)^my = b$. As the matrix $(I-rh^2J)$ is common to both methods, no extra LU factorisations are required. Now Le_{n+1} is an estimate of the error in the lower order method. If we add the local error estimate Le_{n+1} to $y^{[6]}_{n+1}$, we obtain $y^{[8]}_{n+1}$. However, since the sixth order method is P-stable, we could equally well accept these results to advance the step.

The iteration matrix for the eighth order method is $(I-rh^2J)^4$ where, to ensure P-stability, we require $r \ge R^*$, the largest root of the polynomial (11). The iteration matrix for the sixth order methods is $(I-rh^2J)^3$, where, to ensure P-stability, we require $r \ge R^*$, the largest root of the polynomial (16). Since we are prepared to perform at most one LU factorisation per step and since $R^* > R^*$, we take $r \ge R^*$ for both methods.

Here we consider combinations of sixth and eighth order methods which have other common features, with the aim of obtaining further savings. We derive six different pairs and presents some numerical results. Note that other eighth order/sixth order formula pairs may be derived in a similar way.

SHK86A: The eighth order method is the method derived by Khiyal (1991), Khiyal and Thomas (1997a,b) and Thomas and Khiyal (1992) for which $y_{n-\alpha 2}$ and $y_{n-\alpha 3}$ are independent of y_{n+1} , $y_{n-\alpha 1}$ is identically equal to y_{n-1} and the free parameters are chosen so that $\alpha_1 = 1$, $\alpha_3 = 1/2$, $\beta_1 = 1$,

 $\alpha_2 = (-1+\sqrt{2151})/100$ and $r = R^*$. For this method, we must evaluate $f(t_{n-\alpha 2}, y_{n-\alpha 2})$ and $f(t_{n-\alpha 3}, y_{n-\alpha 3})$ once per step. With this eighth order method, we combine a sixth order method such that $y_{n-\alpha 2}$ is independent of y_{m+1} , $\ddot{y}_{n-\alpha 1}$ is identically equal to \ddot{y}_{n-1} and $f(t_{n-\alpha 2}, y_{n-\alpha 2})$ is evaluated once per step. In general $f(t_{n-\alpha 2}, y_{n-\alpha 2})$ has to be evaluated once per step for each of the sixth and eighth order methods. However, here we choose α_2 to be the same for both methods and we also choose the coefficients in the expression (4) for $y_{n-\alpha 2}$ to be the same for both methods. This means that $f(t_{n-\alpha 2}, y_{n-\alpha 2})$ must be evaluated just once per step and may then be used for both the sixth and eighth order methods. The resulting formula pair is as follows:-

Sixth order method given by Eq. (2-3) with

$$\begin{array}{l} A_{-}=0,\,s_{-}=0,\,R_{-}=0,\,Y_{-}=0,\,Z_{-}=0,\,B_{-}=0,\,C_{-}=1,\\ q_{-}=0,\,u_{-}=0,\,L_{-}=1-\alpha_{2},\,T_{-}=\alpha_{2},\,\beta_{2}=(\alpha^{2}_{2}-\alpha^{4}_{2})/20,\\ \beta_{0}=1/12-\beta_{1}-\beta_{2}\alpha^{2}_{2},\,\gamma=1-2\,(\beta_{0}+\beta_{1}+\beta_{2}),\,Z_{+}=[-400\alpha^{2}_{2}\\ (1-\alpha^{2}_{2})^{2}\beta_{1}/(1+\alpha_{2}-\alpha^{2}_{2})][1\,2r^{3}-3r^{2}+r/4-1/360],\\ s_{+}=r^{3}/(\beta_{2}Z_{+}),\,A_{+}=1-12s_{+}-(1+\alpha_{2}-\alpha^{2}_{2})/20/(1-\alpha^{2}_{2})\,\beta_{1},\\ u_{+}=s_{+},\,q_{+}=1-A_{+}-2s_{+},B_{+}=2-2A_{+},\,C_{+}=A_{+}-1,\\ \beta_{2}R_{+}=3r-1/12+\beta_{2}\alpha^{2}_{2}+\beta_{1}\,(1-A_{+}),\,L_{+}=1+\alpha_{2}-2R_{+},\\ T_{+}=R_{+}-\alpha_{2},\,W_{-}+X_{-}=(\alpha^{3}_{2}-\alpha_{2})/6,\,V_{-}=(\alpha^{2}_{2}-\alpha_{2})/2-(W_{-}+X_{-}),\,Y_{+}=(\alpha^{3}_{2}+\alpha^{2}_{2}-R_{+})/12-Z_{+},\,W_{+}+X_{+}=Y_{+}+Z_{+}-(W_{-}+X_{-}),\,V_{+}=(\alpha^{2}_{2}+\alpha_{2})/2-R_{+}-Y_{+}-Z_{+}-(W_{+}+X_{+}),\\ \beta_{1}=1,\,\alpha_{1}=1,\,\alpha_{2}=(-1\pm\sqrt{2151})/100\,\,\text{and}\,\,r=R^{*}. \end{array} \tag{18}$$

Eighth order method given by Eq. (2-5) with

$$\begin{array}{l} A_-=0,\,s_-=0,\,R_-=0,\,Y_-=0,\,Z_-=0,\,D_-=0,\,H_-=0,\\ P_-=0,\,S_-=0,\,\alpha_1=1,\,B_-=0,\,C_-=1,\,q_-=0,\,u_-=0,\\ L_-=1-\alpha_2,\,T_-=\alpha_2,\,E_-=1-\alpha_3,\,W_++X_-=(\alpha_2^3-\alpha_2)/6,\\ G_-=\alpha_3,\,\beta_2=(13-42\alpha_3^2)/840(\alpha_2^4-\alpha_2^2)(\alpha_2^2-\alpha_2^2),\\ \beta_3=(13-42\alpha_2^2)/840(\alpha_3^4-\alpha_3^2)(\alpha_2^2-\alpha_3^2),\,\beta_0=1/12-\beta_1-\beta_2\alpha_2^2-\beta_3\alpha_3^2,\gamma=1-2(\beta_0+\beta_1+\beta_2+\beta_3),\,Q_-=17/3360\\ \beta_3\alpha_3(\alpha_2^3-\alpha_2),M_-=(\alpha_3^3-\alpha_3)/6-\alpha_2Q_-N_-,\,\lambda_3=\alpha_3^2(\alpha_2+\alpha_3)\\ (51\alpha_3^2+13\alpha_2^2+29\alpha_2-35)/(\alpha_2+1)(42\alpha_2^2-13),\\ \lambda_2=\alpha_2^2(\alpha_2+1),\,\lambda_1\beta_1=1/30-\beta_0-\lambda_2\beta_2-\lambda_3\beta_3,\\ S_+=(11/84-12r)/60\beta_3\alpha_2^2(1-\alpha_2^2),\,Z_+=17(1+\alpha_2-\alpha_2^2)/\\ 3360\beta_2(1+\alpha_2)(\alpha_2-\alpha_3)(\lambda_1-1),\,s_+=-r^4/\beta_3S_+Z_+,A_+=\lambda_1-12s_+,\\ C_+=A_+-1,\,\beta_3P_+=-\beta_2Z_+-(\lambda_2-\alpha_2^4)\,\beta_3S_+/(\lambda_1-1),\,u_+=s_+,\\ q_+=1-A_+-s_+-u_+,\,B_+=2-2A_+,\,\lambda_4=[\beta_0(1-\alpha_3)+(28+3\alpha_3)/168-17(\alpha_2^2+\alpha_2+1)/112(\alpha_2+1)+\beta_1(1-\alpha_3)(A_++30s_+)]/\beta_2(\alpha_3-\alpha_2),\,Y_+=-Z_++(\lambda_4-\lambda_2)/18,\,R_+=\lambda_2-12(Y_++Z_+),\\ X_+=Z_+-X_-,\,\beta_3D_+=4r-\beta_0-\beta_1A_+-\beta_2R_+,\,H_+=-P_+-\alpha_2^2S_++(\lambda_3-D_+)/12,\,L_+=1+\alpha_2-2R_+,\,T_+=R_+-\alpha_2,\,W_+=Y_+-W_-,\\ E_+=1+\alpha_3-2D_+,\,V_+=(\alpha_2^2+\alpha_2)/2-R_+-Y_+-W_+-Z_+-X_+,\\ V_-=(\alpha_2^2-\alpha_2)/2-W_--X_-,\,N_+=P_+N_-,\,Q_+=S_+-Q_-,\\ K_-=(\alpha_3^2-\alpha_3)/2-M_-N_-Q_-,\,M_+=H_+-M_-,\,K_+=(\alpha_2^3+\alpha_3)/2-D_+-H_+-M_+-N_+-P_+-Q_+-S_+,\,G_+=D_+-\alpha_3,\,\alpha_3=\frac{1}{2},\,\alpha_2=(-1+\sqrt{2}151)/100,\,\beta_1=1,\,r=R^*,\,13-35\alpha_3-29\alpha_3^3+51\alpha_3^3-9\alpha_2+\\ \end{array}$$

$$29\alpha_2\alpha_3 - 20\alpha_2\alpha_3^2 + 29\alpha_2^2 + 13\alpha_2^2\alpha_3 - 42\alpha_2^2\alpha_3^2 = 0$$

and N_{_} and X_{_} are free parameters. (19)

