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Implicit Second Derivative Hybrid Linear Multistep Method with Nested Predictors for Ordinary Differential Equations

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Abstract

In this paper, we considered an implicit hybrid linear multistep method with nested hybrid predictors for solving first order initial value problems in ordinary differential equations. The derivation of the methods is based on interpolation and collocation approach using polynomial basis function. The region of absolute stability of the method is investigated using the boundary locus approach and the methods have been found to be $A-$stable for step-length $k \leq 6$.

***Keywords*:** Linear multistep methods; hybrid; nesting; interpolation; collocation; boundary locus.

1. Introduction

The conventional linear multistep method (LMM) is defined as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \qquad (1.1)$$

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where α_j and β_j are parameter constants to be determined. The β_k determines if the linear multistep method is explicit or implicit. For explicit LMM (1.1), $\beta_k = 0$ and for implicit methods, $\beta_k \neq 0$. This is a popular method for the numerical approximation of the solutions of initial value problems in ordinary differential equations

$$y' = f(x, y), y(x_0) = y_0 \tag{1.2}$$

Its stability and order are subject to some constraints by [4]. Modification have been made to overcome the barrier, see [2,5,6,7,15,16] among others. Reference [6] introduced a second derivative term into the Adams-type LMM (1.1) to obtain the second derivative linear multistep (SDLMM) of the form

$$y_{n+k} = \alpha_{k-1} y_{n+k-1} + h \sum_{j=0}^{k} \beta_j f_{n+j} + h^2 f'_{n+k} \tag{1.3}$$

Off-step points have been introduced into this linear multistep method to overcome Dahlquist order and stability barrier. Other extension of (1.1) can be found in [10,1,8,3,11,14,16]. Our interest in this paper is to construct an implicit second derivative hybrid linear multistep method of the form

$$y_{n+k} = y_{n+k-1} + h\left(\sum_{j=0}^{k} \beta_j^{(m)} f_{n+j} + \beta_{v_m}^{(m)} f_{n+v_m} \right) + h^2 \lambda_k^{(m)} f'_{n+k} \tag{1.4}$$

which are of order $p = k + 3$ with the hybrids

$$y_{n+v_{l+1}} = y_{n+k} + h\left(\sum_{j=0}^{k} \beta_j^{(l)} f_{n+j} + \beta_{v_l}^{(l)} f_{n+v_l} \right) + h^2 \lambda_{v_l}^{(l)} f'_{n+v_l} \tag{1.5}$$

of order $p^* = k + 4$, where

$$y_{n+v_0} = \sum_{j=0}^{k} \alpha_j^{(-l)} y_{n+j} + h\beta_k^{(-l)} f_{n+k} + h^2 \lambda_k^{(-l)} f'_{n+k} \tag{1.6}$$

of order $p^{**} = k + 2$ for $l = 0(1)\mathrm{m}-1$

This method (1.4) seeks to approximate the solution of (1.2). The idea is to approximate (1.2) through the integration interval $[x_0, \mathrm{x}_N]$ where $y(x):[x_0, \mathrm{x}_N] \to \mathfrak{R}^m$ in which $f:[x_0, \mathrm{x}_N] \times \mathfrak{R}^m$ is smooth.

2. Specification of the hybrid methods (1.4)

The hybrid methods (1.4) with the hybrid predictors (1.5) and (1.6) have constant parameters

$\left\{\beta_j^{(m)}\right\}_{j=0}^{k}, \beta_{v_m}^{(m)}$, $\lambda_k^{(m)}$, $\left\{\beta_j^{(l)}\right\}_{j=0}^{k}, \beta_{v_l}^{(l)}$, $\lambda_{v_l}^{(l)}$, $\left\{\lambda_j^{(-l)}\right\}_{j=0}^{k}$, $\beta_k^{(-l)}$ and $\lambda_k^{(-l)}$ to be determined in such a way that the hybrid method (1.4) become stable. The method (1.4) is the hybrid method of Adams-type equipped with nested functions evaluation of the hybrid predictors (1.5) and (1.6). The hybrid parameters are chosen according as $v_m = k - \frac{1}{2}, v_l = \frac{v_{l+1}+k}{2}, l = 0(1)\mathrm{m}-1,\ v_l \in (0,k),\ v_l \neq j,\ \ j = 0(1)\mathrm{k},\ k = 1,2,3,\dots,$ $m = k-1$

