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$A(\alpha)$ -Stable Linear Multistep Methods for Stiff IVPs in ODEs

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Abstract

In this paper, a class of $A(\alpha)$ -stable linear multistep formulas for stiff initial value problems (IVPs) in ordinary differential equations (ODEs) is developed. The boundary locus of the methods shows that the schemes are A-stable for step number $k \leq 3$ and stiffly stable for k = 4, 5 and 6. Some numerical results are reported to illustrate the method.

Key words: second derivative method, collocation and interpolation, initial value problem, stiff stability, boundary locus

2000 Mathematics Subject Classification: 65L05, 65L06

1 Introduction

Ikhile and Okuonghae [17] introduced a class of stiffly stable continuous extension of second derivative LMM with an off-step point for stiff initial value problems (IVPs) in ordinary differential equations (ODEs)

$$\begin{cases} y' = f(x, y), & x \in [x_0, X], \\ y(x_0) = y_0, \end{cases}$$
 (1)

where the function $f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$. Stiffness in ODEs (1), shows that one or more strong damped modes are present. Stiff problems are very common, and often encountered in simulating electric circuits, fluid power systems, diffusion, pharmaco kinetic theory, heat transfer, and biological sciences, especially in modeling of spread and control of diseases. To solve the above IVPs numerically, we use the Continuous Formula (CF)

$$y(x_n + (t+1)h) = \sum_{j=0}^{k-1} \alpha_{1,j}(t)y_{n+j} + h\beta_v(t)f_{n+v} + h^2\gamma_v(t)f'_{n+v},$$

$$t = k - 1, v = k - \frac{1}{2}, \quad 0 \le v \le k$$
(2)

with the hybrid predictor

$$y(x_n + vh) = \sum_{j=0}^{k-1} \alpha_{2,j}(t)y_{n+j} + h\phi_k(t)f_{n+k} + h^2\delta_k(t)f'_{n+k}, \\ v = t+1, \quad t = k - \frac{3}{2}$$
(3)

to compute the approximate solution y_{n+j} to $y(x_{n+j})$ at the end of a step $[x_n, x_{n+1}]$ of length $h = x_{n+1} - x_n$ for each n = 0, 1, 2, ... and $f_{n+j} = f(x_{n+j})$, y_{n+j}). Note that y_n will depict the exact solution $y(x_n)$. The continuous coefficients $\{\alpha_{1,j}(t), j = 0(1)k - 1\}, \gamma_v(t), \{\alpha_{2,j}(t), j = 0(1)k\}, \beta_v(t), \delta_k(t)$ and $\phi_k(t)$ in t are presumed to be real and satisfying the normalization condition $\alpha_k(t) = 1, \, \alpha_v(t) = 1$ and the scale variable t is $t = (x - x_{n+1})/h$. The method shall be derived for single ordinary differential equations (ODEs), extension to system of ODEs is possible and examples are given in section 5. Continuous linear multistep method gives output at any desire point in the integration interval. For t = k - 1, then $y(x_n + kh)$ in (2) gives y_{n+k} . The method (2) and (3) therefore define an implicit method in y_{n+k} . When (3) is inserted in (2), then resultant expression gives an implicit nonlinear equation in y_{n+k} . The Newton-Raphson method is used in section 5 to resolve this implicitness. Examples of existing stiffly stable formulas for the numerical solution of (1) are in the works of Butcher [1, 2, 3, 4, 5, 6, 7], Enright [9, 10, 11], Fatunla [12], Gear [13, 14], Ikhile and Okuonghae [17], Lambert [18, 19], and Okuonghae [20]. The local truncation errors for (2) and (3) are

$$\mathcal{L}[y(x);h] = \left[y(x_n + (t+1)h) - \sum_{j=0}^{k-1} \alpha_{1,j}(t)y(x_n + jh) - h\beta_v(t)y'(x_n + vh) - h^2\gamma_v(t)y''(x_n + vh)\right]$$
(4)

and

$$\mathcal{L}[y(x);h]_{v} = \left[y(x_{n}+vh) - \sum_{j=0}^{k-1} \alpha_{2,j}(t)y(x_{n}+jh) - h\phi_{k}(t)y'(x_{n}+kh) - h^{2}\delta_{k}(t)y''(x_{n}+kh)\right]$$
(5)

where $y(x_n)$ is any sufficiently differentiable vector valued function. By Taylor series expansion we can show that

$$\mathcal{L}[y(x);h] = ch^{p+1}y^{p+1}(x_n), \quad x_n \le x \le x_{n+1}$$
(6)

for some c, p, and x_n ; where c is regarded as the error constant, while p is the order of the algorithm (2) and (3) respectively. From (4) and (5), we have the order of (2) and (3) to be k + 1 respectively for step number $k \leq 6$. Tables (6) and (7) give the expression of the local truncation errors defined in (4) and (5). The purpose of this article is to use the idea of collocation and interpolation approaches to construct a family of continuous schemes from which discrete algorithms which possesses the following properties: small error constant, zero stability, and large intervals of absolute stability are obtained.

