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The new class of A-stable hybrid multistep methods for numerical solution of stiff initial value problem

M. Mehdizadeh Khalsaraei, M. Molayi
Faculty of Mathematical Science, University of Maragheh, Maragheh, Iran

Abstract
In this paper, we present a class of hybrid multistep methods for the numerical solution of first-order initial value problems. We have used second derivative of solution (similar to second derivative multistep methods of Enright) and an off-step point. The accuracy and stability analysis are discussed. Stability domains of our presented methods have been obtained, showing that this class of efficient numerical methods are A(α)-stable of order up to 10. Numerical results are also given for four test problems.
Keywords: *Initial value problems, Multistep methods, Off-step point, Stability aspects.*

1. Introduction

In recent years, numerous work have focused on the development of more advanced and efficient methods for stiff problems [1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12]. A potentially good numerical method for the solution of stiff systems of ODEs must have good accuracy and some reasonably wide region of absolute stability [3, 13]. A-stability requirement puts a sever limitation on the choice of suitable methods for stiff problems. Dahlquist [3] proved that the order of an A-stable linear multistep method ≤ 2 and that an A-stable multistep method must be implicit. This pessimistic result has encouraged researchers to seek other classes of numerical methods for solving stiff equations. The search for higher order A-stable multi-step methods is carried out in the two main directions. (a) Use higher derivatives of the solutions. (b) Throw in additional stages, off-step point, super-future points and like. This leads into the large field general linear methods. Some known important schemes for stiff systems that will be used for comparison are as follows.

• The Enright [4] k−step second derivative multistep method (SDMM) of order k + 2 which takes the form:

$$y_{n+k} - y_{n+k-1} = h\sum_{j=0}^{k}\beta_j f_{n+j} + h^2\gamma_k g_{n+k},$$

• Special class of SDMM, introduced by Ibrahim and Ismail [7] of the form:

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\beta_k(f_{n+k} - \beta^* f_{n+k-1}) + h^2\gamma^*(g_{n+k} - \beta^* g_{n+k-1}).$$

For $\beta^* = 0, \gamma^* = 0$ this is the same as the SDBDF method.

• MEBDF [2] of order $k+1$ takes the form

$$y_{n+1} + \sum_{j=1}^{k}\alpha_j y_{n+1-j} = h(\beta_2 \overline{f}_{n+2} + \overline{\beta}_1 f_{n+1}) + (\beta_1 - \overline{\beta}_1)\overline{f}_{n+1}.$$

• AEBDF introduced by Hojjati [8] is

$$y_{n+k} - h\widehat{\beta}_k f_{n+k} = -\sum_{j=1}^{k-1}\widehat{\alpha}_j y_{n+j} + h\widehat{\beta}_{k+1}\overline{f}_{n+k+1}.$$

In this paper we introduce a new class of hybrid second derivative multi-step method that has good stability properties.

2. FORMULATION OF THE NEW METHOD

For the numerical solution of

$$\frac{dy}{dx} = f(x; y); \qquad y(0) = y_0, \tag{1}$$

we introduce a class of hybrid second derivative multistep methods (HSDMMs) with one off-step points as follows:

$$\overline{y}_{n+\theta} = h\mu f_{n+1} + \sum_{j=0}^{k-2}\gamma_j y_{n+1-j}, \tag{2}$$

$$y_{n+1}-\sum_{j=0}^{k}\alpha_j y_{n+1-j}=h\beta_\theta \overline{f}_{n+\theta}+h^2\gamma g_{n+1}, \qquad (3)$$

where $g(x,y)=y''=f_x+f_y f$ and coefficients are chosen so that (1) and (2) have order $k-1$ and $k+1$, respectively. To get formula (2) (evaluation the value of $y_{n+\theta}$ at off-step point, i.e. $x_{n+\theta}=x_n+\theta h$) Newton's interpolation formula for nodes x_{n+1} (double node), $x_n, x_{n-1},\ldots,x_{n-k+1}$ (simple nodes) have been used. For more details see [4]. The coefficients of schemes (1) and (2) are given in Table 1 and Table 2 , for $k=1,2,\ldots,8$ with $\theta=\frac{1}{2}$.