SHK86B: In this formula pair, the eighth order method is the method derived by Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992) for which $y_{n-\alpha 1}$ and $y_{n-\alpha 3}$ are independent of y_{n+1} , $\ddot{y}_{n-\alpha 2} = \ddot{y}_{n-1}$, $\alpha_2 = 1$, $\alpha_3 = 1/2$, $\beta_2 = 1$, $\alpha_1 = (-1\pm\sqrt{2151})/100$ and $r=R^*$. For this method we must evaluate $f(t_{n-\alpha 1}, y_{n-\alpha 1})$ and $f(t_{n-\alpha 3}, y_{n-\alpha 3})$ once per step. We combine this method with a sixth order method for which $y_{n-\alpha 1}$ is independent of y_{n+1} and $\ddot{y}_{n-\alpha 2} = \ddot{y}_{n-1}$. The resulting formula pair is as follows:-

Sixth order method given by Eq. (2-4) with

$$\begin{split} A_- &= 0, \ s_- = 0, \ R_- = 0, \ Y_- = 0, \ Z_- = 0, \ \alpha_2 = 1, \ L_- = 0, \\ T_- &= 1, \ V_- = 0, \ W_- = 0, \ X_- = 0, \ B_- = 1 - \alpha_1, \ C_- = \alpha_1, \\ \beta_1 &= (\alpha^2_1 - \alpha^4_1)/20, \ \beta_0 = 1/12 - \beta_2 - \beta_1 \alpha^2_1, \ \gamma = 1 - 2(\beta_0 + \beta_1 + \beta_2), \ u_- &= (\alpha^3_1 - \alpha_1)/6, \ \beta_2 Z_+ = [12r^3 - 3r^2 + r/4 - 1/360]/\alpha^3_1, \ s_+ = r^3/(\beta_2 Z_+), \ X_+ = Z_+, \ u_+ = s_+ - u_-, \\ A_+ &= \alpha^2_1(1 + \alpha_1) - 12s_+, \ B_+ = 1 + \alpha_1 - 2A_+, \ C_+ = A_+ - \alpha_1, \\ q_- &= (\alpha^2_1 - \alpha_1)/2 - u_-, \ q_+ = (\alpha^2_1 + \alpha_1)/2 - A_+ - 2s_+ + u_-, \\ T_+ &= R_+ - 1, \ \beta_2 R_+ = 3r - 1/12 + \beta_2 + \beta_1(\alpha^2_1 - A_+), \\ \beta_2 Y_+ &= (\alpha^2_1 - \alpha_1 - 1)/240(1 - \alpha^2_1) + \beta_2(1 - R_+ - 12\alpha^2_1 Z_+)/12, \\ L_+ &= 2 - 2R_+, \ W_+ = Y_+, \ V_+ = 1 - R_+ - 2Y_+ - 2Z_+, \ \beta_2 = 1, \\ \alpha_2 &= 1, \ \alpha_1 = (-1 \pm \sqrt{2151})/100 \ \text{and} \ r = R^*. \end{split}$$

Eighth order method given by Eq. (2-5) with

```
A_{-} = 0, s_{-} = 0, R_{-} = 0, Y_{-} = 0, Z_{-} = 0, D_{-} = 0, H_{-} = 0,
P_{-} = 0, S_{-} = 0, \alpha_{2} = 1, L_{-} = 0, T_{-} = 1, V_{-} = 0, W_{-} = 0,
X_{-}=0, C_{-}=\alpha_{1}, B_{-}=1-\alpha_{1}, \beta_{1}=(13-42\alpha_{3}^{2})/840(\alpha_{1}^{4}-\alpha_{1}^{2})
(\alpha^2_3 - \alpha^2_1), \beta_3 = (13 - 42\alpha^2_1)/840(\alpha^4_3 - \alpha^2_3)(\alpha^2_1 - \alpha^2_3),
u_{-} = (\alpha_{1}^{3} - \alpha_{1})/6, \beta_{0} = 1/12 - \beta_{1}\alpha_{1}^{2} - \beta_{2} - \beta_{3}\alpha_{3}^{2}, \gamma = 1-2
(\beta_0 + \beta_1 + \beta_2 + \beta_3), N_- = 17/3360 \beta_3 \alpha_3 (\alpha_1^3 - \alpha_1), \lambda_1 = \alpha_1^2
(\alpha_1+1), M_- = (\alpha_3^3 - \alpha_3)/6 - Q_- - \alpha_1 N_-, \lambda_3 = \alpha_3^2 (\alpha_1 + \alpha_3)
(51\alpha^{2}_{3}+13\alpha^{2}_{1}+29\alpha_{1}-35)/(\alpha_{1}+1)(42\alpha^{2}_{1}-13),
\lambda_2 \beta_2 = 1/30 - \beta_0 - \lambda_1 \beta_1 - \lambda_3 \beta_3, \ \beta_2 Z_+ = 17/3360 \alpha_1^2 (1 + \alpha_1)
(1-\alpha_3), s_+ = -r^4/\beta_3 S_+ Z_+, A_+ = \lambda_1 - 12s_+, \beta_3 P_+ = -\beta_2 Z_+ +
(11/84-12r)/60\alpha_1^2(1-\alpha_1^2), S_+ = (1-\alpha_1^2+\alpha_1)(11/84-12r)/(11/84-12r)
60\beta_3(1-\alpha^2_1)(1-\lambda_2), B_1 = 1+\alpha_1+2A_1, C_2 = A_1-\alpha_1
u_{+} = s_{+} - u_{-}, q_{+} = (\alpha^{2} + \alpha_{1})/2 - A_{+} - s_{+} - u_{+}, q_{-} = (\alpha^{2} - \alpha_{1})/2 - u_{-}
\lambda_4 = [\beta_1(\alpha_1 - \alpha_3)(\alpha_1^3 + \alpha_1^2 + 18s_+) + (28 + 3\alpha_3)/168 - 17
(\alpha^2 + \alpha_1 + 1)/112(\alpha_1 + 1) + \beta_0(1 - \alpha_3)/18\beta_2(\alpha_3 - 1),
 Y_{+} = \alpha_{1}^{2}(2-5\alpha_{1}^{2})Z_{+}/3-\lambda_{2}/18 + \lambda_{4}, R_{+} = \lambda_{2}-12(Y_{+} + \alpha_{1}^{2}Z_{+}),
X_{+} = Z_{+}, \beta_{3}D_{+} = 4r - \beta_{0} - \beta_{1}A_{+} - \beta_{2}R_{+}, H_{+} = -\alpha^{2} P_{+} - S_{+} + \beta_{3}P_{+} - \beta_{1}P_{+} - S_{+} + \beta_{2}P_{+} - \beta_{1}P_{+} - \beta_{2}P_{+} - \beta_{1}P_{+} - \beta_{2}P_{+} - \beta_{1}P_{+} - \beta_{2}P_{+} - \beta_{1}P_{+} - \beta_{2}P_{+} - \beta_
(\lambda_3-D_+)/12, L_+=2-2R_+, T_+=R_+-1, E_-=1-\alpha_3, W_+=Y_+
G_{-} = \alpha_3, G_{+} = D_{+} - \alpha_3, V_{+} = 1 - R_{+} - 2Y_{+} - 2Z_{+}, E_{+} = 1 + \alpha_3 - 2D_{+},
N_{+} = P_{+} - N_{-}, Q_{+} = S_{+} - Q_{-}, M_{+} = H_{+} - M_{-}, K_{+} = (\alpha^{2} + \alpha_{3})/(\alpha^{2} + \alpha_{3})
2-D_{+}-H_{+}-M_{+}-N_{+}-P_{+}-Q_{+}-S_{+}, K_{-} = (\alpha^{2}_{3}-\alpha_{3})/2-M_{-}-N_{-}-Q_{-},
\alpha_3 = \frac{1}{2}, \alpha_1 = (-1 + \sqrt{2151})/100, \beta_2 = 1, r = R^*, 13-35
\alpha_3 - 29\alpha_3^2 + 51\alpha_3^3 - 9\alpha_1 + 29\alpha_1\alpha_3 - 20\alpha_1\alpha_3^2 + 29\alpha_1^2 + 13\alpha_1^2
\alpha_3-42\alpha_1^2 \alpha_3^2 = 0 and Q<sub>1</sub> is a free parameter.
                                                                                                                                                                                                             (21)
```