2 Derivation of the continuous formulas

The solution of the IVPs in (1) is approximated by the polynomial

$$y(x) = \sum_{j=0}^{k+1} a_j x^j$$
(7)

where $\{a_j\}_{j=0}^{k+1}$ are the real parameter constants to be determined. From (6) we have

$$y'(x) = f(x,y) = \sum_{j=1}^{k+1} j a_j x^{j-1}$$
(8)

$$y''(x) = f'(x,y) = \sum_{j=2}^{k+1} j(j-1)a_j x^{j-2}$$
(9)

Collocating (7) at $x = x_{n+\nu}$ and interpolating (8) and (9) at $x = x_{n+j}$, j = 0(1)k - 1 and $x = x_{n+\nu}$, we obtain the linear system of equations

$$\begin{pmatrix} 1 & x_n & x_n^2 & \dots & x_{n+1}^{k+1} \\ 1 & x_{n+1} & x_{n+1}^2 & \dots & x_{n+1}^{k+1} \\ \cdot & \cdot & \cdot & \ddots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \ddots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \ddots & \cdot & \cdot \\ 1 & x_{n+k-1} & x_{n+k-1}^2 & \dots & x_{n+k-1}^{k+1} \\ 0 & 1 & 2x_{n+v} & \dots & (k+1)x_{n+v}^k \\ 0 & 0 & 2 & \dots & (k+1)(k)x_{n+v}^{k-1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_{k-1} \\ a_k \\ a_{k+1} \end{pmatrix} = \begin{pmatrix} y_n \\ y_{n+1} \\ \cdot \\ \cdot \\ \cdot \\ y_{n+k-1} \\ f_{n+v} \\ f'_{n+v} \end{pmatrix}$$
(10)

Solving equation (10) for $a'_j s$ and substituting the resulting values into (7) with $x = x_{n+1} + th$ and without loss of generality we can take $x_n = 0$ so that x = h(t+1). Setting $x = x_{n+t+1}$ on the left hand side of (7) yield the continuous method for $k \leq 6$ and t = k - 1. Table (1), below gives explicitly the continuous coefficients of the algorithm in (2) for a fixed k.

| k | j | $\alpha_{1,j}(t)$ | $eta_v(t)$ | $\gamma_v(t)$ |
|---|---------------|---|---|--|
| 1 | 0 | 1 | 0 | 0 |
| | $\frac{1}{2}$ | 0 | 1+t | $\frac{t}{2} + \frac{t^2}{2}$ |
| | 1 | 1 | 0 | 0 |
| 2 | 0 | $-\frac{3t}{13} + \frac{6t^2}{13} - \frac{4t^3}{13}$ | 0 | 0 |
| | 1 | $1 + \frac{3t}{13} - \frac{6t^2}{13} + \frac{4t^3}{13}$ | 0 | 0 |
| | $\frac{3}{2}$ | 0 | $\frac{10t}{13} + \frac{6t^2}{13} - \frac{4t^3}{13}$ | $-\frac{7t}{26}+\frac{t^2}{26}+\frac{4t^3}{13}$ |
| | 2 | 1 | 0 | 0 |
| 3 | 0 | $-\frac{81t}{394} + \frac{171t^2}{394} - \frac{58t^3}{197} + \frac{13t^4}{197}$ | 0 | 0 |
| | 1 | $1 - \frac{216t}{197} - \frac{135t^2}{197} + \frac{216t^3}{197} - \frac{62t^4}{197}$ | 0 | 0 |
| | 2 | $\frac{513t}{394} + \frac{99t^2}{394} - \frac{158t^3}{197} + \frac{49t^4}{197}$ | 0 | 0 |
| | $\frac{5}{2}$ | 0 | $-\frac{100t}{197}$ + $\frac{36t^2}{197}$ + | $\frac{42t}{197} - \frac{23t^2}{197} - \frac{42t^3}{197} +$ |
| | | | $\frac{100t^3}{197} - \frac{36t^4}{197}$ | $\frac{23t^4}{197}$ |
| | 3 | 1 | 0 | 0 |
| 4 | 0 | $\begin{array}{r} -\frac{5900t}{32919}+\frac{13135t^2}{32919}-\frac{6777t^3}{21946}+\\ \frac{6649t^4}{65838}-\frac{394t^5}{32919}\end{array}$ | 0 | 0 |
| | 1 | $\frac{1 - \frac{26875t}{21946} - \frac{11075t^2}{21946} + \frac{55415t^3}{21946} - \frac{10871t^4}{21946} + \frac{730t^5}{10973}}{10973}$ | 0 | 0 |
| | 2 | $\frac{\frac{26650t}{10973}-\frac{5860t^2}{10973}-\frac{38819t^3}{21946}+}{\frac{22693t^4}{21946}-\frac{1754t^5}{10973}}$ | 0 | 0 |
| | 3 | $\begin{array}{l} -\frac{67475t}{65838}+\frac{42115t^2}{65838}+\frac{20181t^3}{21946}-\\ \frac{42115t^4}{65838}+\frac{3466t^5}{32919}\end{array}$ | 0 | 0 |
| | $\frac{7}{2}$ | 0 | $\begin{array}{c ccccc} \frac{4848t}{10973} & - & \frac{3800t^2}{10973} & - \\ \frac{4160t^3}{10973} & + & \frac{3800t^4}{10973} & - \\ \frac{688t^5}{10973} & \end{array}$ | $\begin{array}{r} -\frac{1970t}{10973} + \frac{1689t^2}{10973} + \\ \frac{1618t^3}{10973} - \frac{1689t^4}{10973} + \\ \frac{352t^5}{10973} \end{array}$ |
| | 4 | 1 | 0 | 0 |