2.1 Construction of the Hybrid methods (1.4)

We assume the solution of (1.4) of the form

$$y(\mathrm{x}) = \sum_{j=0}^{k+3} a_j x^j \tag{2.1}$$

where $\left\{a_j\right\}_{j=0}^{k+3}$ are real constant parameters to be determined and $\left(x^j,\ j = o(1)\mathrm{k}+3\right)$ is the polynomial basis function. Differentiating (2.1) twice to obtain

$$y'(\mathrm{x}) = f\left(x,y\right) = \sum_{j=1}^{k+3} j a_j x^{j-1} \tag{2.2}$$

$$y''(\mathrm{x}) = f'(\mathrm{x},\mathrm{y}) = \sum_{j=2}^{k+3} j(\mathrm{j}-1) a_j x^{j-2} \tag{2.3}$$

Interpolating (2.1), (2.2) and (2.3) at $x = x_{n+k}$ and collocating (2.2) at $x = x_{n+j}$, $j = 0(1)\mathrm{k}-2$ and $x = x_{n+v_m}$ we obtain the system of equations

$$\begin{bmatrix} 1 & x_{n+k-1} & x^2_{n+k-1} & . & . & . & x^{k+3}_{n+k-1} \\ 0 & 1 & 2x_n & . & . & . & (k+3)x_n^{k+3} \\ 0 & 1 & 2x^2_{n+1} & . & . & . & (k+3)x_{n+1}^{k+3} \\ . & . & . & . & & & . \\ . & . & . & & . & & . \\ . & . & . & & & . & . \\ 0 & 1 & 2x_{n+k} & . & . & . & (k+3)x_n^{k+3} \\ 0 & 1 & 2x_{n+v_m} & . & . & . & (k+3)x_{n+v_m}^{k+3} \\ 0 & 1 & 2 & . & . & . & (K+3)(k+2)x_{n+k}^{k+3} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ . \\ . \\ . \\ a_{k+1} \\ a_{k+2} \\ a_{k+3} \end{bmatrix} = \begin{bmatrix} y_{n+k-1} \\ f_n \\ f_{n+1} \\ . \\ . \\ . \\ f_{n+k} \\ f_{n+v_m} \\ f'_{n+k} \end{bmatrix} \tag{2.4}$$

Solving equation (2.4) with MATHEMATICA 10.0 Software package, the coefficients

$a_j\,'s\left(j=0(1)k+3\right)$ are obtained. Substituting these coefficients into (2.1) yields the discrete scheme for each k .

3. Construction of the hybrid Predictors

The corresponding hybrid predictor is obtained from the polynomial interpolant

$$y\left(x_n+v_{l+1}h\right)=\sum_{j=0}^{k+4} b_j x^j \tag{3.1}$$

where $\left\{b_j\right\}_{j=o}^{k+4}$ are parameter constants to be determined, $\left\{x^j\right\}_{j=0}^{k+4}$ is the polynomial basis function. Following the approach as in section (3), we obtain the system of equations

$$\begin{bmatrix} 1 & x_{n+k} & x_{n+4}^2 & . & . & . & x_{n+k}^{k+3} \\ 0 & 1 & 2x_n & . & . & . & (k+3)_n^{k+2} \\ 0 & 1 & 2x_{n+1} & . & . & . & (k+3)\,x_{n+1}^{k+2} \\ . & . & . & . & & & . \\ . & . & . & & . & & . \\ . & . & . & & & . & . \\ 0 & 0 & 2x_{n+v} & . & . & . & (k+3)\,x_{n+v}^{k+2} \\ 0 & 0 & 2 & . & . & . & 20k+2x_{n+v}^{k+1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ . \\ . \\ . \\ a_{k+2} \\ a_{k+3} \end{bmatrix} = \begin{bmatrix} y_{n+k} \\ f_n \\ f_{n+1} \\ . \\ . \\ . \\ f_{n+v} \\ f\,'_{n+v} \end{bmatrix} \tag{3.2}$$

Equation (3.2) is solved with MATHEMATICA 10.0 software package to obtain the coefficients of the hybrid predictor (1.5)

