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A Special Family of LMM with Two Hybrid Points for Stiff ODEs

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Abstract

Hybrid methods with one or more off-step points give better stability characteristics and higher order than the conventional linear multistep methods (LMM). Enright (1974) discussed the formulation of the second derivative LMM which was found to be stiffly stable for step number $k \le 7$ for the numerical solution of stiff Initial Value Problems (IVPs) in Ordinary Differential Equations (ODEs). In this paper some second derivative continuous linear multistep methods with two hybrid points are proposed for step number $k \le 9$ for stiff ODEs. The derivation of these methods is based on collocation and interpolation approach of Onumanyi et al (1996) and Arevalo et al (2002). The family of methods is stiffly stable for $k \le 8$ and of comparable accuracy to the Enright's method and the state of-the-art code Ode 15s in MATLAB.

Keywords: , Hybrid points, Continuous LMM, stiffly stable.

1. Introduction:

Methods for solving the initial value problem

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

Whose solution is stiff and where $f\left(x,\ y(x)\right)$ *and* $y(x)$ may be vectors can be based on continuous methods with hybrid points in the interval $\left(x_n\ ,\ x_{n+k}\right)$

Analogous methods are the discrete methods of [2, 3, 4, 6, 7, 9, and 10].

The search for good methods for solving stiff problems is inexhaustible. This paper shows that a slight modification of the Enright method is possible. The modification consists of the addition of two parameters $\alpha_v(t)y_{n+v}$ *and* $\beta_{v^*}(t)f_{n+v^*}$ in (1.2). The inclusion of the hybrid points improves the stability characteristics of the new class of methods. Also the formulation of the new scheme provides numerical solutions at any desired point in the integration interval.

The general form of the Hybrid Second Derivative Continuous Linear Multistep Methods (HSDCLMM) for the numerical solution of (1.1) to be considered is given by

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

The hybrid predictor formulas y_{n+v} and y_{n+v^*} at the hybrid points x_{n+v} and x_{n+v^*} respectively are

$$y_{n+v} = \mu_{k-1}(t)y_{n+k-1} + h\sum_{j=0}^{k}\theta_{1,j}(t)f_{n+j} + h^2\theta_{2,k}(t)f'_{n+k} \tag{1.3}$$

$$y_{n+v^*} = \mu_0(t)y_n + h\sum_{j=0}^{k}\theta_{3,j}(t)f_{n-k+j} \tag{1.4}$$

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where

$$\alpha_j(t),\ \beta_j(t),\ \ \mu_j(t)\ \ ,\theta_{1,j}(t),\ \theta_{2,k}(t)\ \ and\ \ \theta_{3,j}(t)\ \ ,\qquad j=\ 0(1)k$$

are continuous coefficients in t and $f_{n+j}=f\left(x_{n+j}\,,\,y_{n+j}\right)\ ,\ y''_{n+j}=f'_{n+j}=f'(x_{n+j},y_{n+j})$ .The scaled variable is defined as $t=\dfrac{x-x_{n+1}}{h}$ and $h=x_{n+1}-x_n$ is a fixed mesh size. Practical implementation demands that the index of (1.4) be shifted by a unit, that is

$$y_{n+v^*}=\mu_0(t)y_n+\ h\sum_{j=0}^{k}\theta_{3,j}(t)\,f_{n-k+j}\ ;\qquad v=v^*$$

$$n\rightarrow n+1$$

The parameters v and v^* are incorporated to provide off grid collocation points x_{n+v} and x_{n+v^*} in an open interval $\left(x_{n+k-1}\,,\,x_{n+k}\right)\ and\ v=k-\frac{1}{2}$ where k is the step number of the scheme. The resulting scheme (1.2) and the hybrid predictors (1.3) and (1.4) are of order $\left(k+3\right)$, $\left(k+2\right)\ and\ \left(k+1\right)$ respectively.