SHK86C: The eighth order method in this pair is the method derived by Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992) for which $y_{n-\alpha 1}$ and $y_{n-\alpha 3}$ are independent of y_{n+1} , the points $f(t_{n+\alpha 2}, y_{n+\alpha 2})$ and $f(t_{n-\alpha 2}, y_{n-\alpha 2})$ are coincident, $\alpha_2 = 0$, $\alpha_3 = 1/2$, $\beta_2 = 1$, $\alpha_1 = (-2+\sqrt{119})/30$ and $r = R^*$. For this method we must evaluate $f(t_{n-\alpha 1}, y_{n-\alpha 1})$ and $f(t_{n-\alpha 8}, y_{n-\alpha 2})$ once per step. We combine this method with a sixth order method for which $y_{n-\alpha 1}$ is independent of y_{n+1} and the points $(t_{n+\alpha 2}, y_{n+\alpha 2})$ and $(t_{n-\alpha 2}, y_{n-\alpha 2})$ are coincident. The resulting formula pair is as follows:-

Sixth order method given by Eq.(2-3) with

$$\begin{split} &\alpha_3={}^{1}\!\!/_2,\,A_-=0,\,B_-=1\text{-}\alpha_1,\,C_-=\alpha_1,\,s_-=0,\\ &q_-=(3\alpha^2_1\text{-}2\alpha_1\text{-}\alpha^3_1)\!/6,\,u_-=(\alpha^3_1\text{-}\alpha_1)\!/6,\\ &\beta_2Z_+=\left[\text{-}12r^3\text{+}3r^2\text{-}r/4\text{+}1/360\right]\!/2\alpha_1(1\text{+}\alpha_1\text{-}2\alpha^2_1),\\ &X_+=Z_+,\,X_-=X_+,\,Z_-=Z_+,\,s_+=r^3/2\beta_2Z_+,\\ &A_+=2\alpha^3_1\text{-}\alpha_1\text{-}12s_+,\,B_+=1\text{+}\alpha_1\text{-}2A_+,\,C_+=A_+\text{-}\alpha_1,\\ &\beta_1=(\alpha^2_1\text{-}\alpha^4_1)\!/20,\,\beta_0=1\!/12\text{-}\beta_1\alpha^2_1,\,\gamma=1\text{-}2(\beta_0\text{+}\beta_1\text{+}\beta_2),\,q_+=(8\alpha_1\text{+}3\alpha^2_1\text{-}11\alpha^3_1)\!/6\text{+}10s_+,\\ &u_+=s_+\text{-}(\alpha^3_1\text{-}\alpha_1)\!/6,\,\beta_2R_+\text{=}(3r\text{-}\beta_0\text{-}\beta_1A_+)\!/2,\\ &\beta_2Y_+=1\!/720\text{-}\beta_1s_+\!/2\text{-}r\,\beta_2\,\alpha^2_1Z_+\!/8,\,V_+=\text{-}R_+\text{-}2(Y_+\text{+}Z_+),\\ &T_+=R_+,\,R_-=R_+,\,T_-=R_+,\,L_+=1\text{-}2R_+,\,L_-=L_+,\\ &W_+=Y_+,\,Y_-=Y_+,\,W_-=Y_+,\,V_-=V_+,\,\beta_2=1,\\ &\alpha_1=(\text{-}2\text{+}\sqrt{1}19)\!/30,\,\alpha_2=0\,\,\text{and}\,\,r=R^* \end{split} \label{eq:alpha}$$

Eighth order method given by Eq. (2-5) with

```
A_{-} = 0, s_{-} = 0, D_{-} = 0, H_{-} = 0, P_{-} = 0, Q_{-} + S_{-} = 0,
G_{-} = \alpha_{3}, u_{-} = (\alpha_{1}^{3} - \alpha_{1})/6, C_{-} = \alpha_{1}, B_{-} = 1 - \alpha_{1},
\beta_1 = (13-42\alpha_3^2)/840(\alpha_1^4-\alpha_1^2)(\alpha_3^2-\alpha_1^2), \ \beta_3 = (13-42\alpha_1^2)/3
840 (\alpha_3^4 - \alpha_3^2) (\alpha_1^2 - \alpha_3^2), E_- = 1 - \alpha_3, q_- = (\alpha_1^2 - \alpha_1)/2 - u_-
\beta_0 = 1/12 - \beta_1 \alpha_1^2 - \beta_3 \alpha_3^2, \ \gamma = 1 - 2(\beta_0 + \beta_1 + \beta_2 + \beta_3),
N_{-} = 17/3360 \, \beta_3 \alpha_3 (\alpha_1^3 - \alpha_1), \, \lambda_1 = \beta_1 (\alpha_1^4 - 2\alpha_1^3 + \alpha_1) + \beta_3
(\alpha_3^4 - 2\alpha_3^3 + \alpha_3) + 12\beta_3(\alpha_1 - \alpha_1^2)N_{-}, M_{-} = (\alpha_3^3 - \alpha_3)/6 - \alpha_1 N_{-},
\lambda_4 = [24\alpha_1/(\alpha_1^2 - \alpha_1 - 1)][(\alpha_1 + 1)\lambda_1/2\beta_2 - 18(\alpha_1 - 1)(2\alpha_1^3 - 1)(2\alpha_1^3 - 1)][(\alpha_1 + 1)\lambda_1/2\beta_2 - 18(\alpha_1 - 1)(2\alpha_1^3 - 1)(
\alpha^{2}_{1}-3\alpha_{1}-1)Z_{+}, \lambda_{4}\beta_{3}(S_{+}+S_{-})=108r^{2}-864r^{3}+2592r^{4}+
\beta_1(\alpha_1^6 - \alpha_1^4) + \beta_3(\alpha_3^6 - \alpha_3^4), (2\beta_2 Z_+ + \beta_3 N_-)(2\alpha_1^3 - \alpha_1 - \alpha_1^4) = 0,
S_{+} = -r^{4}/2\beta_{3}Z_{+}(S_{+}+S_{-}), A_{+} = 2\alpha_{1}^{3}-\alpha_{1}-12S_{+}, B_{+} = 1+\alpha_{1}-2A_{+},
u_{+} = s_{+} - u_{-}, C_{+} = A_{+} - \alpha_{1}, q_{+} = (\alpha^{2}_{1} + \alpha_{1})/2 - A_{+} - s_{+} - u_{+},
P_{+} = N_{-}(S_{+}+S_{-})\lambda_{1}/\beta_{2}(2\alpha_{1}^{3}-\alpha_{1}-\alpha_{1}^{4}), N_{+} = P_{+}-N_{-}
Q_{+} = S_{+} + 2S_{-}, \beta_{3}\alpha_{3}D_{+} = \beta_{3}\alpha_{3}^{2} + \beta_{1}\alpha_{1}(\alpha_{1} - A_{+}) + 20(\alpha_{1}^{4} - A_{+})
(\alpha_1^2)\beta_3\alpha_3N_+, G_+ = D_+-\alpha_3, K_- = (\alpha_3^2-\alpha_3)/2-M_--N_-, E_+ = 1+
\alpha_3 - 2D_+, H_+ = (2\alpha_3^3 - \alpha_3 - D_+)/12 - \alpha_1^2 P_+ + (\alpha_1^2 - \alpha_1) N_-
M_{+} = H_{+} - M_{-}, L_{+} = 1 - 2R_{+}, K_{+} = (\alpha^{2}_{3} + \alpha_{3})/2 - D_{+} - H_{+} - \alpha^{2}_{3}
M_{+}-N_{+}-P_{+}-2(S_{+}-S_{-}), \beta_{2}R_{+}=2r-(\beta_{0}+\beta_{1}A_{+}+\beta_{3}D_{+})/2,
Y_{+} = -R_{+}/12 - \alpha^{2}_{1}Z_{+} + \lambda_{1}/24\beta_{2}, V_{+} = -R_{+} - 2Y_{+} - 2Z_{+}, T_{+} = R_{+},
X_{+} = Z_{+}, X_{-} = X_{+}, Z_{-} = Z_{+}, W_{+} = Y_{+}, R_{-} = R_{+}, L_{-} = L_{+},
T_{-} = T_{+}, Y_{-} = Y_{+}, V_{-} = V_{+}, W_{-} = W_{+}, 13(1+\alpha_{1}+\alpha_{3}-\alpha_{1}^{2})
64\alpha^{2}_{3}-9\alpha_{1}\alpha_{3}+84\alpha^{2}_{1}\alpha^{2}_{3}+29\alpha^{2}_{1}\alpha_{3}-22\alpha_{1}\alpha^{2}_{3}-51\alpha^{3}_{3}=0
\alpha_2 = 0, \alpha_3 = \frac{1}{2}, \alpha_1 = (-2 + \sqrt{119})/30, \beta_2 = 1, r = R^*
and S<sub>_</sub> is a free parameter.
                                                                                                                                                                                                                                 (23)
```