The corresponding error constants for the hybrid scheme and its hybrid predictors are obtained for each value of k from the Taylor series expansion of (1.4), (1.5) and (1.6) about x_n. These are respectively

$$y_{n+k}-y\left(x_{n+k}\right)=C_{p+1}h^{p+1}y^{p+1}\left(x_n\right)+0\left(h^{p+2}\right) \tag{3.3}$$

$$y_{n+v_{l+1}}-y\left(x_{n+v_{l+1}}\right)=C_{p^*+1}h^{p^*+1}y^{p^*+1}\left(x_n\right)+0\left(h^{p^*+2}\right) \tag{3.4}$$

$$y_{n+v_0}-y\left(x_{n+v_0}\right)=C_{p^{**}+1}h^{p^{**}+1}(\mathrm{x}_n)+0\left(h^{p^{**}+2}\right) \tag{3.5}$$

where $y\left(x_{n+k}\right)$, $y\left(x_{n+v_{l+1}}\right)$ and $y\left(x_{n+v_0}\right)$ are the theoretical solutions; C_{p+1}, C_{p^*+1} and $C_{p^{**}+1}$ are error constants of (1.4) ,(1.5) and (1.6) respectively. Due to the processing speed and the memory capacity of the laptop computer used in the derivation, only few stable members of the family of the method could be obtained. If the method can be derived using higher processor, more stable members can be obtained from step-number $k \geq 10$.

Examples of $A-$stable members of the family of the hybrid methods (1.4) with error constants are:

For $k=1, m=0, \mathrm{v}_0=\frac{1}{2}$

$$y_{n+1}=h\left(\frac{f_n}{6}+\frac{2}{3} f_{n+\frac{1}{2}}+\frac{f_{n+1}}{6}\right)+y_n, \quad C_5=-\frac{1}{2880}$$

with hybrid

$$y_{n+\frac{1}{2}}=-\frac{3}{8} h f_{n+1}+\frac{y_n}{8}+\frac{7 y_{n+1}}{8}+\frac{1}{16} h^2 f'_{n+1}, \quad C_6=\frac{-1}{384}$$

For $k=2, m=1, \mathrm{v}_1=\frac{3}{2}$

$$y_{n+2}=h\left(-\frac{f_n}{720}+\frac{11 f_{n+1}}{60}+\frac{28}{45} f_{n+\frac{3}{2}}+\frac{47 f_{n+1}}{240}\right)+y_{n+1}-\frac{1}{120} h^2 f'_{n+2}, \quad C_6=-\frac{1}{14400}$$

with hybrids $v_1=\frac{3}{2}, \mathrm{v}_0=\frac{7}{4}$

$$y_{n+\frac{3}{2}}=h\left(\frac{f_n}{3920}-\frac{f_{n+1}}{135}-\frac{2516}{6615} f_{n+\frac{7}{4}}-\frac{9 f_{n+2}}{80}\right)+y_{n+2}+\frac{29}{1260} f_{n+\frac{7}{4}}, C_7=\frac{7}{40960}$$

$$y_{n+\frac{7}{4}}=-h \frac{231 f_{n+2}}{1024}-\frac{3 y_n}{2048}+\frac{7 y_{n+1}}{256}+\frac{1995 y_{n+2}}{2048}+\frac{21 h^2 f'_{n+2}}{90}, \quad C_6=-\frac{1}{50812}$$

For $K=3, m=2, \mathrm{v}_2=\frac{5}{2}, p=6$

$$y_{n+3}=y_{n+2}+h\left(\frac{f_n}{5400}-\frac{f_{n+1}}{360}+\frac{23 f_{n+2}}{120}+\frac{136}{225} f_{n+\frac{5}{2}}+\frac{223 f_{n+3}}{1080}\right)-\frac{1}{90} h^2 f'_{n+3}, \quad C_7=-\frac{13}{604800}$$

with hybrids $v_2 = \frac{5}{2}, \mathrm{v}_1 = \frac{11}{4}, \mathrm{v}_0 = \frac{23}{8}$