2.0 Derivation of the HSDCLMM

Let us assume that the numerical solution of (1.1) is in the form of the polynomial interpolant

$$y(x)\ =\ \sum_{j=0}^{m}a_jx^j \tag{2.1}$$

In the derivation of HSDCLMM, let $m=k+3$

then

$$y'(x)\ =\ \sum_{j=1}^{k+3}j\ a_jx^{j-1}\qquad\text{and}\qquad y''(x)=\sum_{j=2}^{k+3}j(j-1)\,a_jx^{j-2} \tag{2.2}$$

Collocating (2.2) at the points $x=x_{n+k}\ ,\ x_{n+v}\ ,\ x_{n+v+1}$ and interpolating at $x_{n+j}\ ,\ j=0(1)k$ we obtain the linear system of equations

$$\begin{bmatrix} 0 & 1 & 2x_n & 3x_n^2 & \cdots & (k+3)x_n^{k+2} \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & \cdots & (k+3)x_{n+1}^{k+2} \\ 0 & 1 & 2x_{n+2} & 3x_{n+2}^2 & \cdots & (k+3)x_{n+2}^{k+2} \\ 0 & 1 & 2x_{n+3} & 3x_{n+3}^2 & \cdots & (k+3)x_{n+3}^{k+2} \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 1 & 2x_{n+k} & 3x_{n+k}^2 & \cdots & (k+3)x_{n+k}^{k+2} \\ 0 & 1 & 2x_{n+v^*} & 3x_{n+v^*}^2 & \cdots & (k+3)x_{n+v^*}^{k+2} \\ 1 & x_{n+k-1} & x_{n+k-1}^2 & x_{n+k-1}^3 & \cdots & x_{n+k-1}^{k+3} \\ 1 & x_{n+v} & x_{n+v}^2 & x_{n+v}^3 & \cdots & x_{n+v}^{k+3} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_k \\ a_{k+1} \\ a_{k+2} \\ a_{k+3} \end{bmatrix} = \begin{bmatrix} f_n \\ f_{n+1} \\ f_{n+2} \\ f_{n+3} \\ \vdots \\ f_{n+k} \\ f_{n+v^*} \\ y_{n+k-1} \\ y_{n+v} \end{bmatrix} \tag{2.3}$$

After evaluating (2.3) using MATHEMATICA, the resulting values of $\{a_j\}_{j=0}^{k+3}$ are substituted into (2.1) to give the continuous coefficients $\alpha_j(t)$, $\beta_j(t)$ which are shown in Table 1 for the first three values of k

3.0 Derivation of the Implicit and Explicit Hybrid Predictors

Following the pattern in section 2.0 the implicit hybrid predictor (1.3) and the explicit hybrid predictor (1.4) at the hybrid points x_{n+v} and x_{n+v^*} are derived using the polynomial interpolant (2.1) by setting $m = k+2$ and $m = k+1$ respectively. The continuous coefficients for the two hybrid predictors are given in Table 2 and Table 3 respectively .

4.0 Stability of the Methods

Substituting the hybrid solutions y_{n+v} *and* y_{n+v+1} at the points x_{n+v} *and* x_{n+v+1} respectively into the method (1.2) for a corresponding k and applying the resultant method to the scalar test problem $y' = \lambda y$, $\mathrm{Re}(\lambda h) < 0$, $z = \lambda h$ with an arbitrary initial value we obtain the stability polynomial

$$\pi(r, z) = r^k - \alpha_{k-1} r^{k-1} - z\sum_{j=0}^{k}\beta_j r^j - \alpha_v\left(r^{k-1} + z\sum_{j=0}^{k}\theta_{1,j} r^j + z^2\theta_{2,k} r^k \right) - z\beta_{v^*}(1 + z\sum_{j=0}^{k}\beta_j r^j)$$

The root locus plot of the stability polynomial shows that the new methods are stiffly stable for $k \le 8$. It is unstable for $k \ge 9$. Figures 1-9 are the graphs of the root loci of the method (1.2). The step number, the interval of absolute stability, the error constant and the order of methods are given in Table 4.