SHK86D: For the eighth order method derived by Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992) for which $y_{n-\alpha 1}$ and $y_{n-\alpha 3}$ are independent of y_{n+1} , $\ddot{y}_{n-\alpha 2}=\ddot{y}_n$, $\alpha_1=(-2+\sqrt{119})/30$, $\alpha_2=0$, $\alpha_3=1/2$, $\beta_2=1$ and $r=R^*$. For this method we must evaluate $f(t_{n-\alpha 1},y_{n-\alpha 1})$ and $f(t_{n-\alpha 3},y_{n-\alpha 3})$ once per step. We combine this method with a sixth order method for which $y_{n-\alpha 1}$ is independent of y_{n+1} and $\ddot{y}_{n-\alpha 2}=\ddot{y}_n$. The resulting formula pair is as follows:-Sixth order method given by Eq. (2-4) with

$$\begin{split} &A_{-}=0,\,B_{-}=1\text{-}\alpha_{1},\,C_{-}=\alpha_{1},\,s_{-}=0,\,q_{-}=(3\alpha^{2}_{1}\text{-}2\alpha_{1}\text{-}\alpha^{3}_{1})/6,\\ &u_{-}=(\alpha^{3}_{1}\text{-}\alpha_{1})/6,\,R_{-}=0,\,T_{-}=0,\,L_{-}=1,\,Y_{-}=0,\,W_{-}=0,\\ &V_{-}=0,\,X_{-}=0,\,Z_{-}=0,\,\beta_{1}=(\alpha^{2}_{1}\text{-}\alpha^{4}_{1})/20,\,\beta_{0}=1/12\text{-}\beta_{1}\alpha^{2}_{1},\\ &\gamma=1\text{-}2\,(\beta_{0}\text{+}\beta_{1}\text{+}\beta_{2}),\,\beta_{2}\,Z_{+}=[12r^{3}\text{-}3r^{2}+r/4\text{-}1/360]/\\ &\alpha_{1}(2\alpha^{2}_{1}\text{-}\alpha_{1}\text{-}1),\,X_{+}=Z_{+},\,s_{+}=r^{3}/\beta_{2}Z_{+},\,A_{+}=2\alpha^{3}_{1}\text{-}\alpha_{1}\text{-}12s_{+},\\ &B_{+}=1\text{+}\alpha_{1}\text{-}2A_{+},\,C_{+}=A_{+}\text{-}\alpha_{1},\,q_{+}=(8\alpha_{1}\text{+}3\alpha^{2}_{1}\text{-}11\alpha^{3}_{1})/\\ &6+10s_{+},\,u_{+}=s_{+}\text{-}(\alpha^{3}_{1}\text{-}\alpha_{1})/6,\,\beta_{2}R_{+}=3r\text{-}\beta_{0}\text{-}\beta_{1}A_{+},\\ &\beta_{2}Y_{+}=1/360\text{-}\beta_{1}s_{+}\text{-}r/4\text{-}\beta_{2}\,\alpha^{2}_{1}Z_{+},\,V_{+}=\text{-}R_{+}\text{-}2(Y_{+}\text{+}Z_{+}),\\ &T_{+}=R_{+},\,L_{+}=1\text{-}2R_{+},\,W_{+}=Y_{+},\,\beta_{2}=1,\\ &\alpha_{1}=(\text{-}2\text{+}\sqrt{1}19)/30,\,\alpha_{2}=0\,\,\text{and}\,\,r=R^{*}. \end{split}$$

