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The Numerical Integration of Stiff Systems of ODEs using Stiffly Stable Continuous Second Derivative Hybrid Methods

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Abstract

A class of continuous second derivative hybrid methods is developed and the stability of these methods is investigated using the root locus plot. The k-step stiffly stable schemes of order $k+2$ are suitable for stiff systems of equations for $k \le 14$. These schemes have been implemented and some numerical results are presented.

Keywords *:* Continuous Linear Multistep Methods, Hybrid Predictor, Stiff Stability, Root Locus.

1.0 Introduction

Let us consider the initial value problem

$$y' = f(x, y(x)),\ y(a) = y_0,\ x \in (a, b) \tag{1.1}$$

whose solution is stiff. The class of stiffly stable continuous second derivative hybrid methods of interest for the numerical solution of (1.1) is given by

$$y_{n+k} = y_{n+k-1} + h\sum_{j=0}^{k} \beta_{1,j}(t)\, f_{n+j} + h\beta_{1,v}(t) f_{n+v} \tag{1.2}$$

and the hybrid predictor

$$y_{n+v} = \sum_{j=0}^{k} \alpha_j(t) y_{n+j} + h\beta_{2,k}(t) f_{n+k} + h^2 \beta_{3,k}(t)\, f'_{n+k} \tag{1.3}$$

where $t = \dfrac{x - x_{n+1}}{h}$ *and* $v = k - \frac{1}{2}$

Equation (1.2) is an extension of [5]

Our purpose is to derive hybrid methods in continuous form which possess good characteristics such as small error constant, high order and minimum function evaluation. The use of the second derivative in the hybrid predictor enhances stability characteristics. The methods have been obtained using a means of interpolation and collocation. Continuous collocation methods are found in, [1], [2], [3], [4], [7], [9], [11], [12], [13], [14].

The derivation of the class of methods and its hybrid predictor is found in section 2. The determination of the stability of the method using the root locus is contained in section 3. In section 4 some numerical results are presented.

2.0 The Derivation of the Class of Methods and its Hybrid Predictor

The polynomial interpolant

$$y(x) = \sum_{j=0}^{k+2} a_j x^j \tag{2.1}$$

is assumed to represent the numerical solution of (1.1). Substituting (2.1) into (1.2) we obtain the linear system of equations. The values of $a'_j s$ are determined by solving the above system of equations. Setting $x = x_{n+1} + th$ and putting the resulting values a_j in (2.1) yield the coefficients $\beta_{1,0}(t),\ \beta_{1,1}(t), \beta_{1,2}(t), \cdots, \beta_{1,k}(t)$ *and* $\beta_{1,v}(t)$ for a fixed value of k with $t = k-1$. In Table A we have the continuous coefficients of the schemes for $k = 1, 2, 3$.

In a similar manner using the interpolant

$$y_{n+v}^{(x)} = \sum_{j=0}^{k+2} b_j x^j \tag{2.3}$$

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$$
\begin{bmatrix}
0 & 1 & 2x_n & 3x_n^2 & \cdots & (k+2)x_n^{k+1} \\
0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & \cdots & (k+2)x_{n+1}^{k+1} \\
0 & 1 & 2x_{n+2} & 3x_{n+2}^2 & \cdots & (k+2)x_{n+2}^{k+1} \\
0 & 1 & 2x_{n+3} & 3x_{n+3}^2 & \cdots & (k+2)x_{n+3}^{k+1} \\
0 & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & 1 & 2x_{n+k} & 3x_{n+k}^2 & \cdots & (k+2)x_{n+k}^{k+1} \\
0 & 1 & 2x_{n+v} & 3x_{n+v}^2 & \cdots & (k+2)x_{n+v}^{k+1} \\
1 & x_{n+k-1} & x_{n+k-1}^2 & x_{n+k-1}^3 & \cdots & x_{n+k-1}^{k+2}
\end{bmatrix}
\begin{bmatrix}
a_0 \\ a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ a_k \\ a_{k+1} \\ a_{k+2}
\end{bmatrix}
=
\begin{bmatrix}
f_n \\ f_{n+1} \\ f_{n+2} \\ f_{n+3} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ f_{n+k} \\ f_{n+v} \\ y_{n+k-1}
\end{bmatrix}
\qquad (2.2)
$$