Table 1 The continuous coefficients of CF in (2). $v = k - \frac{1}{2}$

| k | j | $\alpha_{1,j}(t)$ | $\beta_v(t)$ | $\gamma_v(t)$ |
|---|---------------|---|--|---|
| 5 | 0 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 1 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 2 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 3 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 4 | $\begin{array}{c} \frac{2599891t}{2606628} & - & \frac{1715105t^2}{1737752} & - \\ \frac{1804039t^3}{2606628} & + & \frac{4985819t^4}{5213256} & - \\ \frac{66321t^5}{217219} & + & \frac{19937t^6}{651657} \end{array}$ | 0 | 0 |
| | $\frac{9}{2}$ | 0 | $\begin{array}{r} -\frac{266848t}{651657} & +\\ \frac{849520t^2}{1954971} + \frac{515120t^3}{1954971} -\\ \frac{273040t^4}{651657} + \frac{285424t^5}{1954971} -\\ \frac{30400t^6}{1954971} \end{array}$ | $\frac{\frac{34048t}{217219} - \frac{112144t^2}{651657} - \frac{62600t^3}{651657} + \frac{35880t^4}{217219} - \frac{39544t^5}{651657} + \frac{4504t^6}{651657}$ |
| | 5 | 1 | 0 | 0 |
| 6 | 0 | $\begin{array}{r} -\frac{19290069t}{141667595} + \frac{193448871t^2}{566670380} - \\ \frac{368244713t^3}{1133340760} + \frac{26122729t^4}{170001114} - \\ \frac{131446469t^5}{3400022280} + \frac{8431667t^6}{1700011140} - \\ \frac{217219t^7}{850005570} \end{array}$ | 0 | 0 |
| | 1 | $\frac{1 - \frac{170790345t}{113334076} - \frac{27438479t^2}{226668152} + \frac{7696982581t^3}{6120040104} - \frac{1722620983t^4}{2040013368} + \frac{1514216965t^5}{6120040104} - \frac{35223037t^6}{1020006684} + \frac{2869771t^7}{1530010026}$ | 0 | 0 |

 ${\bf Table \ 1} \ \ {\rm The \ Continuous \ Coefficients \ of \ CF \ in \ (2) \ (continued)}$

| k | j | $\alpha_{1,j}(t)$ | $\beta_v(t)$ | $\gamma_v(t)$ |
|---|----------------|--|---|--|
| | 2 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 3 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 4 | $\frac{\frac{69077727t}{28333519} - \frac{323751749t^2}{113334076} - \frac{7670551471t^3}{6120040104} + \frac{674853809t^4}{255001671} - \frac{7166970445t^5}{6120040104} + \frac{214350505t^6}{1020006684} - \frac{20816779t^7}{1530010026}$ | 0 | 0 |
| | 5 | $\begin{array}{r} -\frac{575349399t}{566670380}+\frac{1417489173t^2}{1133340760}+\\ \frac{530504683t^3}{1133340760}-\frac{781502957t^4}{680004456}+\\ \frac{1837449149t^5}{3400022280}-\frac{172476367t^6}{1700011140}+\\ \frac{5783299t^7}{850005570}\end{array}$ | 0 | 0 |
| | <u>11</u> 2 | 0 | $\begin{array}{c c} \frac{10988800t}{28333519} & -\\ \frac{13976256t^2}{28333519} & -\\ \frac{41612704t^3}{255001671} & +\\ \frac{38224480t^4}{85000557} & -\\ \frac{56509600t^5}{255001671} & +\\ \frac{3704288t^6}{85000557} & -\\ \frac{776896t^7}{255001671} \end{array}$ | $\begin{array}{rrrr} -\frac{3970368t}{28333519} & + \\ \frac{5134256t^2}{28333519} & + \\ \frac{4737112t^3}{85000557} & - \\ \frac{4656440t^4}{28333519} & + \\ \frac{7069864t^5}{85000557} & - \\ \frac{477816t^6}{28333519} + \\ \frac{104128t^7}{85000557} \end{array}$ |
| | 6 | 1 | 0 | 0 |

 ${\bf Table \ 1} \ \ {\rm The \ Continuous \ Coefficients \ of \ CF \ in \ (2) \ (continued)}$