$$y_{n+\frac{5}{2}} = h\left(-\frac{13 f_n}{232320} + \frac{3 f_{n+1}}{4480} - \frac{167 f_{n+2}}{17280} - \frac{44048}{144345} f_{n+\frac{11}{4}} - \frac{203}{1920} f_{n+3} \right) + y_{n+3} + \frac{2}{99} h^2 f'_{n+\frac{11}{4}}$$

$$C_8 = \frac{1}{107520}$$

$$y_{n+\frac{11}{4}} = h\left(-\frac{77 f_n}{16250880} + \frac{359 f_{n+1}}{6912000} - \frac{269 f_{n+2}}{501760} - \frac{16032868}{87483375} f_{n+\frac{23}{8}} - \frac{407 f_{n+1}}{6144} \right) + y_{n+3} + \frac{286 h^2}{36225} f'_{n+\frac{23}{8}}$$

$$C_8 = \frac{1513}{1651507200}$$

$$y_{n+\frac{23}{8}} = -\frac{47495 h f_{n+3}}{393216} + \frac{35 y_n}{589824} - \frac{161 y_{n+1}}{262144} + \frac{345 y_{n+2}}{65536} + \frac{2348185 y_{n+3}}{2359296} + \frac{805 h^2 f'_{n+3}}{131072}, \; C_7 = \frac{161}{12582912}$$

4. Stability of the Hybrid Schemes (1.4)

This section considers some important definitions and stability properties of the hybrid schemes.

Definition 1:

A numerical scheme (1.4) is $A-$stable if the region of absolute stability lies entirely in the open left half of the complex plane.

Definition 2:

The numerical scheme (1.4) is $A(\alpha)-$Stable for some $\alpha \in \left[0, \frac{\pi}{2}\right]$, if the wedge $s_\alpha = \left\{ z : | Arg(-z) | < \alpha, z \neq 0 \right\}$ is contained in the region of absolute stability. The largest $\alpha_{\max}$ is the angle of absolute stability.

Definition 3:

The numerical scheme (1.4) is stiffly stable if (i) it is absolutely stable in the Region $R_1 = \left\{ z : | \mathrm{Re(z)} | \leq D_L \right\}$ and (ii) accurate in the region $R_2 = \left\{ z : \mathrm{D}_L < | \mathrm{Re}(z) | < \mathrm{D}_R ;\ | \mathrm{Im}(z) | < \mathrm{D}_1 \right\}$, such that the stability region is contained in the region $R_1 \cup R_2$.

The numerical scheme is Zero-Stable since the roots of the first characteristics polynomial

$$\rho(r) = r^k - r^{k-1}$$

satisfy $|\,\mathrm{r}_i\,| \leq 1$ with roots of $[r_i] = 1$ being simple.

To investigate the stability properties of the family of the hybrid multistep methods (1.4), we employ the boundary locus approach discussed in[14].

Substituting the hybrid predictors in (1.6) into (1.5) then into (1.4) at the hybrid points to yield a scheme, the resulting scheme for fixed k is applied to the scalar test problem $y' = \lambda y,\quad y'' = \lambda^2 y,\ \mathrm{Re}(\lambda) < 0$ which yields the stability polynomials as

$$\pi(r,z) = r^k - r^{k-1} - z\left(\sum_{j=0}^{k} \beta_j^{(m)} r^j + \beta_{v_m}^{(m)}\left(H_p(r,z) - z^2 \lambda_k^{(m)} r^k\right)\right) \tag{5.1}$$

where

$$H_p(r,z) = r^k - z\left(\sum_{j=0}^{k} \beta_j^{(l)} r^k + \beta_{v_l}^{(l)}\left(\ldots\left(\sum_{j=0}^{k} \beta_j^{(-l)} r^j + z\beta_k^{(-l)} + z^2 \lambda_k^{(-l)} r^k + z^2 \lambda_{v_l}^{(l)}\left(\ldots(T)\ldots\right)\right)\right)\right) \text{ and}$$

$$T = \sum_{j=0}^{k} \beta_j^{(-l)} r^j + z\beta_k^{(-l)} + z^2 \lambda_k^{(-l)} r^k$$

The boundary plots are obtained from the stability polynomials for various k.

5. The Stability Plots of the hybrid method

The following are the boundary plots of the implicit hybrid scheme derived in:

The boundary loci reveal that the scheme (1.4) is zero-stable. For $k \leq 6$, it is A-Stable and $A(\alpha)$-Stable for $k > 6$ to k=9.