the coefficients $\alpha_0^*(t), \alpha_1^*(t), \ \alpha_2^*(t), \cdots, \alpha_k^*(t), \ \ \beta_{2,k}(t)$ *and* $\beta_{3,k}(t)$ of the hybrid predictor (1.3) are derived. For $k = 1, 2, 3$ its continuous coefficients are given in Table B. Likewise for $k \in 4(1)14$, the continuous coefficients for the schemes (1.2) and (1.3) can be gotten.

Table 1: Continuous Coefficients of the New Class of Methods.

k	t	j	$\alpha_j(t)$	$\alpha_j(k-1)$	$\beta_{1,j}(t)$	$\beta_{1,j}(k-1)$
1	0	0	1	1	$\frac{1}{6}+\frac{t^2}{2}+\frac{2}{3}t^3$	$\frac{1}{6}$
		$\frac{1}{2}$	0	0	$\frac{2}{3}-2t^2-\frac{4}{3}t^3$	$\frac{2}{3}$
		1	1	1	$\frac{1}{6}+t+\frac{3}{2}t^2+\frac{2}{3}t^3$	$\frac{1}{6}$
2	1	0	0	0	$-\frac{t^2}{12}+\frac{t^3}{6}-\frac{t^4}{12}$	0
		1	1	1	$t-t^2-\frac{t^3}{3}+\frac{t^4}{2}$	$\frac{1}{6}$
		$\frac{3}{2}$	0	0	$\frac{4t^2}{3}-\frac{2t^4}{3}$	$\frac{2}{3}$
		2	1	1	$-\frac{t^2}{4}+\frac{t^3}{6}+\frac{t^4}{4}$	$\frac{1}{6}$

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3	2	0	0	0	$\frac{31}{1800}-\frac{t^2}{10}+\frac{13t^3}{90}-\frac{3t^4}{40}+\frac{t^5}{75}$	$-\frac{1}{1800}$
		1	0	0	$-\frac{151}{360}+t-\frac{7t^2}{12}-\frac{2t^3}{9}+\frac{7t^4}{24}-\frac{t^5}{15}$	$\frac{1}{360}$
		2	1	1	$-\frac{109}{120}+\frac{3t^2}{2}-\frac{t^3}{6}-\frac{5t^4}{8}+\frac{t^5}{5}$	$\frac{19}{120}$
		$\frac{5}{2}$	0	0	$\frac{88}{225}-\frac{16t^2}{15}+\frac{16t^3}{45}+\frac{8t^4}{15}-\frac{16t^5}{75}$	$\frac{152}{225}$
		3	1	1	$-\frac{29}{360}+\frac{t^2}{4}-\frac{t^3}{9}-\frac{t^4}{8}+\frac{t^5}{15}$	$\frac{59}{360}$

Table 2: Continuous Coefficients of the Hybrid Predictor

K	t	j	$\alpha^*_j(t)$	$\alpha^*_j(k-\frac{3}{2})$	$\beta_{2,k}(t)$	$\beta_{2,k}(k-\frac{3}{2})$	$\beta_{3,k}(t)$	$\beta_{3,k}(k-\frac{3}{2})$
1	$-\frac{1}{2}$	0	$-t^3$	$\frac{1}{8}$	0	0	0	0
		$\frac{1}{2}$	1	1	0	0	0	0
		1	$1+t^3$	$\frac{7}{8}$	$1-t^3$	$-\frac{3}{8}$	$\frac{t^2}{2}+\frac{t^3}{2}$	$\frac{1}{16}$
2	$\frac{1}{2}$	0	$-\frac{t}{8}+\frac{3t^2}{8}-\frac{3t^3}{8}+\frac{t^4}{8}$	$\frac{-1}{128}$	0	0	0	0
		1	$1-2t+2t^3-t^4$	$\frac{3}{16}$	0	0	0	0
		$\frac{3}{2}$	1	1	0	0	0	0
		2	$\frac{17t}{8}-\frac{3t^2}{8}-\frac{13t^3}{8}+\frac{7t^4}{8}$	$\frac{105}{128}$	$-\frac{5t}{4}+\frac{3t^2}{4}+\frac{5t^3}{4}-\frac{3t^4}{4}$	$-\frac{21}{64}$	$\frac{t}{4}-\frac{t^2}{4}-\frac{t^3}{4}+\frac{t^4}{4}$	$\frac{3}{64}$
3	$\frac{3}{2}$	0	$-\frac{4t}{27}+\frac{10t^2}{27}-\frac{t^3}{3}+\frac{7t^4}{54}-\frac{t^5}{54}$	$\frac{1}{576}$	0	0	0	0