| k | t | ы | $\gamma_v(t)$ | $eta_v(t)$ | $lpha_{1,6}(t)$ | $lpha_{1,5}(t)$ | $lpha_{1,4}(t)$ | $lpha_{1,3}(t)$ | $lpha_{1,2}(t)$ | $lpha_{1,1}(t)$ | $lpha_{1,0}(t)$ |
|---|--------|----------------|----------------------------|-----------------------------|-----------------|-----------------------------|------------------------------|-----------------------------|-----------------------------|----------------------------|----------------------------|
| 1 | 0 | $\frac{1}{2}$ | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1 |
| 5 | - | 5 3 | $\frac{1}{13}$ | $\frac{12}{13}$ | 0 | 0 | 0 | 0 | 1 | $\frac{141}{13}$ | $-\frac{1}{13}$ |
| 3 | 5 | <u>7</u> | $\frac{168}{197}$ | $\frac{24}{197}$ | 0 | 0 | 0 | 1 | $\frac{231}{197}$ | $-\frac{39}{197}$ | $\frac{5}{197}$ |
| 4 | 3 | $\frac{7}{2}$ | $\frac{8640}{10973}$ | $\frac{1704}{10973}$ | 0 | 0 | 1 | $\frac{14072}{10973}$ | $-\frac{4002}{10973}$ | $\frac{1040}{10973}$ | $-\frac{137}{10973}$ |
| 5 | 4 | $\frac{9}{2}$ | $\frac{39680}{217219}$ | $\frac{472960}{651657}$ | 0 | 1 | $\frac{304895}{217219}$ | $-\frac{1130590}{1954971}$ | $\frac{49390}{217219}$ | $-rac{13055}{217219}$ | $\frac{14491}{1954971}$ |
| 9 | 5 L | $\frac{11}{2}$ | $\frac{5842560}{28333519}$ | $\frac{18905600}{28333519}$ | 1 | $\frac{43473174}{28333519}$ | $-\frac{71374295}{85000557}$ | $\frac{12544580}{28333519}$ | $-\frac{4984665}{28333519}$ | $\frac{3692882}{85000557}$ | $-\frac{139099}{28333519}$ |

Table 2The discrete coefficients of the continuous formulas in (2)

3 The derivation of the continuous hybrid predictor

Similarly, the corresponding hybrid predictor

$$y(x_n+vh) = \sum_{j=0}^{k-1} \alpha_{2,j}(t) y_{n+j} + h\phi_k(t) f_{n+k} + h^2 \delta_k(t) f'_{n+k}, \quad v = t+1, \quad t = k-3/2$$
(11)

for $f(x_{n+v})$ and $f'(x_{n+v})$ in (2) are obtained from the polynomial interpolant

$$y(x_{n+v}) = \sum_{j=0}^{k+1} b_j x^j.$$
 (12)

where $\{b\}_{j=0}^{k+1}$ are the real parameter constants to be determined. Following the same procedure as in section 2, the unknown continuous coefficients of the hybrid predictors in (3) are obtained. Tables (3) and (4), below show the continuous and the discrete coefficients of the predictor (3) for $k \leq 6$ respectively.

| k | j | $\alpha_{2,j}(t)$ | $\beta_k(t)$ | $\delta_k(t)$ |
|---|---------------|---|--|---|
| 1 | 0 | 1 | 0 | 0 |
| | $\frac{1}{2}$ | 0 | 0 | 0 |
| | 1 | 0 | 1+t | $-\frac{1}{2} + \frac{t^2}{2}$ |
| 2 | 0 | $-\frac{3t}{7} + \frac{3t^2}{7} - \frac{t^3}{7}$ | 0 | 0 |
| | 1 | $1 + \frac{3t}{7} - \frac{3t^2}{7} + \frac{t^3}{7}$ | 0 | 0 |
| | $\frac{3}{2}$ | 1 | 0 | 0 |
| | 2 | 0 | $\frac{4t}{7} + \frac{3t^2}{7} - \frac{t^3}{7}$ | $-\frac{5t}{14} - \frac{t^2}{7} + \frac{3t^3}{14}$ |
| 3 | 0 | $-\frac{22t}{85} + \frac{39t^2}{85} - \frac{41t^3}{170} + \frac{7t^4}{170}$ | 0 | 0 |
| | 1 | $1 - \frac{64t}{85} - \frac{72t^2}{85} + \frac{64t^3}{85} - \frac{13t^4}{85}$ | 0 | 0 |
| | 2 | $\frac{86t}{85} + \frac{33t^2}{85} - \frac{87t^3}{170} + \frac{19t^4}{170}$ | 0 | 0 |
| | $\frac{5}{2}$ | 1 | 0 | 0 |
| | 3 | 0 | $\frac{-\frac{23t}{85} + \frac{6t^2}{85} + \frac{23t^3}{85} - \frac{6t^4}{85}}{\frac{6t^4}{85}}$ | $\frac{\frac{14t}{85} - \frac{11t^2}{170} - \frac{14t^3}{85} + \frac{11t^4}{170}$ |

Table 3 The continuous coefficients of the hybrid predictor (3)