Eighth order method given by Eq. (2-5) with

```
A_{-} = 0, s_{-} = 0, R_{-} = 0, L_{-} = 1, T_{-} = 0, Y_{-} = 0, V_{-} = 0,
X_{-} = 0, Z_{-} = 0, D_{-} = 0, H_{-} = 0, P_{-} = 0, S_{-} = 0, G_{-} = \alpha_{3},
u_{-} = (\alpha_{1}^{3} - \alpha_{1})/6, C_{-} = \alpha_{1}, B_{-} = 1 - \alpha_{1}, q_{-} = (\alpha_{1}^{2} - \alpha_{1})/2 - u_{-},
E_{-} = 1 - \alpha_{3}, \beta_{1} = (13 - 42\alpha_{3}^{2})/840(\alpha_{1}^{4} - \alpha_{1}^{2})(\alpha_{3}^{2} - \alpha_{1}^{2}),
\beta_3 = (13-42\alpha_1^2)/840(\alpha_3^4-\alpha_3^2)(\alpha_1^2-\alpha_3^2), \ \beta_0 = 1/12-\beta_1
\alpha^{2}_{1}-\beta_{3}\alpha^{2}_{3}, \gamma = 1-2(\beta_{0}+\beta_{1}+\beta_{2}+\beta_{3}), N_{-}=17/3360\beta_{3}
\alpha_3(\alpha_1^3 - \alpha_1), \beta_2 \lambda_1 = \beta_1(\alpha_1^4 - 2\alpha_1^3 + \alpha_1) + \beta_3(\alpha_3^4 - 2\alpha_3^3 + \alpha_3)
+12\beta_3(\alpha_1-\alpha_1^2)N_{-}, M_{-} = (\alpha_3^3-\alpha_3)/6-\alpha_1N_{-}, \lambda_4 = [12\alpha_1/(\alpha_1^2)]
-\alpha_1-1][(\alpha_1+1)\lambda_1-18(\alpha_1-1)(2\alpha_1^3-\alpha_1^2-3\alpha_1-1)Z_+],
s_{+} = -r^{4}/\beta_{3}Z_{+}S_{+}, W_{-} = 0, (\beta_{2}Z_{+} + \beta_{3}N_{-})(2\alpha_{1}^{3} - \alpha_{1} - \alpha_{1}^{4}) = 0,
\lambda_4\beta_3S_+=108r^2-864r^3+2592r^4+\beta_1(\alpha^{6}_{1}-\alpha^{4}_{1})+\beta_3(\alpha^{6}_{3}-\alpha^{4}_{3}),
A_{+} = 2\alpha_{1}^{3} - \alpha_{1} - 12s_{+}, B_{+} = 1 + \alpha_{1} - 2A_{+}, u_{+} = s_{+} - u_{-}
C_{+} = A_{+} - \alpha_{1}, q_{+} = (\alpha^{2} + \alpha_{1})/2 - A_{+} - s_{+} - u_{+}, P_{+} = N_{-} - S_{+} \lambda_{1}/2
(2\alpha_{_{1}}^{_{3}}\text{-}\alpha_{_{1}}\text{-}\alpha_{_{1}}^{_{4}}),\;\beta_{_{3}}\alpha_{_{3}}D_{_{+}}\equiv\beta_{_{3}}\alpha_{_{3}}^{_{2}}+\beta_{_{1}}\alpha_{_{1}}(\alpha_{_{1}}\text{-}A_{_{+}})+20(\alpha_{_{1}}^{_{4}}\text{-}\alpha_{_{1}}^{_{2}})
\beta_3 \alpha_3 N_+, N_+ = P_+ - N_-, Q_+ = S_+ - Q_-, G_+ = D_+ - \alpha_3,
K_{-} = (\alpha_{3}^{2} - \alpha_{3})/2 - M_{-} - N_{-} - Q_{-}, E_{+} = 1 + \alpha_{3} - 2D_{+},
H_{+} = (2\alpha_{3}^{3} - \alpha_{3} - D_{+})/12 - \alpha_{1}^{2}P_{+} + (\alpha_{1}^{2} - \alpha_{1})N_{-}, M_{+} = H_{+} - M_{-},
X_{+} = Z_{+}, L_{+} = 1-2R_{+}, K_{+} = (\alpha^{2} + \alpha_{3})/2-D_{+}-H_{+}-M_{+}-N_{+}
P_+-S_+-Q_+, V_+=-R_+-2Y_+-2Z_+, T_+=R_+, W_+=Y_+,
\beta_2 R_+ = 4r - (\beta_0 + \beta_1 A_+ + \beta_3 D_+), Y_+ = -R_+ / 12 - \alpha^2 Z_+ + \lambda_1 / 12,
13(1+\alpha_1+\alpha_3-\alpha_1^2)-64\alpha_3^2-9\alpha_1\alpha_3+84\alpha_1^2\alpha_3^2+29\alpha_1^2\alpha_3-22
\alpha_1 \alpha_3^2 - 51 \alpha_3^3 = 0, \alpha_2 = 0, \alpha_3 = \frac{1}{2}, \alpha_1 = (-2 + \sqrt{119})/30,
\beta_2 = 1, r = R^* and Q_i is a free parameter.
```

SHK86E: Here, the eighth order method is the method derived by Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992) for which $y_{n-\alpha 2}$ and $y_{n-\alpha 3}$ are independent of y_{n+1} , the points $f(t_{n+\alpha 1}, y_{n+\alpha 1})$ and $f(t_{n-\alpha 1}, y_{n-\alpha 1})$ are coincident, $\alpha_1 = 0$, $\alpha_3 = 1/2$, $\alpha_2 = (-2+\sqrt{119})/30$, $\beta_1 = 1$

and $r=R^*$. For this method we must evaluate $f(t_{n-\alpha 2}, y_{n-\alpha 2})$ and $f(t_{n-\alpha 3}, y_{n-\alpha 3})$ once per step. We combine this method with a sixth order method for which $y_{n-\alpha 2}$ is independent of y_{n+1} and the points $(t_{n+\alpha 1}, y_{n+\alpha 1})$ and $(t_{n-\alpha 1}y_{n})_{\alpha 1}$ are coincident. The resulting formula pair is as follows:-Sixth order method given by Eq. (2-3) with

 $\begin{array}{l} R_-=0,\ T_-=\alpha_2, L_-=1-\alpha_2,\ X_-+Z_-=0,\ \beta_2=(\alpha_2^2-\alpha_2^4)/20,\\ \beta_0=1/12-\beta_2\alpha_2^2,\ Z_++Z_-=\left[240\alpha_2(1+\alpha_2)\beta_1/(1+\alpha_2-\alpha_2^2)\beta_2\right]\left[r^3-r^2/4+r/48-1/4320\right],\ \gamma=1-2(\beta_0+\beta_1+\beta_2),\\ W_-=(\alpha_3^2-\alpha_2)/6,\ Y_-=0,\ A_+=\left[r/8-3r^2/2-1/720\right]/\beta_2\\ (Z_++Z_-),V_-=(3\alpha_2^2-2\alpha_2-\alpha_3^2)/6,\ s_+=(1+\alpha_2-\alpha_2^2)/480\alpha_2\\ (1+\alpha_2)\beta_1-A_+/12,\ B_+=1-2A_+,\ C_+=A_+,\ X_+=Z_++2Z_-,\\ u_+=s_+,\ q_+=-A_+-2s_+,\ A_-=A_+,\ B_-=B_+,\ C_-=C_+,\ s_-=s_+,\\ \beta_2R_+=3r-1/12+\beta_2\alpha_2^2-2\beta_1A_+,\ q_-=q_+,\ u_-=u_+,\\ Y_+=(2\alpha_2^3-\alpha_2-R_+)/12,\ T_+=R_+-\alpha_2,\ L_+=1+\alpha_2-2R_+,\\ W_+=Y_+-W_-,\ V_+=-R_+-2Y_+-2(Z_++Z_-)+(\alpha_2^3+3\alpha_2^2+2\alpha_2)/6,\\ \beta_1=1,\ \alpha_2=(-2+\sqrt{119})/30,\ \alpha_1=0,\ r=R^*\ \text{and}\\ Z_-\ \text{is a free parameter}. \end{array} \label{eq:condition}$