5.0 Implementation of the Derived Methods

For $k = 1$, (1.2) becomes

$$y_{n+1} = \frac{1}{19}(-13 y_n + 32 y_{n+\frac{1}{2}}) + h(-\frac{17}{114} f_n + \frac{13}{38} f_{n+1} - \frac{2}{57} f_{n+\frac{3}{2}}) \quad , \qquad p = 4 \qquad (5.1)$$

Where

$$y_{n+\frac{1}{2}} = y_n + \frac{h}{24}(7 f_n + 5 f_{n+1}) - \frac{h^2}{12} f'_{n+1} \quad , \qquad p = 3$$

$$y_{n+\frac{3}{2}} = y_{n+1} + \frac{h}{8}(- f_{n+1} + 5 f_{n+2}) \quad , \qquad p = 2$$

To test and compare the derived methods with [5] and Ode 15s Code of MATLAB in [8], (5.1) is used to solve the following IVPs:

The nonlinear chemical problem of [5]

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

$$y_2' = 0.04 y_1 - 10^4 y_2 y_3 - 3\times 10^7 y_2^2 \ , \ y(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$y_3' = 3 \times 10^7 y_2^2$$

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

and the linear problem of [5]

$$y' = \begin{bmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -100 \end{bmatrix} y \ , \quad y(0) = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

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

The graphs showing the accuracy of the scheme when compared with Enright's method and Ode 15s Code of MATLAB are given in Figures 10 and 11.

Table 1: Continuous Coefficients of HSDCLMM.

k	t	j	$\alpha_j(t)$	$\alpha_j(k-1)$	$\beta_j(t)$	$\beta_j(k-1)$
1	0	0	$-\frac{13}{19}+\frac{48t^2}{19}-\frac{32t^3}{19}-\frac{48t^4}{19}$	$-\frac{13}{19}$	$-\frac{17}{114}+\frac{73t^2}{114}-\frac{6t^3}{19}-\frac{46t^4}{57}$	$-\frac{17}{114}$
		$\frac{1}{2}$	$\frac{32}{19}-\frac{48t^2}{19}+\frac{32t^3}{19}+\frac{48t^4}{19}$	$\frac{32}{19}$	0	0
		1	1	1	$\frac{13}{38}+t+\frac{9t^2}{38}-\frac{22t^3}{19}-\frac{14t^4}{19}$	$\frac{13}{38}$
		$\frac{3}{2}$	0	0	$-\frac{2}{57}+\frac{22t^2}{57}+\frac{12t^3}{19}+\frac{16t^4}{57}$	$-\frac{2}{57}$
2	1	0	0	0	$-\frac{9t^2}{260}+\frac{3t^3}{26}-\frac{7t^4}{65}+\frac{2t^5}{65}$	$\frac{1}{260}$
		1	$1-\frac{1440t^2}{247}+\frac{640t^3}{247}+\frac{720t^4}{247}-\frac{384t^5}{247}$	$-\frac{217}{247}$	$t-\frac{1912t^2}{741}+\frac{493t^3}{741}+\frac{956t^4}{741}-\frac{148t^5}{247}$	$-\frac{166}{741}$
		$\frac{3}{2}$	$\frac{1440t^2}{247}-\frac{640t^3}{247}-\frac{720t^4}{247}+\frac{384t^5}{247}$	$\frac{464}{247}$	0	0
		2	1	1	$-\frac{369t^2}{988}+\frac{329t^3}{494}+\frac{77t^4}{247}-\frac{74t^5}{247}$	$\frac{301}{988}$
		$\frac{5}{2}$	0	0	$\frac{272t^2}{3705}-\frac{112t^3}{741}-\frac{136t^4}{3705}+\frac{112t^5}{1235}$	$-\frac{88}{3705}$