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		1	$1-\frac{3t}{2}-\frac{t^2}{4}+\frac{11t^3}{8}-\frac{3t^4}{4}+\frac{t^5}{8}$	$\frac{-5}{256}$	0	0	0	0
		2	$4t-2t^2-3t^3+\frac{5t^4}{2}-\frac{t^5}{2}$	$\frac{15}{64}$	0	0	0	0
		$\frac{5}{2}$	1	1	0	0	0	0
		3	$-\frac{127t}{54}+\frac{203t^2}{108}+\frac{47t^3}{24}-\frac{203t^4}{108}+\frac{85t^5}{216}$	$\frac{1805}{2304}$	$\frac{14t}{9}-\frac{25t^2}{18}-\frac{5t^3}{4}+\frac{25t^4}{18}-\frac{11t^5}{36}$	$\frac{-115}{384}$	$-\frac{t}{3}+\frac{t^2}{3}+\frac{t^3}{4}-\frac{t^4}{3}+\frac{t^5}{12}$	$\frac{5}{128}$

3.0 The Stability of the Methods

The stability of the methods is determined using the root locus approach. Lambert [10] and Otunta et al [13] discussed the general graphical form of the root locus plot. Substituting the hybrid solution y_{n+v} at point x_{n+v} into the LMM (1.2) for a corresponding k and applying the resultant method to the scalar test problem $y' = \lambda y,\ \mathrm{Re}(\lambda h) < 0, \quad z = \lambda h$ with an arbitrary initial value we have the stability polynomial

$$\pi(r,\, z) = r^k - r^{k-1} - z\sum_{j=0}^{k}\beta_{1,j}r^j - z\beta_{1,v}\left(\sum_{j=0}^{k}\alpha_j r^j + z\beta_{2,k}r^k + z^2\beta_{3,k}r^k\right)$$

Applying the root locus method to $\pi(r,\, z) = 0$ shows that the methods in (1.2) are stiffly stable for $k \le 14$. The root Loci are shown in figures 1-15. For any given value of k, the interval of absolute stability of the methods are deduced in Table 3.