Eighth order method given by Eq. (2-5) with

 $R_{-} = 0$, $Y_{-} = 0$, $X_{-} + Z_{-} = 0$, $D_{-} = 0$, $H_{-} = 0$, $S_{-} = 0$, $\beta_2 = (13-42\alpha_3^2)/840(\alpha_2^4-\alpha_2^2)(\alpha_3^2-\alpha_2^2), \beta_3 = (13-42\alpha_3^2)/840(\alpha_3^4-\alpha_3^2)(\alpha_3^2-\alpha_3^2), \beta_3 = (13-42\alpha_3^2)/840(\alpha_3^4-\alpha_3^2), \beta_3 = (13-4\alpha_3^2)/840(\alpha_3^4-\alpha_3^2), \beta_3 = (13-4\alpha_3^2)/840(\alpha_3^4-\alpha_3^2)$ $42\alpha_{2}^{2}$)/840(α_{3}^{4} - α_{3}^{2})(α_{2}^{2} - α_{3}^{2}), $\beta_{0} = 1/12 - \beta_{2}\alpha_{2}^{2} - \beta_{3}\alpha_{3}^{2}$, $\gamma = 1 - 2(\beta_0 + \beta_1 + \beta_2 + \beta_3), Q_- = 17/3360\beta_3\alpha_3(\alpha_2^3 - \alpha_2),$ $\lambda_1 = \beta_2(\alpha_2^4 - 2\alpha_2^3 + \alpha_2) + \beta_3(\alpha_3^4 - 2\alpha_3^3 + \alpha_3) + 12\beta_3(\alpha_2 - \alpha_2^2)$ $Q_{-}, N_{-}+P_{-}=0, M_{-}=(\alpha^{3}_{3}-\alpha_{3})/6-\alpha_{2}Q_{-}, Z_{+}+Z_{-}=17\beta_{1}$ $(1+\alpha_2-\alpha_2^2)/3360\beta_2\lambda_1(\alpha_2-\alpha_3)(1+\alpha_2), W_- = (\alpha_2^3-\alpha_2)/6,$ $V_{-} = (\alpha^{2} - \alpha_{2})/2 - W_{-}$ $E_{-} = 1 - \alpha_{3}$ $K_{-} = (\alpha^{2} - \alpha_{3})/2 - M_{-}O_{-}$ $\lambda_4 = 12(\alpha_2^4 - \alpha_2^2) - 153(1 + \alpha_2 - \alpha_2^2) / 140\beta_2(\alpha_2 - \alpha_3)(1 + \alpha_2),$ $G_{-} = \alpha_3, L_{-} = 1 - \alpha_2, T_{-} = \alpha_2, \lambda_4 \beta_3 S_{+} = 108r^2 - 864r^3 + 2592r^4$ $+\beta_2(\alpha_2^6-\alpha_2^4)+\beta_3(\alpha_3^6-\alpha_3^4), Q_+ = S_+-Q_-, \beta_3(P_++P_-) = -\beta_2(Z_+$ $+Z_{-})-\beta_{1}\beta_{3}S_{+}(2\alpha_{2}^{3}-\alpha_{2}-\alpha_{2}^{4})/\lambda_{1},\;s_{+}=-r^{4}/2\beta_{3}S_{+}(Z_{+}+Z_{-}),$ $A_{+} = -12s_{+} + \lambda_{1}/2\beta_{1}, R_{+} = [1/12 + (\alpha_{3}-1)\beta_{0} + \alpha_{3}(2\beta_{1}A_{+}-4r)]$ $+20\beta_3\alpha_3(\alpha_2^4-\alpha_2^2)Q_+/\beta_2(\alpha_2-\alpha_3), X_+ = Z_++Z_--X_-, C_+ = A_+,$ $u_{+} = s_{+}, N_{+} = P_{+} + P_{-} - N_{-}, B_{+} = 1 - 2A_{+}, q_{+} = -A_{+} - 2s_{+},$ $Y_{+} = (2\alpha_{2}^{3} - \alpha_{2} - R_{+})/12$, $T_{+} = R_{+} - \alpha_{2}$, $A_{-} = A_{+}$, $B_{-} = B_{+}$, $C_{-} = C_{+}, s_{-} = s_{+}, u_{-} = u_{+}, L_{+} = 1 + \alpha_{2} - 2R_{+}, W_{+} = Y_{+} - W_{-}$ $q_{-} = q_{+}, V_{+} = (\alpha^{2}_{2} + \alpha_{2})/2 - R_{+} - Y_{+} - W_{+} - 2(Z_{+} + Z_{-}),$ $\beta_3 D_+ = 4r - (\beta_0 + 2\beta_1 A_+ + \beta_2 R_+), E_+ = 1 + \alpha_3 - 2D_+,$ $G_{+} = D_{+} - \alpha_{3}, H_{+} = (2\alpha_{3}^{3} - \alpha_{3} - D_{+})/12 - \alpha_{2}^{2}S_{+} + (\alpha_{2}^{2} - \alpha_{2})Q_{-},$ $M_{+} = H_{+} - M_{-}, K_{+} = (\alpha^{2}_{3} + \alpha_{3})/2 - D_{+} - H_{+} - M_{+} - S_{+} - Q_{+}$ $2(P_{+}+P_{-}),13(1+\alpha_{2}+\alpha_{3}-\alpha_{2}^{2})-64\alpha_{3}^{2}-9\alpha_{2}\alpha_{3}+84\alpha_{2}^{2}\alpha_{3}^{2}+$ $29\alpha_{2}^{2}\alpha_{3}-22\alpha_{2}\alpha_{3}^{2}-51\alpha_{3}^{3}=0, \alpha_{1}=0, \alpha_{3}=\frac{1}{2}, \alpha_{2}=(-2)$ $+\sqrt{119}/30$, $\beta_1 = 1$, $r = R^*$ and Z and P are free parameters. (27)

SHK86F: In this formula pair, the eighth order method is the method derived by Khiyal (1991), Khiyal and Thomas (1997a), Thomas and Khiyal (1992) for which $y_{n-\alpha 2}$ and $y_{n-\alpha 3}$ are independent of y_{n+1} , $\ddot{y}_{n-\alpha 1} = \ddot{y}_{n}$, $\alpha_1 = 0$, $\alpha_2 = (-2+\sqrt{119})/30$,

 $\alpha_3=1/2,~\beta_1=1~\text{and}~r=R^*.$ For this method we must evaluate $f(t_{n\cdot\alpha2},y_{n\cdot\alpha2})$ and $f(t_{n\cdot\alpha3},y_{n\cdot\alpha3})$ once per step. We combine this method with a sixth order method for which $y_{n\cdot\alpha2}$ is independent of y_{n+1} and $\ddot{y}_{n\cdot\bar{\alpha}1}\ddot{y}_{n}$. The resulting formula pair is

Sixth order method given by Eq. (2-3) with

 $\begin{array}{l} R_-=0,\ T_-=\alpha_2,\ L_-=1-\alpha_2,\ Z_-=0,\ Y_-=0,\ A_-=0,\\ B_-=1,\ C_-=0,\ s_-=0,\ q_-=0,\ u_-=0,\ \beta_2=(\alpha^2_2-\alpha^4_2)/20,\\ Z_+=\left[240\alpha_2(1+\alpha_2)\beta_1/(1+\alpha_2-\alpha^2_2)\beta_2\right]\left[r^3-r^2/4+r/48-1/4320\right],\\ \beta_0=1/12-\beta_2\alpha^2_2,\ \gamma=1-2\ (\beta_0+\beta_1+\beta_2),\ A_+=\left[r/4-3r^2-1/360\right]/\beta_2Z_+,\ s_+=\left(1+\alpha_2-\alpha^2_2\right)/240\alpha_2(1+\alpha_2)\beta_1-A_+/12,\\ B_+=1-2A_+,\ \beta_2R_+=3r-1/12+\beta_2\alpha^2_2-\beta_1A_+,\ L_+=1+\alpha_2-2R_+,\\ T_+=R_+-\alpha_2,\ C_+=A_+,\ Y_+=(2\alpha^3_2-\alpha_2-R_+)/12,\ W_-=(\alpha^3_2-\alpha_2)/6,\ W_+=Y_+-W_-,\ q_+=-A_+-2s_+,\ u_+=s_+,\ X_+=Z_+-X_-,\\ V_++X_+=(\alpha^2_2+\alpha_2)/2-R_+-Y_+-W_+-Z_+,\ V_-+X_-=(3\alpha^2_2-2\alpha_2-\alpha^3_2)/6,\ \beta_1=1,\ \alpha_2=(-2+\sqrt{119})/30,\ \alpha_1=0,\ r=R^* \\ \text{and }X_-\text{ is a free parameter.} \end{array} \label{eq:Reconstruction}$