| k | j | $\alpha_{2,j}(t)$ | $eta_k(t)$ | $\delta_k(t)$ |
|---|---------------|---|---|--|
| 4 | 0 | $\begin{array}{r} -\frac{333t}{1660}+\frac{1383t^2}{3320}-\frac{2897t^3}{9960}+\\ \frac{277t^4}{3320}-\frac{17t^5}{1992}\end{array}$ | 0 | 0 |
| | 1 | $\frac{1 - \frac{891t}{830} - \frac{261t^2}{415} + \frac{428t^3}{415} - \frac{154t^4}{415} + \frac{7t^5}{166}}$ | 0 | 0 |
| | 2 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 3 | $\begin{array}{rrrr} -\frac{549t}{830} + \frac{141t^2}{415} + \frac{766t^3}{1245} - \\ \frac{141t^4}{415} + \frac{23t^5}{498} \end{array}$ | 0 | 0 |
| | $\frac{7}{2}$ | 1 | 0 | 0 |
| | 4 | 0 | $\frac{\frac{31t}{166} - \frac{45t^2}{332} - \frac{55t^3}{332} + \frac{45t^4}{332} - \frac{7t^5}{332}$ | $\begin{array}{rrrr} -\frac{87t}{830} &+& \frac{137t^2}{1660} &+\\ \frac{149t^3}{1660} &-& \frac{137t^4}{1660} &+& \frac{5t^5}{332} \end{array}$ |
| 5 | 0 | $\begin{array}{r} -\frac{1996t}{12019}+\frac{13693t^2}{36057}-\frac{45107t^3}{144228}+\\ \frac{11423t^4}{96152}-\frac{3055t^5}{144228}+\frac{415t^6}{288456}\end{array}$ | 0 | 0 |
| | 1 | $\frac{1 - \frac{46366t}{36057} - \frac{29161t^2}{72114} + \frac{336715t^3}{288456} - \frac{169321t^4}{288456} + \frac{34213t^5}{288456} - \frac{2491t^6}{288456}$ | 0 | 0 |
| | 2 | $\frac{30024t}{12019} - \frac{8538t^2}{12019} - \frac{41453t^3}{24038} + \frac{57159t^4}{48076} - \frac{3288t^5}{12019} + \frac{1031t^6}{48076}$ | 0 | 0 |
| | 3 | $\begin{array}{r} -\frac{19478t}{12019}+\frac{91225t^2}{72114}+\frac{374053t^3}{288456}-\\ \frac{118997t^4}{96152}+\frac{93419t^5}{288456}-\frac{7909t^6}{288456}\end{array}$ | 0 | 0 |
| | 4 | $\frac{\frac{20716t}{36057}-\frac{19111t^2}{36057}-\frac{61559t^3}{144228}+}{\frac{149089t^4}{288456}-\frac{21305t^5}{144228}+\frac{3799t^6}{288456}}$ | 0 | 0 |
| | $\frac{9}{2}$ | 1 | 0 | 0 |
| | 5 | 0 | $\begin{array}{rrrr} -\frac{1761t}{12019} + \frac{1805t^2}{12019} + \\ \frac{4745t^3}{48076} - \frac{6995t^4}{48076} + \\ \frac{2299t^5}{48076} - \frac{225t^6}{48076} \end{array}$ | $\begin{array}{c c} \frac{912t}{12019} & - & \frac{1931t^2}{24038} & - \\ \frac{2355t^3}{48076} & + & \frac{3725t^4}{48076} & - \\ \frac{1293t^5}{48076} & + & \frac{137t^6}{48076} \end{array}$ |

Table 3 The continuous coefficients of the hybrid predictor (3) (continued)

| k | j | $\alpha_{2,j}(t)$ | $\beta_k(t)$ | $\delta_k(t)$ |
|---|----------------|---|--|--|
| 6 | 0 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 1 | $\frac{1 - \frac{235525t}{161868} - \frac{60715t^2}{323736} + \frac{400241t^3}{323736} - \frac{126893t^4}{161868} + \frac{17585t^5}{80934} - \frac{9235t^6}{323736} + \frac{67t^7}{46248}$ | 0 | 0 |
| | 2 | $\frac{\frac{81325t}{26978} - \frac{443605t^2}{323736} - \frac{418147t^3}{215824} + \\ \frac{\frac{289547t^4}{161868} - \frac{185401t^5}{323736} + \frac{8793t^6}{107912} - \\ \frac{403t^7}{92496}$ | 0 | 0 |
| | 3 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 4 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 0 | 0 |
| | 5 | $\begin{array}{rrrr} -\frac{29285t}{53956} &+& \frac{208717t^2}{323736} &+\\ \frac{148187t^3}{539560} -\frac{96833t^4}{161868} +\frac{10733t^5}{40467} -\\ \frac{5017t^6}{107912} +& \frac{667t^7}{231240} \end{array}$ | 0 | 0 |
| | $\frac{11}{2}$ | 1 | 0 | 0 |
| | 6 | 0 | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ |

Table 3 The continuous coefficients of the hybrid predictor (3) (continued)