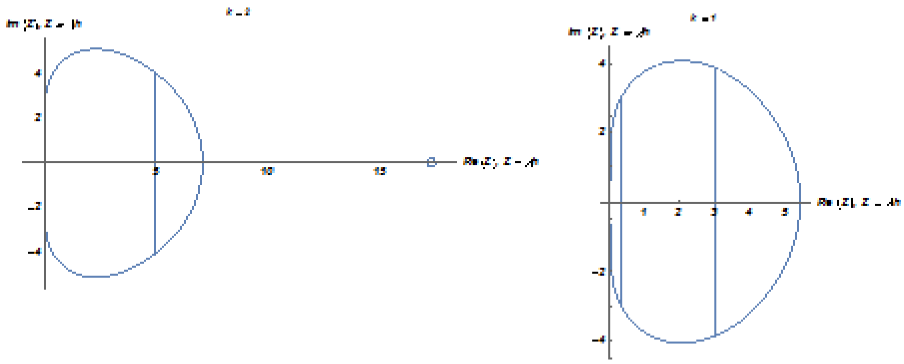

Figure 4

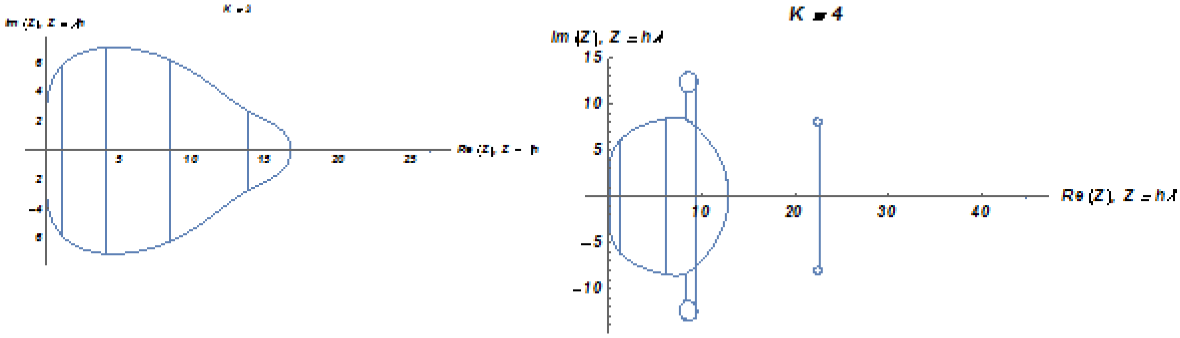

Figure 5

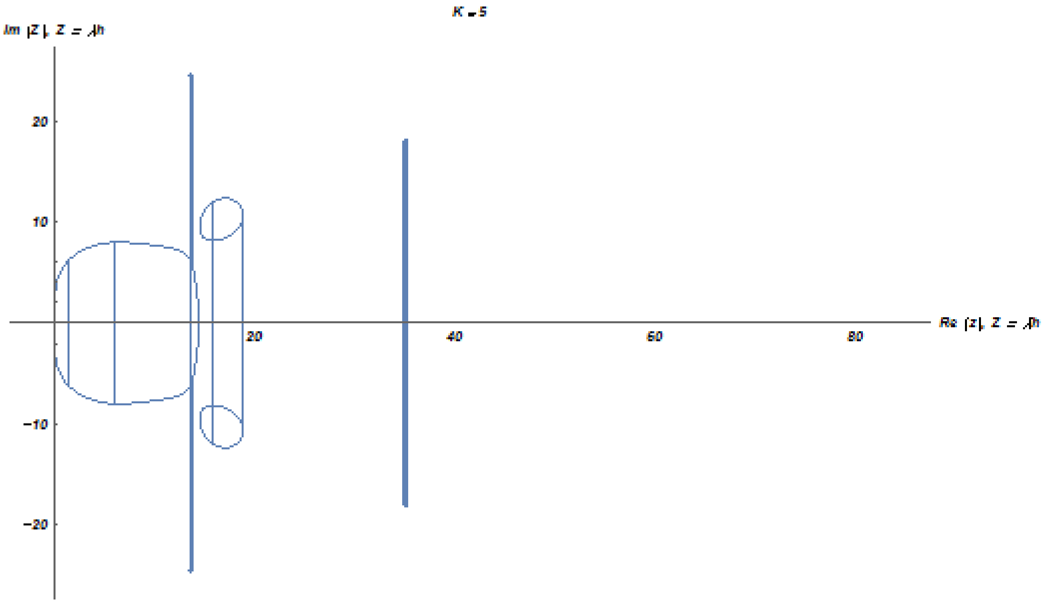

Figure 6

6. Numerical implementations

This section considers numerical implementation of the new hybrid methods (1.4) on some stiff initial value problems in ordinary differential equations. Since the method is an implicit method, the implicitness is resolved by applying the Newton scheme

$$y_{n+k}^{[r+1]} = y_{n+k}^{[r]} - J\left(y_{n+k}^{[r]}\right)^{-1} F\left(y_{n+k}^{[r]}\right), r = 0,1,2,3,... \tag{6.1}$$

or a modification of (6.1) where $J\left(y_{n+k}^{[r]}\right)$ is the Jacobian matrix of the new hybrid method. The (6.1) requires starting value and is generated from the explicit scheme