3	2	0	0	0	$\frac{291}{31976}-\frac{270t^2}{3997}+\frac{4313t^3}{35973}-\frac{8257t^4}{95928}+\frac{673t^5}{23982}-\frac{247t^6}{71946}$	$-\frac{35}{41112}$
		1	0	0	$-\frac{8133}{22840}+t-\frac{9509t^2}{11420}-\frac{127t^3}{3426}+\frac{1727t^4}{4568}-\frac{203t^5}{1142}+\frac{437t^6}{17130}$	$\frac{697}{68520}$
		2	$-\frac{837}{571}+\frac{4800t^2}{571}-\frac{2880t^3}{571}-\frac{1920t^4}{571}+\frac{1728t^5}{571}-\frac{320t^6}{571}$	$-\frac{581}{571}$	$-\frac{7857}{4568}+\frac{7595t^2}{1713}-\frac{10816t^3}{5139}-\frac{7911t^4}{4568}+\frac{4669t^5}{3426}-\frac{2467t^6}{10278}$	$-\frac{11657}{41112}$
		$\frac{5}{2}$	$\frac{1408}{571}-\frac{4800t^2}{571}+\frac{2880t^3}{571}+\frac{1920t^4}{571}-\frac{1728t^5}{571}+\frac{320t^6}{571}$	$\frac{1152}{571}$	0	0
		3	1	1	$-\frac{939}{4568}+\frac{1925t^2}{2284}-\frac{6625t^3}{10278}-\frac{4049t^4}{13704}+\frac{1325t^5}{3426}-\frac{863t^6}{10278}$	$\frac{11669}{41112}$
		$\frac{7}{2}$	0	0	$\frac{792}{19985}-\frac{10384t^2}{59955}+\frac{5200t^3}{35973}+\frac{216t^4}{3997}-\frac{1040t^5}{11991}+\frac{3904t^6}{179865}$	$-\frac{472}{25695}$

Table 2: Continuous Coefficients of the Implicit Hybrid Predictor.

k	t	j	$\mu_j(t)$	$\mu_j(k-\frac{3}{2})$	$\theta_{1,j}(t)$	$\theta_{1,j}(k-\frac{3}{2})$	$\theta_{2,k}(t)$	$\theta_{2,k}(k-\frac{3}{2})$
1	$-\frac{1}{2}$	0	1	1	$\frac{1}{3}+\frac{t^3}{3}$	$\frac{7}{24}$	0	0
		$\frac{1}{2}$	1	1	0	0	0	0
		1	0	0	$\frac{2}{3}+t-\frac{t^3}{3}$	$\frac{5}{24}$	$\frac{-1}{6}+\frac{t^2}{2}+\frac{t^3}{3}$	$-\frac{1}{12}$
2	$\frac{1}{2}$	0	0	0	$-\frac{t^2}{8}+\frac{t^3}{6}-\frac{t^4}{16}$	$-\frac{11}{768}$	0	0
		1	1	1	$t-\frac{t^2}{2}-\frac{t^3}{3}+\frac{t^4}{4}$	$\frac{67}{192}$	0	0
		$\frac{3}{2}$	1	1	0	0	0	0
		2	0	0	$\frac{5t^2}{8}+\frac{t^3}{6}-\frac{3t^4}{16}$	$\frac{127}{768}$	$-\frac{t^2}{4}+\frac{t^4}{8}$	$-\frac{7}{128}$
3	$\frac{3}{2}$	0	0	0	$\frac{23}{1080}-\frac{t^2}{9}+\frac{4t^3}{27}-\frac{5t^4}{72}+\frac{t^5}{90}$	$\frac{71}{17280}$	0	0
		1	0	0	$-\frac{9}{20}+t-\frac{t^2}{2}-\frac{t^3}{4}+\frac{t^4}{4}-\frac{t^5}{20}$	$-\frac{21}{640}$	0	0
		2	1	1	$-\frac{29}{40}+t^2-\frac{3t^4}{8}+\frac{t^5}{10}$	$\frac{247}{640}$	0	0
		$\frac{5}{2}$	1	1	0	0	0	0
		3	0	0	$\frac{83}{540}-\frac{7t^2}{18}+\frac{11t^3}{108}+\frac{7t^4}{36}-\frac{11t^5}{180}$	$\frac{2467}{17280}$	$-\frac{11}{180}+\frac{t^2}{6}-\frac{t^3}{18}-\frac{t^4}{12}+\frac{t^5}{30}$	$-\frac{61}{1440}$