| $lpha_{2,0}(t)$ | $\begin{array}{c c} \alpha_{2,1}(t) & \alpha_{2,0}(t) \\ 0 & 1 \\ \hline \frac{9}{8} & -\frac{1}{8} \end{array}$ | | $\frac{21}{544}$ | $-\frac{361}{21248}$ | $\frac{7955}{879104}$ | $\frac{42859}{7892992}$ | |
|-----------------|--|---------------|-------------------|-----------------------|--------------------------|----------------------------|--|
| $lpha_{2,1}(t)$ | | | $-rac{73}{272}$ | $\frac{651}{5312}$ | $-rac{62685}{879104}$ | $\frac{93115}{1973248}$ | |
| $lpha_{2,2}(t)$ | 0 | 0 | $\frac{669}{544}$ | $-\frac{9079}{21248}$ | $\frac{113157}{439552}$ | $\frac{734085}{3946496}$ | |
| $lpha_{2,3}(t)$ | 0 0 | | 0 | $\frac{7021}{5312}$ | $-rac{527235}{879104}$ | $\frac{442079}{986624}$ | |
| $lpha_{2,4}(t)$ | 0 | 0 | 0 | 0 | $\frac{1234755}{879104}$ | $-\frac{6190635}{7892992}$ | |
| $lpha_{2,5}(t)$ | 0 0 | | 0 | 0 | 0 | $\frac{2921391}{1973248}$ | |
| $lpha_{2,6}(t)$ | 0 | 0 | 0 | 0 | 0 | 0 | |
| $lpha_v(t)$ | 1 | 1 | 1 | 1 | 1 | 1 | |
| $\phi_{\ k}(t)$ | $ \begin{array}{c c} \delta_k(t) & \phi_k(t) \\ -\frac{3}{16} & -\frac{3}{2} \\ -\frac{3}{16} & 3 \\ \end{array} $ | | $\frac{21}{68}$ | $\frac{2835}{10624}$ | $\frac{104355}{439552}$ | $\frac{2921391}{1973248}$ | |
| $\delta_k(t)$ | | | $-\frac{69}{544}$ | $-\frac{1029}{10624}$ | $-\frac{34695}{439552}$ | $\frac{132165}{1973248}$ | |
| v | $\frac{1}{2}$ | $\frac{3}{2}$ | <u>2</u> 2 | $\frac{7}{2}$ | $\frac{9}{2}$ | $\frac{11}{2}$ | |
| t | $-\frac{1}{2}$ | 2 | 5 3 | $\frac{5}{2}$ | $\frac{1}{2}$ | $\frac{3}{2}$ | |
| k | 1 | 2 | 3 | 4 | 5 | 9 | |

Table 4The discrete coefficients of the hybrid predictor in (3)

4 Stability of the methods in (2)

In this section, we investigate the stability properties of the discrete version of the CF defined in (2) for a given value of $k \leq 6$. In examining the stability property of (2), we give the following definitions:

Definition 1 A linear multistep method (LMM) is said to be zero stable if the roots of $\rho(r) = 0$ are inside the unit circle with simple roots on the unit circle, where $\rho(r) = \sum_{j=0}^{k} \alpha_j r^j$ is the first characteristics polynomial for the numerical integrator (2) for a fixed t.

Definition 2 A LMM is said to be A-stable if the absolute value of the root(s) of the stability polynomial of the numerical integrator lies in the open left half of the z-plane of the stability region.

Examples of A-stable methods can be found in the work of Butcher [1, 2, 4, 5], Dalhquist [8], Enright [9], Gear and [13, 14].

Definition 3 (cf. Gear [13], and Fatunla [12]) A numerical scheme is said to be stiffly stable (i) if it is absolutely stable in the region $R_1 = \{z : |\operatorname{Re}(z)| \le D_L\}$, (ii) and accurate in the region $R_2 = \{z : D_L < |\operatorname{Re}(z)| < D_R; |\operatorname{Im}(z)| < D_L\}$, such that the stability region contains a region of the form $R_1 \cup R_2$.

The diagrammatical interpretation of conditions (i) and (ii) in boundary locus form is nicely given in the appendix. Also see Gear [14], Enright [9] and Fatunla [12].

Definition 4 A numerical algorithm is said to be $A(\alpha)$ stable for some $\alpha \in [0, \frac{\pi}{2}]$ if the wedge $S_{\alpha} = \{z : |\operatorname{Arg}(-z)| < \alpha, z \neq 0\}$ is contained in its region of absolute stability.

The largest $\alpha(\alpha_{\max})$ is regarded as the angle of absolute stability on the argument of stability. The definition of stiffly stability given in the spirit of Gear [13, 14] show that stiff stability implies $A(\alpha)$ -stability. Also see Fatunla [12], Hairer[15] and Widlund [22]. Applying the discrete version of CF (2) for a fixed step number k to the scalar test problem $y' = \lambda y$, $\operatorname{Re}(\lambda) < 0$, and substituting the hybrid solution (3), y_{n+v} at the hybrid point x_{n+v} for a corresponding k gives the stability polynomial

$$\pi(r,z) = r^{k} - \sum_{j=0}^{k-1} \alpha_{1,j} r^{j} - \beta_{v} \left(\sum_{j=0}^{k} \alpha_{1,j} r^{j} + z r^{k} \phi_{k} + z^{2} \delta_{k} r^{k} \right) z$$
$$- \gamma_{v} \left(\sum_{j=0}^{k} \alpha_{1,j} r^{j} + r^{k} z \phi_{k} + z^{2} \delta_{k} r^{k} \right) z^{2}, \quad z = \lambda h.$$
(13)

Fig. 1 show the loci of (2) and (3) for $k \leq 6$. Following Definition 4, observe that for $1 \leq k \leq 3$ the CF in (2) are A-stable and stiffly stable when $4 \leq k \leq 6$

respectively. At k = 7, no stable process was found. It is conjectured that the method (2) is unstable for $k \ge 8$.



Fig. 1 The boundary locus of the stability domain of the method (2) for $k \le 6$. At $k \ge 7$, instability sets in. See the graphs of k = 7 and k = 8 below.



Fig. 2 The boundary locus of the stability domain of the method (2) for k = 7.



Fig. 3 The boundary locus of the stability domain of the method (2) for k = 8.