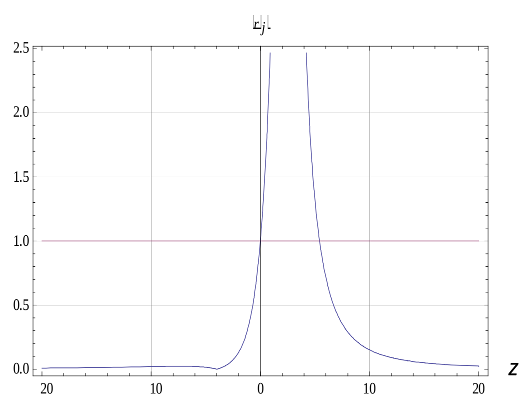

Figure 1: Root Locus for k=1

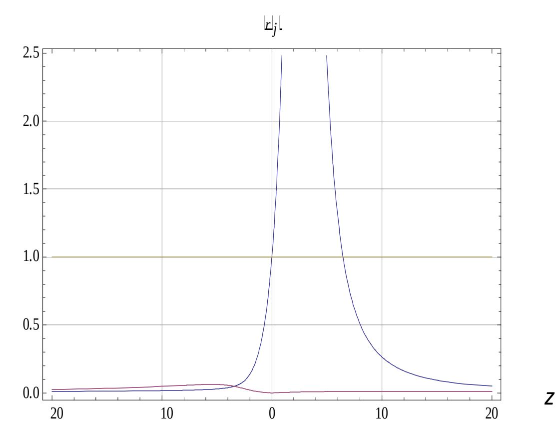

Figure 2: Root Locus for k=2

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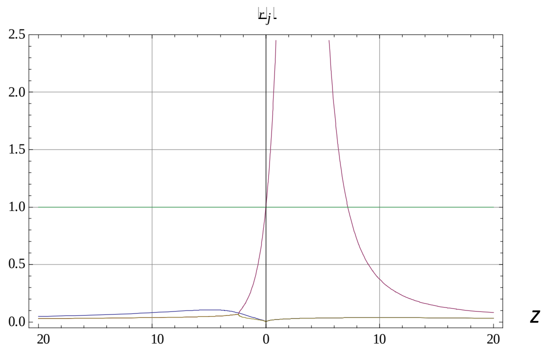