Table3: Continuous Coefficients of the Explicit Hybrid Predictor.

k	t	j	$\mu_j(t)$	$\mu_j(-\frac{1}{2})$	$\theta_{3,j}(t)$	$\theta_{3,j}(-\frac{1}{2})$
1	$-\frac{1}{2}$	0	1	1	$-\frac{1}{2}-t-\frac{t^2}{2}$	$-\frac{1}{8}$
		$\frac{1}{2}$	1	1	0	0
		1	0	0	$\frac{3}{2}+2t+\frac{t^2}{2}$	$\frac{5}{8}$
2	$-\frac{1}{2}$	0	1	1	$\frac{5}{12}+t+\frac{3t^2}{4}+\frac{t^3}{6}$	$\frac{1}{12}$
		$\frac{1}{2}$	1	1	0	0
		1	0	0	$-\frac{4}{3}-3t-2t^2-\frac{t^3}{3}$	$-\frac{7}{24}$
		2	0	0	$\frac{23}{12}+3t+\frac{5t^2}{4}+\frac{t^3}{6}$	$\frac{17}{24}$
3	$-\frac{1}{2}$	0	1	1	$-\frac{3}{8}-t-\frac{11t^2}{12}-\frac{t^3}{3}-\frac{t^4}{24}$	$-\frac{25}{384}$
		$\frac{1}{2}$	1	1	0	0
		1	0	0	$\frac{37}{24}+4t+\frac{7t^2}{2}+\frac{7t^3}{6}+\frac{t^4}{8}$	$\frac{107}{384}$
		2	0	0	$-\frac{59}{24}-6t-\frac{19t^2}{4}-\frac{4t^3}{3}-\frac{t^4}{8}$	$-\frac{187}{384}$
		3	0	0	$\frac{55}{24}+4t+\frac{13t^2}{6}+\frac{t^3}{2}+\frac{t^4}{24}$	$\frac{99}{128}$

Table 4: 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 (1.0.2) + (1.0.3) + (1.0.4)	Method (1.0.2)	Method (1.0.3)	Method (1.0.4)	$P_1(1.0.2)$	$P_2(1.0.3)$	$P_3(1.0.4)$
1	0	$(-\infty, 0) \cup (6.33, \infty)$	$\frac{1}{960}$	$\frac{11}{1152}$	$\frac{1}{12}$	4	3	2
2	1	$(-\infty, 0) \cup (8.72, \infty)$	$\frac{49}{142272}$	$\frac{71}{23040}$	$\frac{25}{384}$	5	4	3
3	2	$(-\infty, 0) \cup (10.56, \infty)$	$\frac{10583}{69068160}$	$\frac{109}{76800}$	$\frac{157}{2880}$	6	5	4
4	3	$(-\infty, 0) \cup (12.10, \infty)$	$\frac{1837}{2281574}$	$\frac{101}{129024}$	$\frac{243}{5120}$	7	6	5
5	4	$(-\infty, 0) \cup (13.40, \infty)$	$\frac{251069713}{5325481728000}$	$\frac{6971}{14450688}$	$\frac{40997}{967680}$	8	7	6
6	5	$(-\infty, 0) \cup (14.60, \infty)$	$\frac{22360231}{750319897600}$	$\frac{1191389}{3715891200}$	$\frac{1191619}{30965760}$	9	8	7
7	6	$(-\infty, 0) \cup (15.66, \infty)$	$\frac{38355465191}{1923058319616000}$	$\frac{1505863}{6688604160}$	$\frac{4111117}{116121600}$	10	9	8
8	7	$(-\infty, 0) \cup (16.62, \infty)$	$\frac{38083306453823}{2729190168430387200}$	$\frac{28877507}{175177728000}$	$\frac{122224747}{3715891200}$	11	10	9
9	8	Unstable	$\frac{717673306641629327}{709510539218697216000}$	$\frac{299132723}{2397988454400}$	$\frac{755300059}{24524881920}$	12	11	10