In Tab. 5, we give explicitly the values of angle (α) of the method in (2) and (3) for $k \leq 6$.

| k | 1 | 2 | 3 | 4 | 5 | 6 |
|----------|--------------|--------------|--------------|--------------|--------------|--------------|
| Order(2) | 2 | 3 | 4 | 5 | 6 | 7 |
| Order(3) | 2 | 3 | 4 | 5 | 6 | 7 |
| D | 0 | 0 | 0 | 0.2 | 0.5 | 1.7 |
| α | 90° | 90° | 90° | 85° | 77° | 48° |

Tab. 5 The step-number, scaled variable t and the angle (α) of CF

Tab. 6 and 7 show the step number, the continuous and the discrete versions of the error constants of the scheme (2) and (3). Constants c_{p+1} and c_{p+1}^* in Tab. 6 and 7 are the discrete error constants for the CF (2) and hybrid predictor (3) respectively.

| | | | | | | | | | c_{p+1}^* | $\frac{7}{48}$ | $\frac{5}{128}$ | $\frac{361}{21760}$ | $\frac{11137}{1274880}$ | $\frac{128577}{24614912}$ | $\frac{1502457}{442007552}$ |
|--|--|--|--|---|--|---|---|---|--|------------------------------------|--|---|--|---|--|
| Continuous and Discrete Error Constants of CF(2) | Continuous error constant $(c_{p+1}(t))$ c_{p+1} | $\frac{(1+t)(1+2t+4t^2)}{24}h^3y^{(3)}(x_n)$ | $\frac{t(1+t)\left(17-38t+26t^2\right)}{624}h^4 y^{(4)}(x_n) \qquad \qquad$ | $\frac{(-1+t)t(1+t)(2403+t(-2709+788t))}{94560}h^5y^{(5)}(x_n)$ | $ \frac{(-2+t)(-1+t)t(1+t)(652075+8t(-59485+10973t))}{63204480} h^6 y^{(6)}(x_n) \frac{14491}{2633520} $ | $\frac{3+t)(-2+t)(-1+t)t(1+t)\left(11984371-6436822t+868876t^2\right)}{4379135040}h^{7}y^{(7)}(x_n) \left \begin{array}{c} 139099\\ 36492792\\ 36492792\\ \end{array} \right $ | $\frac{3+t)(-2+t)(-1+t)t(1+t)(627493311+t(-266276781+28333519t))}{1142407486080}h^8y^{(8)}(x_n)\left(\frac{4447381}{1586677064}\right)$ | Continuous and Discrete Error Constants of $Predictor(3)$ | Continuous error constant $(c_{p+1}(t^*))$ | $rac{1}{6}(1+t^3)h^3y^{(3)}(x_n)$ | $\frac{1}{168}t(1+t)(17+t(-20+7t))h^4y^{(4)}(x_n)$ | $\frac{1}{10200}(-1+t)t(1+t)(508+t(-406+85t))h^5y^{(5)}(x_n)$ | $\frac{1}{298800}(-2+t)(-1+t)t(1+t)(4779+5t(-558+83t))h^{6}y^{(6)}(x_{n})$ | $\frac{1}{575760}(-3+t)(-2+t)(-1+t)t(1+t)(228784+t(-104372+12019t))h^{7}y^{(7)}(x_{n})$ | $\frac{180}{180}(-4+t)(-3+t)(-2+t)(-1+t)t(1+t)(384925+7t(-20530+1927t))h^8y^{(8)}(x_n) = \frac{1}{44}$ |
| 6 Th | | | | | | · | (-4+t) | 7 The | | | | | | • | $\frac{1}{54387}$ |
| Iab. | t | 0 | Η | 7 | 3 | 4 | Ŋ | Tab. | t | $-\frac{1}{2}$ | 7 <mark>1</mark> | 0 0 | 2 <mark>0</mark> | <u>5</u> -4 | 00 |
| | k | 1 | 2 | 3 | 4 | IJ | 9 | Ľ. | k | 1 | 2 | 3 | 4 | 5 | 9 |
| | | | | | | | | | | | | | | | |

5 Numerical experiments

In this section we shall test the discrete version of the new scheme (CF) of order 6 and compare it with the Ode15s of MATLAB for the following IVPs:

Prob. 1: A stiff system of Van der Pol equations discussed in [15]

$$y'_1 = y_2, \ y'_2 = 1000(1 - y_1^2) - y_1, \quad y(x) = \begin{pmatrix} 2\\ 0 \end{pmatrix}, \quad x \in [0, 10]$$

Prob. 2: Nonlinear chemical problem solved in [9] and [16]

$$y_1' = -0.04y_1 + 10^4 y_2 y_3, \qquad y_2' = -400y_1 + 10^4 y_2 y_3 - 3 \times 10^7 y_2^2,$$
$$y_3' = 3 \times 10^7 y_2^2, y(0) = \begin{pmatrix} 1\\0\\0 \end{pmatrix}$$

with $x \in [0,3]$ and h = 0.0001 for Prob.2. The method defined by (2) and (3) is as follows. From (2) and (3)