$$y_{n+1}^{r} = y_n + \frac{h}{2}\left(f_{n-1} + f_n\right), p = 2 \tag{6.2}$$

Using fixed step-size h. The following problems are considered for implementation.

Problem [1]

The Chemical reaction problems in [17]

$$y'_1 = -0.04y_1 + 10^4 y_2 y_3, \quad y_1(0) = 1$$

$$y'_2 = 0.04y_1 - 10^4 y_2 y_3 - 3.10^7 y_2^2, \quad y_2(0) = 0$$

$$y'_3 = 3.10^7 y_2^2, \quad y_3(0) = 0$$

$$h = 10^{-6}, x \in [0,3]$$

Problem [2]

The non linear moderately stiff problems in [9]

$$y'_1 = -0.1y_1 - 199.9y_2, \quad y_1(0) = 2$$

$$y'_2 = -200y_2, \quad y_2(0) = 1$$

$h = 0.0001$ with exact solution $y_1(x) = e^{-0.1x} + e^{-200x}$ and $y_2(\mathrm{x}) = e^{-200x}$

Problem [3]

The Van der pol equation in [12]

$$y'_1 = y_2, \qquad y_1(0) = 2$$

$$y'_2 = \left(\left(1 - y_1^2\right) y_2 - y_1\right) / \varepsilon, \quad y_2(0) = 0$$