Eighth order method given by Eq. (2-5) with

 $A_{-} = 0$, $B_{-} = 1$, $C_{-} = 0$, $s_{-} = 0$, $q_{-} = 0$, $u_{-} = 0$, $R_{-} = 0$, $Y_{-} = 0$, $Z_{-} = 0$, $D_{-} = 0$, $H_{-} = 0$, $S_{-} = 0$, $P_{-} = 0$, $\beta_2 = (13-42\alpha_3^2)/840(\alpha_2^4-\alpha_2^2)(\alpha_3^2-\alpha_2^2), \ \beta_3 = (13-42\alpha_2^2)/3$ $840(\alpha_3^4 - \alpha_3^2)(\alpha_2^2 - \alpha_3^2), \beta_0 = 1/12 - \beta_2 \alpha_2^2 - \beta_3 \alpha_3^2, \gamma = 1-2$ $(\beta_0 + \beta_1 + \beta_2 + \beta_3), Q_- = 17/3360\beta_3\alpha_3(\alpha_2^3 - \alpha_2), \lambda_1 = \beta_2(\alpha_2^4)$ $-2\alpha_{2}^{3}+\alpha_{2}+\beta_{3}(\alpha_{3}^{4}-2\alpha_{3}^{3}+\alpha_{3})+12\beta_{3}(\alpha_{2}-\alpha_{2}^{2})Q_{-}, M_{-}=(\alpha_{3}^{3}+\alpha_{3})+12\beta_{3}(\alpha_{2}-\alpha_{3}^{2})Q_{-}$ $-\alpha_3$)/6- α_2 Q_-, E_ = 1- α_3 , λ_4 = 12 (α_2^4 - α_2^2)-153(1+ α_2 $-\alpha_2^2$ /140 $\beta_2(\alpha_2-\alpha_3)(1+\alpha_2)$, G₋ = α_3 , L₋ = 1- α_2 , Z₊ = 17 β_1 $(1+\alpha_2-\alpha_2^2)/3360\beta_2\lambda_1(\alpha_2-\alpha_3)(1+\alpha_2)$, $s_+=-r^4/\beta_3S_+Z_+$ $u_{+} = s_{+}, C_{+} = A_{+}, T_{-} = \alpha_{2}, \lambda_{4}\beta_{3}S_{+} = 108r^{2}-864r^{3}+2592r^{4}+$ $\beta_2(\alpha_2^6 - \alpha_2^4) + \beta_3(\alpha_3^6 - \alpha_3^4)$, $A_+ = -12s_+ + \lambda_1/\beta_1$, $B_+ = 1-2A_+$, $\beta_{3}P_{+} = -\beta_{2}Z_{+} - \beta_{1}\beta_{3}S_{+}(2\alpha_{2}^{3} - \alpha_{2} - \alpha_{2}^{4})/\lambda_{1}, K_{-} = (\alpha_{3}^{2} - \alpha_{3})/2 - M_{-}$ $Q_{-}N_{-}, Q_{+} = S_{+}-Q_{-}, R_{+} = [1/12+(\alpha_{3}-1)\beta_{0}+\alpha_{3}(\beta_{1}A_{+}-4r)]$ $+20\beta_3\alpha_3(\alpha_2^4-\alpha_2^2)Q_+/\beta_2(\alpha_2-\alpha_3), q_+=-A_+-2s_+, V_-=(\alpha_2^2-\alpha_3)$ α_2 /2-W_-X_, $Y_+ = (2\alpha_2^3 - \alpha_2 - R_+)/12$, $\beta_3 D_+ = 4r - (\beta_0 + \beta_1 A_+)/12$ $+\beta_2 R_+$), $L_+ = 1 + \alpha_2 - 2R_+$, $T_+ = R_+ - \alpha_2$, $W_+ = Y_+ - W_ X_{+} = Z_{+} - X_{-}, M_{+} = H_{+} - M_{-}, G_{+} = D_{+} - \alpha_{3}, H_{+} = (2\alpha_{3} - \alpha_{3} - D_{+})$ $/12-\alpha_2^2S_++(\alpha_2^2-\alpha_2)Q_-$, $V_+=(\alpha_2^2+\alpha_2)/2-R_+-Y_+-W_+-Z_+-X_+$, $E_{+} = 1 + \alpha_{3} - 2D_{+}, N_{+} = P_{+} - N_{-}, K_{+} = (\alpha^{2} + \alpha_{3})/2 - D_{+} - H_{+} - M_{+}$ $S_{+}-Q_{+}-P_{+}-N_{+}$, $W_{-}=(\alpha_{2}^{3}-\alpha_{2})/2$, $13(1+\alpha_{2}+\alpha_{3}-\alpha_{2}^{2})-64\alpha_{3}^{2}-64\alpha_{3}^{2}$ $9\alpha_2\alpha_3 + 84\alpha_2^2\alpha_3^2 + 29\alpha_2^2\alpha_3 - 22\alpha_2\alpha_3^2 - 51\alpha_3^3 = 0$, $\alpha_1 = 0$, $\alpha_3 = \frac{1}{2}$, $\alpha_2 = (-2 + \sqrt{119})/30$, $\beta_1 = 1$, $r = R^*$ and X_ and N_ are free parameters. (29)

Observe that, for all the pairs derived, $f(t_{n-\alpha i},y_{n-\alpha i})$ is common to both the sixth and eighth order methods.

NUMERICAL RESULTS

We present some numerical results for the formula pairs. We are mainly concerned with solving oscillatory stiff initial value problems. We have tried a number of explicit scalar (nonstiff) test problems of the form (1). They give similar results and so we restrict our attention to one oscillatory example.

Example 1: $\ddot{y}+\sinh(y) = 0$, y(0) = 1, $\dot{y}(0) = 0$.

This is a pure oscillation problem whose solution has maximum amplitude unity and period approximately six.

To verify that our techniques work for systems, we use as a test problem a moderately stiff system of two equations.

Example 2:
$$\ddot{y}_1 + \sinh(y_1 + y_2) = 0$$
, $y_1(0) = 1$, $\dot{y}_1(0) = 0$; $\ddot{y}_2 + 10^4 y_2 = 0$, $y_2(0) = 10^{-8}$, $\dot{y}_2(0) = 0$:

For this example we have deliberately introduced coupling from the stiff (linear) equation to the nonstiff (nonlinear) equation. Our intention here is that the stiff oscillatory component y_2 should be present only at the noise level as otherwise we would expect to choose the stepsize to resolve y_2 .

Both Examples 1 and 2 have been solved for t∈[0,6] and both were also used by Khiyal and Thomas (1997a). Following Khiyal and Thomas (1997a), the stepsize is chosen initially to be h=1 as this is more or less on scale for the problems. However, to ensure that the iterations set up by the starting technique converge and that the local error test is satisfied, this stepsize is reduced automatically by the codes.

The error at the end point is obtained by comparing the computed solution with the solution obtained by using a fixed step code with a small stepsize for Example 1 and for the first equation of Example 2. For the second equation of Example 2, we have used the exact solution. We denote the error at the end point by MAXERR where for the scalar equation it is Error at t = 6 and for the system it is |Error| at t = 6.

We present the results for the cases where the maximum number of iterations permitted for the direct hybrid method, PMAX, is 10. As we have seen, at least one extra starting value is required by all our methods. We allow the methods which are used for the starting technique to take a maximum of ten iterations to achieve convergence. This initial relaxation of PMAX for the starting technique is designed to avoid rejecting steps at this stage simply because convergence is slow.

In each case, we present some statistics on the performance of the methods. These are important when comparing the cost of the methods. The notation used in the Tables are as follows.

 Number of evaluations of the differential equations right hand side f, FCN;

- Number of evaluations of the Jacobian ∂f=∂y, JCB;
- Number of iterations overall, NIT;
- Number of iterations on steps where the iteration converges, NSIT;
- Number of steps overall, NST;
- Number of successful steps to complete the integration, NSST;
- Number of failed steps, NFST;
- Number of steps where the stepsize is changed, NCST;
- Number of LU factorisations of the iteration matrix, NFAC:
- Number of function evaluations required on a per step basis, rather than on each iteration, NFPS;
- Number of iterations overall for the higher order method, NITH.

The results are given in Table 1-8. The cost of the starting technique is not included in the tables. We present the results for the case where the eighth order method is used to advance the step. (We have also tested an approach in which the sixth order method is used to advance the step but this is more expensive, in general.) Thus, the sixth order method is used as a predictor for the eighth order method and to form the error estimate. As a predictor for the sixth order method, we use an interpolant of degree five. That is, we define $y^{(0)}_{n+1} = p_{5,n}(t_n+h)$, where p_{5,n}(t) is the polynomial of degree five which interpolates to $(t_{n,i}, y_{n,i}, \ddot{y}_{n,i})$, i = 0, 1, 2. This predictor can be used only if information from two previous steps is available. On a change of stepsize, we need to compute approximations for y and ÿ at previous points. We obtain these approximations by using the polynomial of degree eight, $p_{8,n}(t)$, which interpolates to $(t_{n-i}, y_{n-i}, \ddot{y}_{n-i})$, i = 0, 1, 2, 3 and for which $p_{8,n}(t_{n-4}) = y_{n-4}$. Note that this interpolant has the same order (locally) as the eighth order direct hybrid method.

Before we can employ this error estimation technique, we need a special starting technique to obtain the values y_1 , y_2 , y_3 and y_4 . Thus we take four steps with the eighth order, four stage implicit Runge-Kutta method. To solve the resulting system of nonlinear equations, we use the iteration scheme proposed by Cooper and Butcher (1983).