Figure 3: Root Locus for k=3

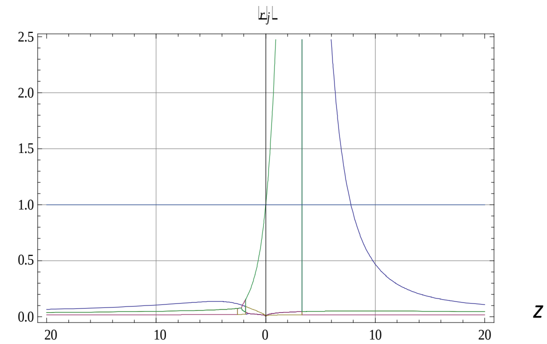

Figure 4: Root Locus for k=4

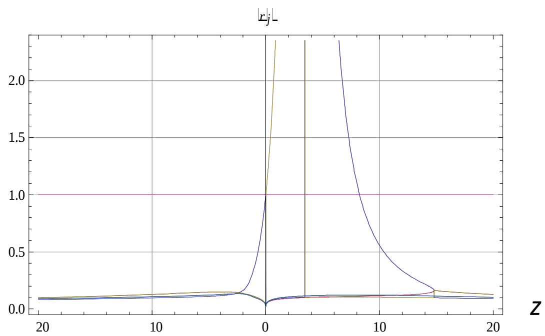

Figure 5: Root Locus for k=5

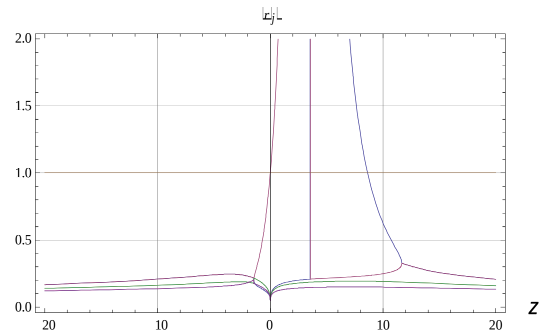

Figure 6: Root Locus for k=6

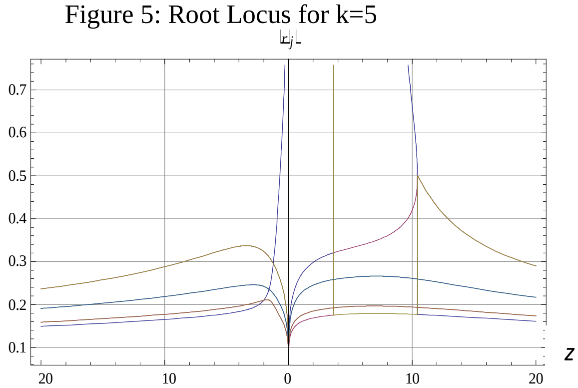

Figure 7: Root Locus for k=7

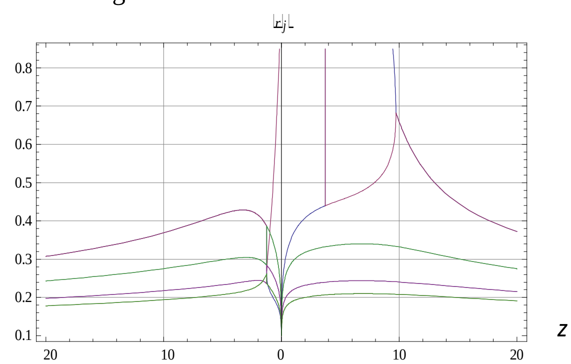

Figure 8: Root Locus for k=8

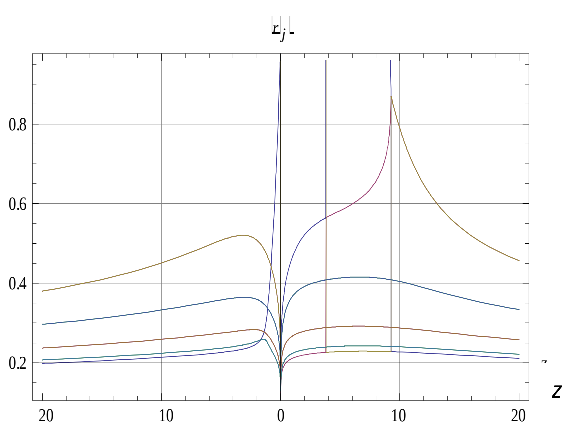

Figure 9: Root Locus for k=9

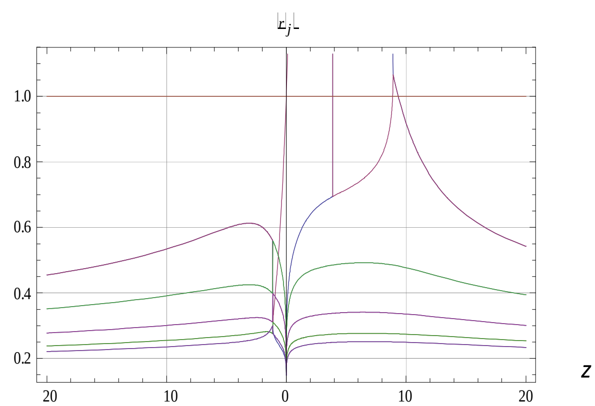

Figure 10: Root Locus for k=10

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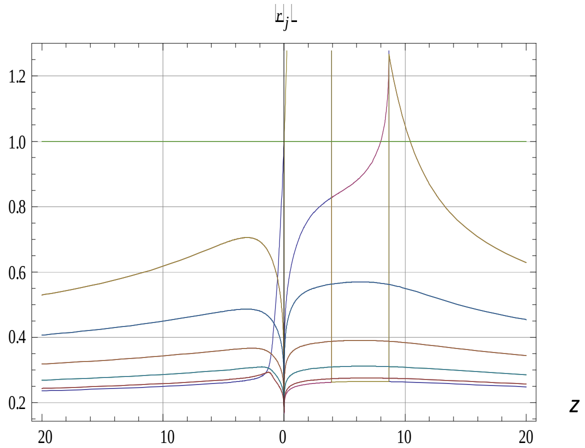