[__]

$$F(y_{n+k}^{[s]}) =$$

= $y(x_{n+k}^{[s]}) - \sum_{j=0}^{k-1} \alpha_{1,j}(t)y_{n+j} - h\beta_v(t)f(x_{n+v}, y_{n+v}^{[s]}) - h^2\gamma_v(t)f'(x_{n+v}, y_{n+v}^{[s]})$

where,

$$y_{n+v}^{[s]} = \sum_{j=0}^{k-1} \alpha_{2,j}(t) y_{n+j} + h\phi_k(t) f(x_{n+k}, y_{n+k}^{[s]}) + h^2 \delta_k(t) f'(x_{n+k}, y_{n+k}^{[s]}).$$

The solution of the above stiff problems leads to solving implicit set of nonlinear equations which demands the use of Newton Raphson method

$$y_{n+k}^{[s+1]} = y_{n+k}^{[s]} - J^{-1}(y_{n+k}^{[s]})F(y_{n+k}^{[s]}),$$
(14)

where $J^{-1}(y_{n+k}^{[s]})$ is the Jacobian matrix. The explicit trapezoidal rule is used to obtain the starting value for the Newton Raphson iterative scheme in (14). The numerical solution given by (2) and that of the *Ode15s* code are given in the Fig. 4 and Fig. 5.

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Fig. 4 The numerical solution of $y_1(x)$ component in Prob. 1



Fig. 5 The numerical solution of $y_2(x)$ component in Prob. 2

Conclusion

In this paper, a new family of $A(\alpha)$ numerical methods for stiff differential equation (ODEs) in initial value problems is presented. The new formulas are found to be A-stable for $k \leq 3$ and stiffly stable for $4 \leq k \leq 6$. The SSF were tested on two standard stiff IVPs and the resulting nonlinear system is solved using Newton Raphson scheme. The numerical solution graphs in Fig. 4 of the method in (2) on Prob. 1 coincide and show that the method in (2) compares with the state-of the-art of *MATLAB ode15s* code and in Fig. 5, the numerical solution shows that SSF outperformed the popular Ode15s code in [16] on Prob. 2.

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References

- [1] Butcher, J. C.: The Numerical Analysis of Ordinary Differential Equation: Runge Kutta and General Linear Methods. *Wiley*, Chichester, 1987.
- Butcher, J. C.: High Order A-stable Numerical Methods for Stiff Problems. Journal of Scientific Computing 25 (2005), 51–66.
- [3] Butcher, J. C., Hojjati, G.: Second derivative methods with RK stability Numer. Algorithms 40 (2005), 415–429.
- [4] Butcher, J. C.: Forty-five years of A-stability.. In: Numerical Analysis and Applied Mathematics: International Conference on Numerical Analysis and Applied Mathematics 2008. AIP Conference Proceedings 1048 (2008).
- [5] Butcher, J. C.: Numerical Methods for Ordinary Differential Equations. sec. edi., Wiley, Chichester, 2008.
- [6] Butcher, J. C.: General linear methods for ordinary differential equations. Mathematics and Computers in Simulation 79 (2009), 1834–1845.
- [7] Butcher, J. C.: Trees and numerical methods for ordinary differential equations. Numerical Algorithms 53 (2010), 153–170.
- [8] Dahlquist, G.: A special stability problem for linear multistep methods. BIT 3 (1963), 27–43.
- [9] Enright, W. H.: Second derivative multistep methods for stiff ODEs. SIAM J. Num. Anal. 11 (1974), 321–331.
- [10] Enright, W. H.: Continuous numerical methods for ODEs with defect control. J. Comput. Appl. Math. 125 (2000), 159–170.
- [11] Enright, W. H., Hull, T. E., Linberg, B.: Comparing numerical Methods for Stiff of ODEs systems. BIT 15 (1975), 1–48.
- [12] Fatunla, S. O.: Numerical Methods for Initial Value Problems in ODEs. Academic Press, New York, 1978.
- [13] Gear, C. W.: The automatic integration of stiff ODEs. In: Morrell A.J.H. (ed.) Information processing 68: Proc. IFIP Congress, Edinurgh, 1968 Nort-Holland, Amsterdam, 1968, 187–193.
- [14] Gear, C. W.: The automatic integration of ODEs. Comm. ACM 14 (1971), 176–179.
- [15] Hairer, E., Wanner, G.: Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems. Springer-Verlag, Berlin, 1996.
- [16] Higham, J. D., Higham, J. N.: Matlab Guide. SIAM, Philadelphia, 2000.
- [17] Ikhile, M. N. O., Okuonghae, R. I.: Stiffly stable continuous extension of second derivative LMM with an off-step point for IVPs in ODEs. J. Nig. Assoc. Math. Phys. 11 (2007), 175–190.
- [18] Lambert, J. D.: Numerical Methods for Ordinary Differential Systems. The Initial Value Problems. Wiley, Chichester, 1991.
- [19] Lambert, J. D.: Computational Methods for Ordinary Differential Systems. The Initial Value Problems. Wiley, Chichester, 1973.
- [20] Okuonghae, R. I.: Stiffly Stable Second Derivative Continuous LMM for IVPs in ODEs. Ph.D. Thesis, Dept. of Maths. University of Benin, Benin City. Nigeria, 2008.
- [21] Selva, M., Arevalo, C., Fuherer, C.: A Collocation formulation of multistep methods for variable step-size extensions. Appl. Numer. Math. 42 (2002), 5–16.
- [22] Widlund, O.: A note on unconditionally stable linear multistep methods. BIT 7 (1967), 65–70.