Having completed four steps with a uniform stepsize, we form an estimate of the local error. If this is too big, we reduce the stepsize and return to the start. If the local error test is satisfied, we use the eighth order direct hybrid method for subsequent steps. At the end of each step, we form the error estimate Le_{n+1} . The stepsize for the next step (or for the repeated step in the case of an error test failure) is given by

Table 1:Result for Example 1. initially H = 1.0, PMAX = 10, $TOL = 10^{-4}$

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Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	1.19×10 ⁻⁴	2.80×10 ⁻⁵	5.77×10 ⁻⁵	1.54×10 ⁻⁵	9.25×10 ⁻⁵	5.15×10 ⁻⁵
FCN	254	217	261	291	506	242
JCB	1	1	1	2	1	1
NIT	65	54	68	78	116	65
NSIT	56	54	54	58	112	57
NST	20	19	19	21	52	16
NSST	17	18	17	18	51	14
NCST	4	2	4	3	1	4
NFST	3	1	2	3	1	2
NFPS	38	37	37	39	104	31
NITH	21	18	20	18	54	16

Table 2:Result For Example 2. Initially H = 1.0, PMAX = 10, $TOL = 10^{-4}$

Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	3.71×10^{-4}	3.63×10^{-4}	7.28×10 ⁻⁵	7.25×10 ⁻⁵	2.12×10^{-4}	8.98×10 ⁻⁴
FCN	3342	4364	4162	4162	2748	4086
JCB	2	12	6	6	2	10
NIT	832	1083	1040	1040	684	1021
NSIT	778	991	999	999	678	951
NST	273	363	344	344	231	336
NSST	264	344	333	333	230	319
NCST	10	15	8	8	1	12
NFST	9	19	11	11	1	17
NFAC	15	44	22	22	4	38
NFPS	544	721	684	684	462	666
NITH	302	394	358	358	234	357

Table 3: Result for Example 1. Initially H = 1.0, PMAX = 10, $TOL = 10^{-6}$

Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	3.90×10^{-6}	1.03×10^{-6}	1.85×10^{-6}	1.86×10^{-6}	1.81×10^{-6}	1.60×10 ⁻⁵
FCN	368	361	338	338	1627	473
JCB	1	1	1	1	1	1
NIT	99	93	92	92	366	131
NSIT	85	92	83	83	320	86
NST	23	28	20	20	173	24
NSST	21	27	19	19	163	19
NCST	3	1	2	2	11	8
NFST	2	1	1	1	10	5
NFPS	46	55	40	40	346	48
NITH	25	27	22	22	183	32

Table 4: Result for Example 2. Initially H = 1.0, PMAX = 10, $TOL = 10^{-6}$

	zatampre za matamy z	1 110,1111111 10,10				
Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	3.51×10 ⁻⁵	9.40×10 ⁻⁶	2.96×10 ⁻⁶	2.87×10 ⁻⁶	1.38×10^{-6}	1.62×10^{-6}
FCN	3340	5585	4013	4085	5585	3698
JCB	1	5	10	9	3	8
NIT	831	1392	999	1016	1360	921
NSIT	777	1347	929	952	1339	867
NST	272	464	328	336	499	304
NSST	265	456	316	325	495	295
NCST	10	7	11	10	4	8
NFST	7	8	12	11	4	9
NFAC	11	18	31	28	9	24
NFPS	544	928	655	671	998	607
NTTH	303	481	361	366	507	328

$$\hat{h} = h(TOL/2|Le_{n+1}|_{\infty})^{1/7},$$

where TOL is the local error tolerance and h is the current stepsize. We do not allow the stepsize to decrease by more than a factor ρ_1 or increase by more than a factor ρ_3 . These restrictions help to avoid large fluctuations in the stepsize caused by local changes in the error estimate. Also, we do not increase the stepsize at all unless it can

be increased by a factor of at least ρ_2 , where $\rho_2 < \rho_3$. This restriction is designed to avoid the extra function and Jacobian evaluations involved in changing the stepsize unless a worthwhile increase is predicted. Following Thomas (1987), in our tests we take ρ_1 = 0.1, ρ_2 = 2 and ρ_3 = 10.

Comparing the results given in Table 1-8 with those presented by Khiyal and Thomas (1997a), for which a

Table 5: Result for Example 1. Initially H = 1.0, PMAX = 10, $TOL = 10^{-8}$

Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	4.33×10^{-7}	4.43×10^{-7}	2.82×10 ⁻⁷	2.82×10 ⁻⁷	3.27×10 ⁻⁸	1.23×10 ⁻⁵
FCN	1348	1345	861	861	5705	976
JCB	1	1	1	1	1	1
NIT	356	355	228	428	1275	259
NSIT	201	218	173	173	1219	168
NST	82	83	55	55	622	60
NSST	58	63	47	47	608	45
NCST	36	32	14	14	16	23
NFST	24	20	8	8	14	15
NFPS	164	166	110	110	1244	120
NITH	116	114	67	67	636	79

Table 6: Result for Example 2. Initially H = 1.0, PMAX = 10, $TOL = 10^{-8}$

Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	1.55×10^{-7}	1.81×10^{-7}	3.02×10^{-7}	3.02×10^{-7}	1.20×10^{-7}	2.67×10 ⁻⁷
FCN	3609	3847	4282	3629	8226	3630
JCB	1	7	10	6	1	6
NIT	900	956	1068	907	1829	906
NSIT	863	903	967	827	1829	844
NST	298	319	346	292	913	297
NSST	292	311	328	278	913	286
NCST	11	10	23	20	2	15
NFST	6	8	18	14	0	11
NFAC	12	22	42	31	3	26
NFPS	596	638	692	584	1826	594
NITH	313	341	386	324	913	318

Table 7: Result for Example 1. Initially H = 1.0, PMAX = 10, $TOL = 10^{-10}$

Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	7.07×10 ⁻¹¹	2.73×10 ⁻¹¹	1.02×10^{-9}	1.02×10^{-9}	6.22×10 ⁻¹¹	5.28×10 ⁻⁸
FCN	1160	1202	1070	1070	15750	1151
JCB	1	1	1	1	1	1
NIT	308	315	283	283	3508	305
NSIT	280	304	272	272	3436	266
NST	77	85	73	73	1736	76
NSST	72	83	71	71	1718	69
NCST	8	4	4	4	20	10
NFST	5	2	2	2	18	7
NFPS	154	170	146	146	3472	152
NITH	82	87	75	75	1754	84

Table 8: Result for Example 2. Initially H = 1.0, PMAX = 10, $TOL = 10^{-10}$

Methods	SHK86A	SHK86B	SHK86C	SHK86D	SHK86E	SHK86F
MAXERR	5.43×10 ⁻⁹	8.04×10 ⁻⁹	1.67×10 ⁻⁹	1.67×10 ⁻⁹	1.34×10^{-9}	1.67×10 ⁻⁹
FCN	6888	7143	6076	5941	20152	7079
JCB	2	7	13	10	1	6
NIT	1718	1783	1519	1485	4479	1770
NSIT	1674	1733	1411	1398	4475	1730
NST	569	590	487	479	2238	583
NSST	564	582	471	467	2237	577
NCST	8	8	16	13	2	7
NFST	5	8	16	12	1	6
NFAC	11	22	42	32	3	18
NFPS	1138	1180	974	958	4476	1166
NITH	596	614	545	28	2239	603

predictor-corrector approach is used to estimate the local error, we find that in general the formula pair approach is cheaper for Example 2 while the predictor corrector approach is usually cheaper for example 1. However, even for Example 1, the formula pair approach requires fewer steps than the predictor-corrector approach but is more expensive overall because the integration has to be performed with two (P-stable) methods on each step.

We believe that the performance of all these methods would be improved considerably by using a more satisfactory interpolant. At present, we use the interpolating polynomial of degree eight, $p_{\delta,n}(t)$ to calculate the back values on a change of stepsize. We notice that when the stepsize is increased during the computation, the approximations calculated by $p_{\delta,n}(t)$ are unfortunately not very good (since this is extrapolation

rather than interpolation) and this means more computational effort is required to ensure convergence of the iterations.

CONCLUSIONS

In the study, we have derived some formula pairs, consisting of a sixth order and an eighth order direct hybrid method. The two methods in each pair have been chosen to have some features in common, so that the computational cost of using the formula pair is reduced. The formula pairs provide an estimate of the local error and this allows the stepsize to be varied so that the size of the local error is controlled.

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