Figure 11: Root Locus for k=11

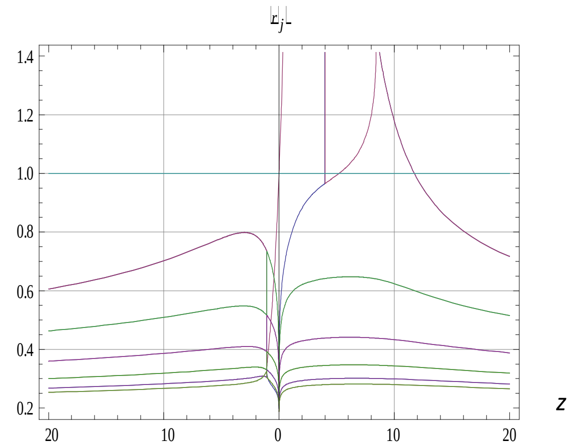

Figure 12: Root Locus for k=12

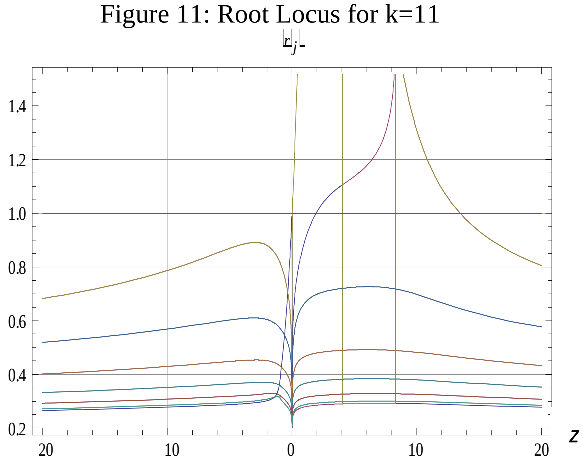

Figure 13: Root Locus for k=13

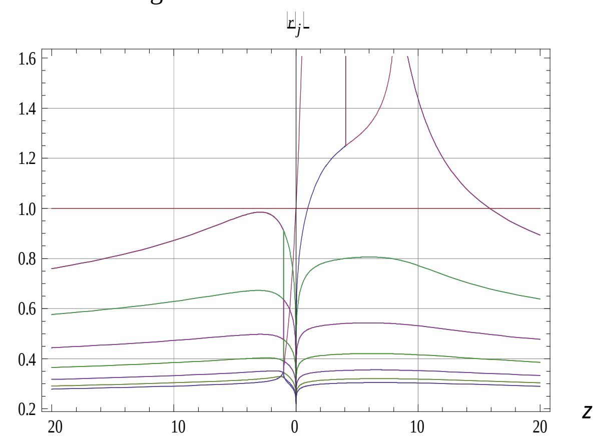

Figure 14: Root Locus for k=14

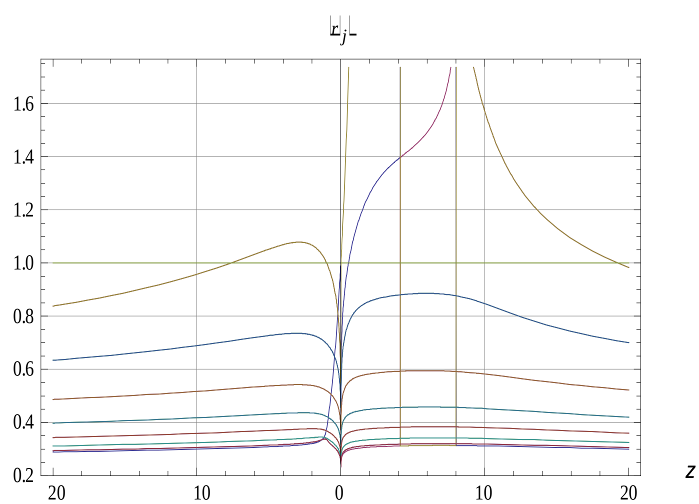

Figure 15: Root Locus for k=15

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Table 3: The step number, interval of absolute stability, error constant and order of methods.