$$h = 0.001, \quad \varepsilon = 10^{-1}$$

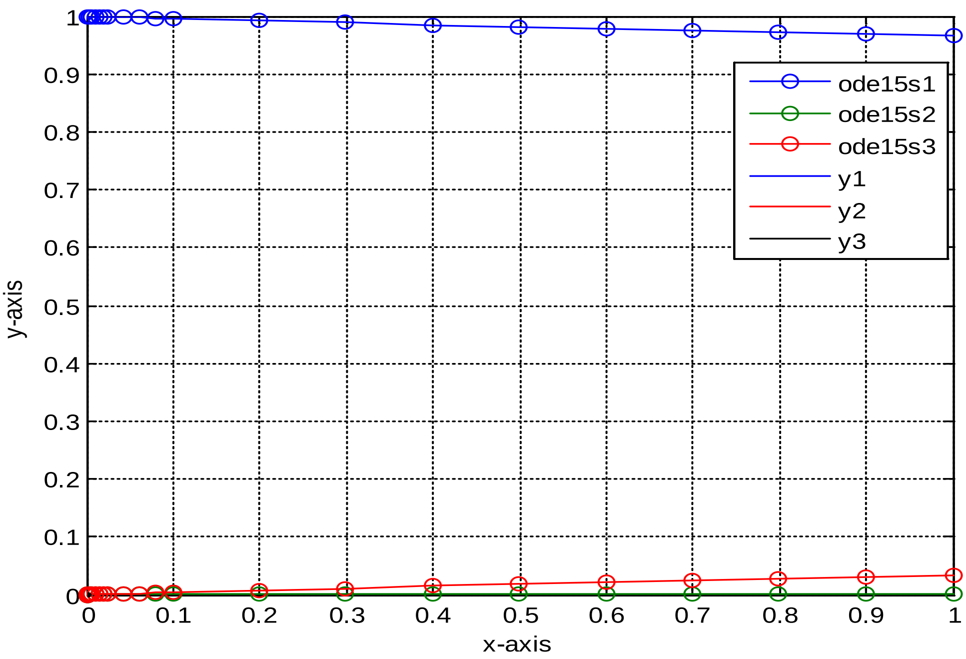

Figure 1: Graphical solution of problem1

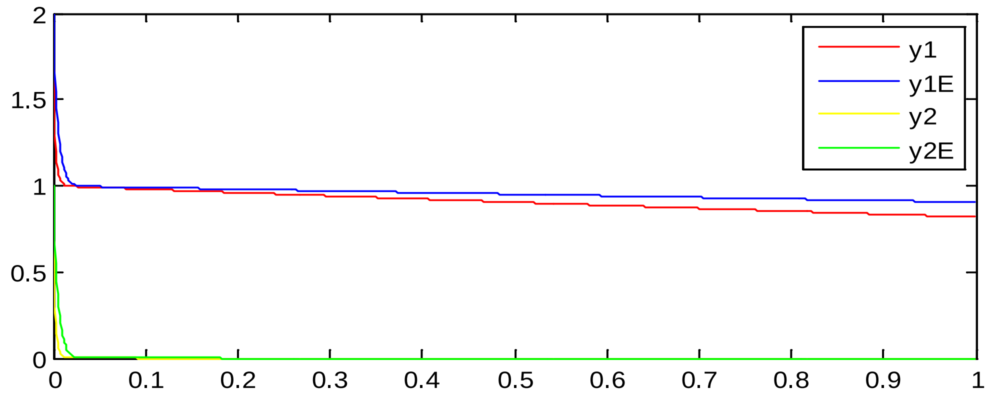

Figure 2: Graphical solution of problem 2

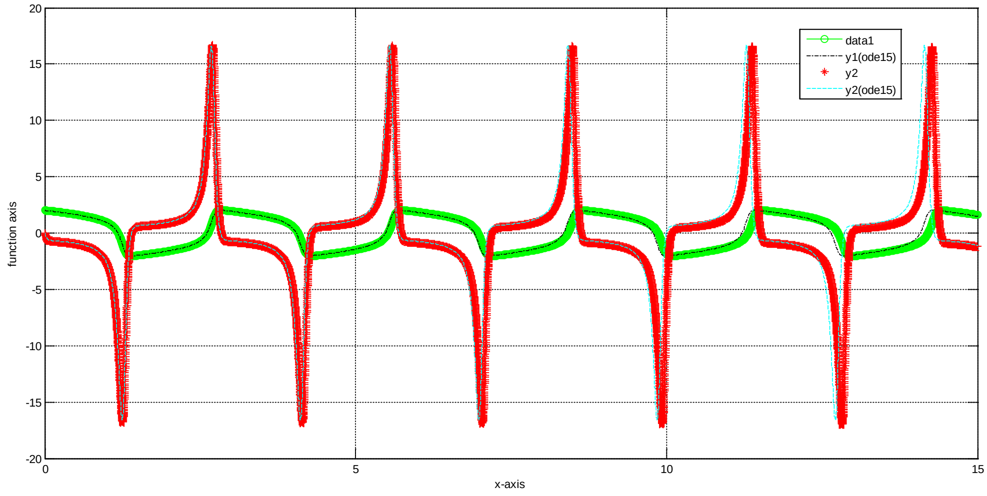

Figure 3: Graphical solution of problem3

7. Conclusion

This paper has presented a class of hybrid linear multistep methods (1.4) with nested hybrid predictors (1.5) for stiff initial value problems in ordinary differential equations. The hybrid scheme has high order stability and is seen to overcome Dahlquist order barrier on linear multistep methods (1.1). The scheme has been implemented on three stiff problems and the results in figures 1 and 3 show that the scheme (1.4) compares favourably with ODE15s of MATLAB in [13]. In figure 2, the graph is in alignment with the exact solution of the ODE.

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