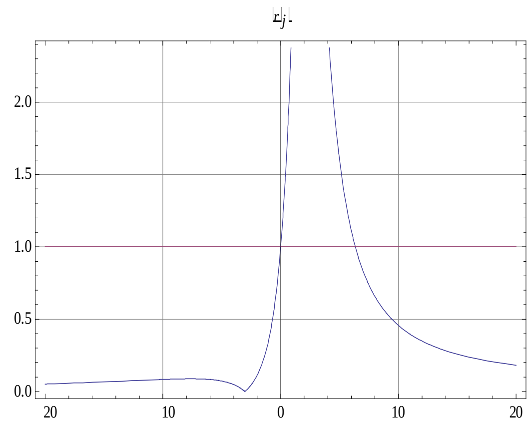

Figure 1: Root Locus for k=1

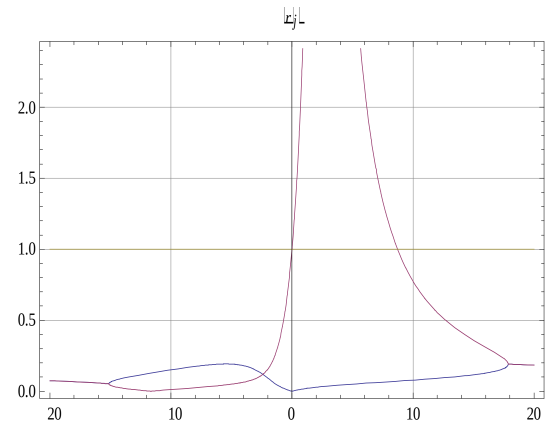

Figure 2: Root Locus for k=2

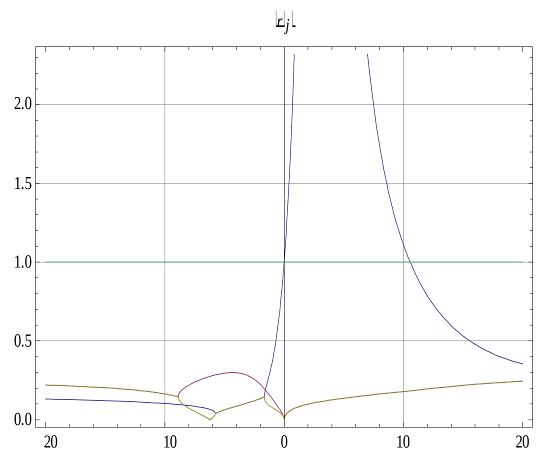

Figure 3: Root Locus for k=3

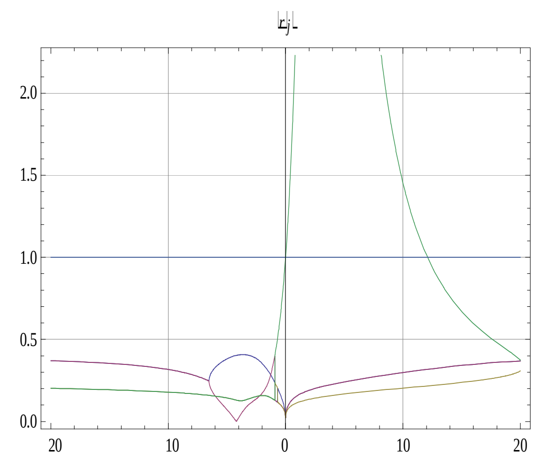

Figure 4: Root Locus for k=4

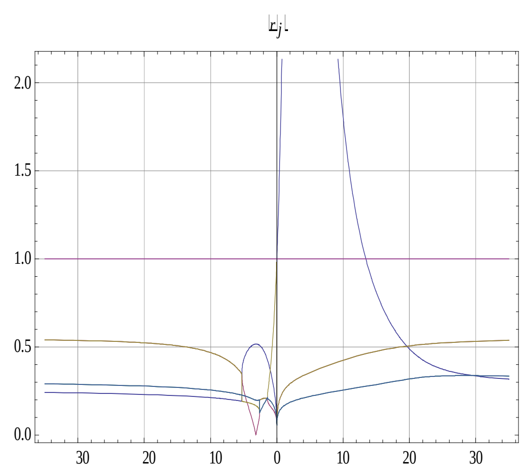

Figure5: Root Locus for k=5

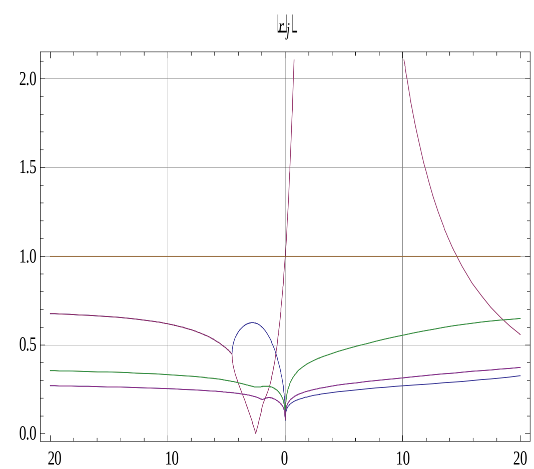

Figure 6: Root Locus for k=6

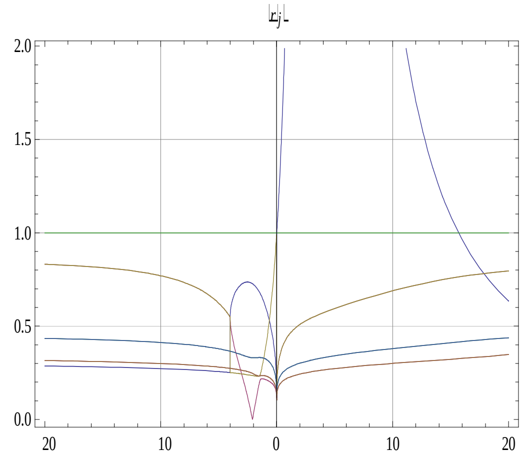

Figure7: Root Locus for k=7

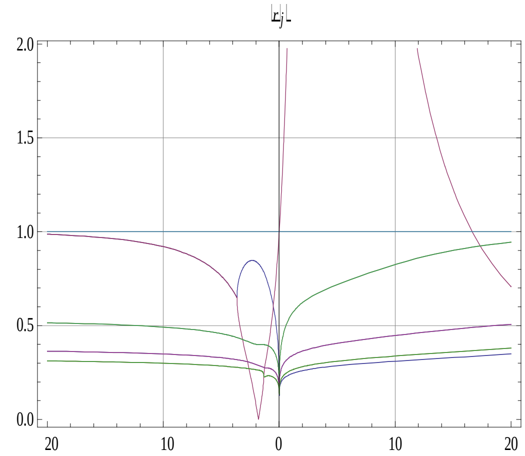

Figure8: Root Locus for k=8