k	Interval of Absolute stability for z		Error Constants		Order	
	t	Method (1.2) + (1.3)	Method (1.2)	Method (1.3)	$P_1(1.2)$	$P_2(1.3)$
1	0	$(-\infty, 0) \cup (4, \infty)$	$-\frac{1}{2880}$	$-\frac{1}{384}$	4	3
2	1	$(-\infty, 0) \cup (5.85, \infty)$	$-\frac{1}{2880}$	$-\frac{1}{1280}$	4	4
3	2	$(-\infty, 0) \cup (7.2, \infty)$	$-\frac{1}{3600}$	$\frac{-1}{3072}$	5	5
4	3	$(-\infty, 0) \cup (9.2, \infty)$	$-\frac{5}{24192}$	$\frac{-1}{6144}$	6	6
5	4	$(-\infty, 0) \cup (8.25, \infty)$	$-\frac{1}{70560}$	$\frac{-3}{32768}$	7	7
6	5	$(-\infty, 0) \cup (9.25, \infty)$	$-\frac{3499}{29030400}$	$\frac{-11}{196608}$	8	8
7	6	$(-\infty, 0) \cup (8.93, \infty)$	$-\frac{1039}{10886400}$	$\frac{-143}{3932160}$	9	9
8	7	$(-\infty, 0) \cup (9.12, \infty)$	$-\frac{369689}{4790016000}$	$\frac{-13}{524288}$	10	10
9	8	$(-\infty, 0) \cup (9.15, \infty)$	$-\frac{83711}{1317254400}$	$\frac{-221}{12582912}$	11	11
10	9	$(-\infty, 0) \cup (9.35, \infty)$	$-\frac{555959297}{10461394944000}$	$\frac{-323}{25165824}$	12	12
11	10	$(-\infty, 0) \cup (10.46, \infty)$	$-\frac{102086969}{2266635571200}$	$\frac{-323}{33554432}$	13	13
12	11	$(-\infty, 0) \cup (11.75, \infty)$	$-\frac{16966329803}{439378587648000}$	$\frac{-7429}{1006632960}$	14	14
13	12	$(-\infty, 0) \cup (13.5, \infty)$	$-\frac{2623916993}{78460462080000}$	$\frac{-37145}{6442450944}$	15	15
14	13	$(-\infty, 0) \cup (15.75, \infty)$	$-\frac{1496727730 6931}{5121898964 58240000}$	$\frac{-19665}{4294967296}$	16	16
15	14	Instable	$-\frac{2000818289471}{7774310928384 0000}$	$\frac{-63365}{17179869184}$	17	17

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4.0 Numerical Experiment

Let us consider the following initial value problems:

Problem 1: Linear problem, Enright [5]

$$y' = \begin{bmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{bmatrix} y, \; y(0) = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \; y(x) = \begin{bmatrix} e^{-0.1x} \\ e^{-10x} \\ e^{-100x} \\ e^{-1000x} \end{bmatrix}$$

with x in the range [0,3] and $h = 0.0001$

Problem 2: Nonlinear chemical problem, Enright [5]

$$y_1' = -0.04y_1 + 10^4 y_2 y_3$$

$$y_2' = 400y_1 + 10^4 y_2 y_3 - 3\times10^7 y_2^2, \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$y_3' = 3\times10^7 y_2^2$$

$$x \in 0(0.0001)3$$

For $k = 1$, the proposed class of methods is used to solve the above problems. The implicitness in the methods is resolved by applying the Newton Raphson iterative scheme as reported in [5], [6], [9] ,[10] and [13]. The inverse Euler method in [6] is used to generate the starting values for the iterative schemes. The numerical results of the first component of problem 1 and the second component of problem 2 are of comparable accuracy to that of [5] and ODE 15s code in MATLAB discussed in [8] as seen figure 16 and figure 17.

5.0 Conclusion

A class of continuous second derivative linear multistep methods with one hybrid point of step number $k \le 14$ is considered. The stability graphs in figures 1-15 show that the methods are stiffly stable for $k \le 14$ and unstable for $k = 15$. The order and the error constant of the methods and its corresponding second derivative hybrid are given in table 3. The graphs in figure 16 and figure 17 show the accuracy of the new formulas when compared to results from Enright's methods and the state of-the-art code, ODE 15s in MATLAB.

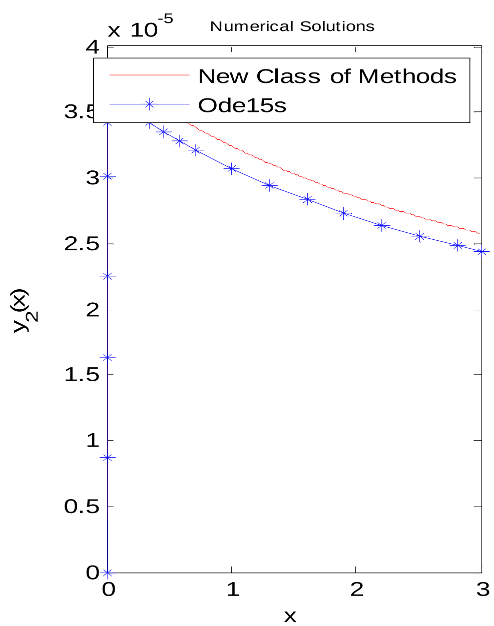

Figure 16: The plot of the numerical solutions of the component $y_1(x)$ of problem 1.

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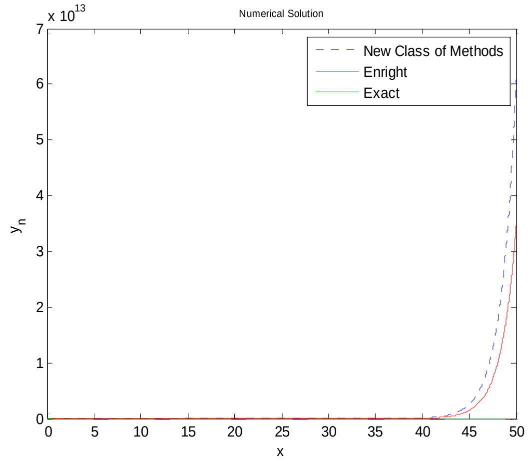

Figure 17: The plot of the numerical solutions of the component $y_2(x)$ of problem 2.

References

[1] **Arevalo**, C. Fuherer, C. and Seva, M., (2002), A Collocation Formulation of Multistep methods for Variable Step-size Extensions. Appl. Numer. Math, Vol. 42, pp. 5-16.

[2] Burrage, K. and Tian, T. (2001), Stiffly Accurate Runge Kutta Methods for Stiff Stochastic Differential Equations, Comput, Phys. Commun., Vol. 142, pp. 186-190.

[3] Butcher, J. C. and Chen, D. J. L. (2001), On the Implementation of ESIRK methods for Stiff IVPs, Numer. Math. Vol. 26, pp, 477-489.

[4] Butcher, J. C. (2002). The A-stability of Methods with Pade and Generalized Stability Functions. Numer. Algorithms; Vol. 31, pp. 47-58.

[5] Enright, W. H. (1974), Second Derivative Multistep Methods for Stiff Ordinary Differential Equations. SIAM. J. Numerical Analysis Vol. 1., No. 2.

[6] Fatunla, S. O. (1988), Numerical Methods for Initial Value Problems in Ordinary Differential Equation, Academics Press Inc.

[7] Hairer, E. and Lubeich. C. H. (2004), Symmetric Multistep Methods Over Long Times. Numer. Math. Vol. 32, pp. 373-379.

[8] Higham, J. D. and Higham J. N. (2000), Matlab Guide. SIAM Philadelphia.

[9] Ikhile, M. N. O. and Okuonghae, R. I. (2007), Stiffly Stable Continuous Extension Second Derivative LMM with an off-step Point for IVPs in ODEs Journal of the Nigerian Association of mathematical Physics, Vol. 11, pp. 175-190.

[10] Lambert, J. D. (1991), Computational Methods in Ordinary Differential Equations; John Wiley and Sons, New York.

*Corresponding author: Tel. +2348056743776

[11] Okuonghae, R. I. (2008), Stiffly Stable Second Derivative Continuous Linear Multi Step Methods for Initial Value Problems in Ordinary Differential Equations Ph.D. Thesis. Department of Mathematics, University of Benin, Benin City, Nigeria.

[12] Onumanyi, P., Sirisena, U. W. and Awoyemi, D. O. (1996), A new Family of Predictor-Corrector Methods. Spectrum Journal. Vol. 3, No. 1& 2.

[13] Otunta, F. O. Ikhile, M. N. O. and Okuonghae, R. I. (2007), Second Derivative Continuous Linear Multi Step Methods for the Numerical Integration of Stiff Ordinary Differential Equations. Journal of the Nigerian Association Mathematical Physics, Vol. 11, pp.159-174.

[14] Sirisena, U. W., Onumanyi, P. and Chollon, J. P. (2001), Continuous Hybrid Methods Through Multistep Collocation ABACUS, Vol. 28; No. 2; pp. 58-66.

*Corresponding author: Tel. +2348056743776

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