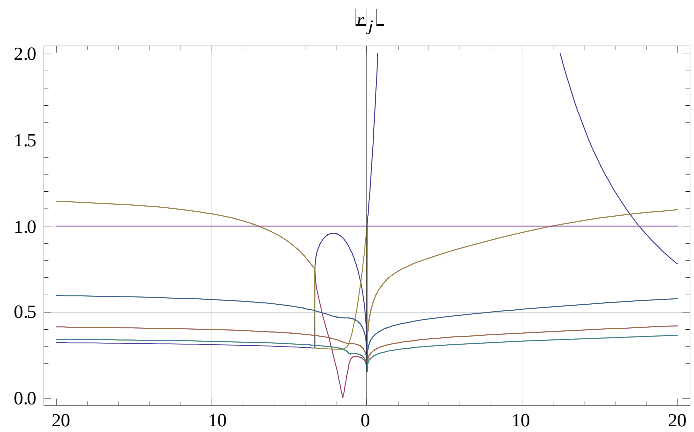

Figure9: Root Locus for k=9

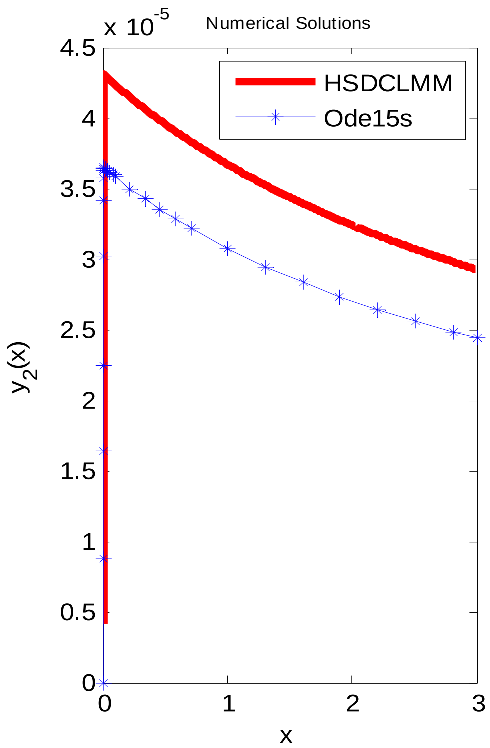

Figure 10: The plot of numerical solution of the component $y_2(x)$ of the nonlinear chemical problem of [5].

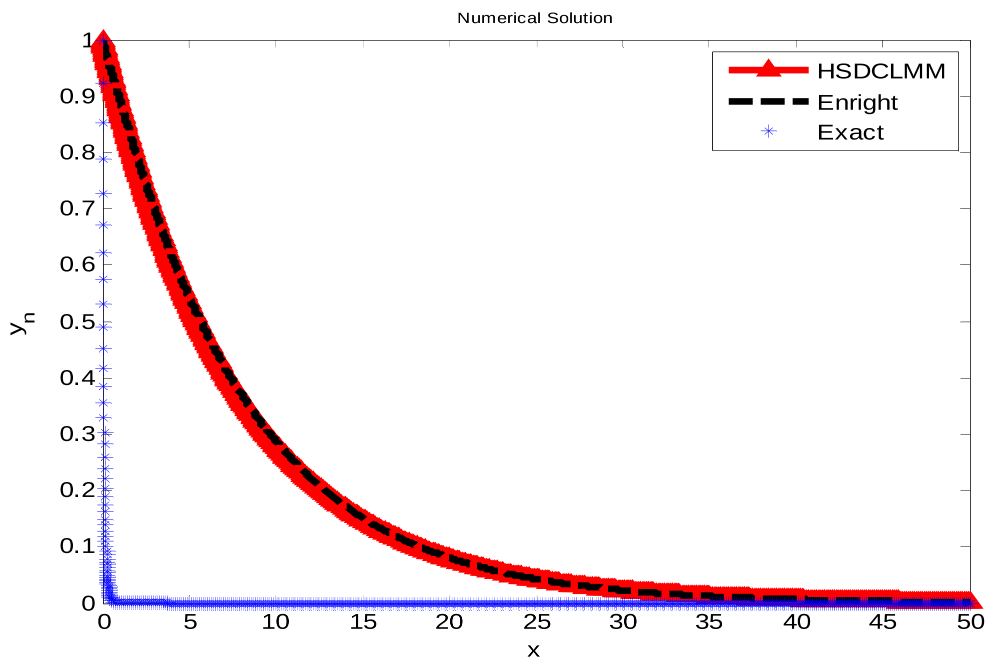

Figure 11: The plot of numerical solution of the component $y_1(x)$ of the linear problem of [5]

6.0 Conclusion

In this paper, a family of stiffly stable second derivative continuous linear multistep methods with two hybrid points is derived for the numerical solution of the initial value problem (1.1). The scheme employs collocation and interpolation as alternative to integration and differentiation method of deriving computational methods for IVPs in ODEs. The root loci in Figures 1-9 show that the methods are stiffly stable for $k \leq 8$ and unstable for $k \geq 9$.The graph of the numerical results in Figure 10 shows that HSDCLMM and Ode 15s Code of MATLAB are of comparable performance while the numerical results in Figure 11 show that HSDCLMM coincides with Enright's method.

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