Table 1. Coefficients in (2)

k	2	3	4	5	6	7	8
r	1	4	32	192	3072	10240	40960
μ	$-\frac{1}{r}$	$-\frac{1}{r}$	$-\frac{6}{r}$	$-\frac{30}{r}$	$-\frac{420}{r}$	$-\frac{1260}{r}$	$-\frac{4620}{r}$
γ_0	$\frac{1}{r}$	$\frac{3}{r}$	$\frac{21}{r}$	$\frac{115}{r}$	$\frac{1715}{r}$	$\frac{5397}{r}$	$\frac{20559}{r}$
γ_1		$\frac{1}{r}$	$\frac{12}{r}$	$\frac{90}{r}$	$\frac{1680}{r}$	$\frac{6300}{r}$	$\frac{27720}{r}$
γ_2			$-\frac{1}{r}$	$-\frac{30}{r}$	$-\frac{8960}{r}$	$-\frac{2100}{r}$	$-\frac{11150}{r}$
γ_3				$\frac{2}{r}$	$\frac{112}{r}$	$\frac{840}{r}$	$\frac{6160}{r}$
γ_4					$-\frac{15}{r}$	$-\frac{225}{r}$	$-\frac{2475}{r}$
γ_5						$\frac{28}{r}$	$\frac{616}{r}$
γ_6							$-\frac{70}{r}$

Table 2. Coefficients in (3)

k	1	2	3	4	5	6	7	8
r	1	25	277	20085	273243	13951028	358345319	31746201805
γ	0	$\frac{1}{r}$	$\frac{12}{r}$	$\frac{852}{r}$	$\frac{11160}{r}$	$\frac{547740}{r}$	$\frac{13552560}{r}$	$\frac{1159880400}{r}$
β_θ	$\frac{1}{r}$	$\frac{24}{r}$	$\frac{264}{r}$	$\frac{19200}{r}$	$\frac{263040}{r}$	$\frac{13547520}{r}$	$\frac{351267840}{r}$	$\frac{31419924480}{r}$
α_1	$-\frac{1}{r}$	$-\frac{26}{r}$	$-\frac{291}{r}$	$-\frac{20984}{r}$	$-\frac{280905}{r}$	$-\frac{13997124}{r}$	$-\frac{348440337}{r}$	$-\frac{29727911520}{r}$
α_2		$\frac{1}{r}$	$\frac{15}{r}$	$\frac{894}{r}$	$\frac{3110}{r}$	$-\frac{630765}{r}$	$-\frac{44902809}{r}$	$-\frac{7267840680}{r}$
α_3			$\frac{1}{r}$	$\frac{24}{r}$	$\frac{6990}{r}$	$\frac{1123160}{r}$	$\frac{63367955}{r}$	$\frac{10329123616}{r}$
α_4				$-\frac{19}{r}$	$-\frac{2865}{r}$	$-\frac{593730}{r}$	$-\frac{42026355}{r}$	$-\frac{8281573650}{r}$
α_5					$\frac{427}{r}$	$\frac{168012}{r}$	$\frac{17412381}{r}$	$\frac{4510487520}{r}$
α_6						$-\frac{20581}{r}$	$-\frac{4210843}{r}$	$-\frac{1623353480}{r}$
α_7							$\frac{454689}{r}$	$\frac{348835680}{r}$
α_8								$-\frac{33939291}{r}$

3. ACCURACY AND STABILITY ANALYSIS

We now prove the following lemma regarding the order of accuracy of (3) used in the way described by stages (2) and (3).

Theorem 1. Let

(i) formula (2) is of order $k-1$,

(ii) formula (3) is of order $k+1$, are solved using an iteration scheme iterated to convergence,

then scheme (2-3) has order k .

Proof. The local truncation error for (2) of order $k-1$ is

$$y\left(x_{n+\theta}\right)-\bar{y}_{n+\theta}=C_1h^ky^{(k)}\left(x_n\right)+O(h^{k+1}), \qquad (4)$$

where $x_{n+\theta}=x_n+\theta h, 0<\theta<1$, and C_1 is the error constant when the method is being used to get $\bar{y}_{n+\theta}$. Similarly, the truncation error for method (3) of order $k+1$ is

$$y\left(x_{n+1}\right)-y_{n+1}=Ch^{k+2}y^{(k+2)}\left(x_n\right)+O(h^{k+3}), \qquad (5)$$

where C is the error constant of the method (2). Assuming that $y_{n+1-j}, j=1,2,\ldots,k$, be exact, then from (2) and (3) the difference operator associated with method (2) is

$$y\left(x_{n+1}\right)-y_{n+1}=Ch^{k+2}y^{(k+2)}\left(x_n\right)+h\beta_\theta\left[f\left(x_{n+\theta},y\left(x_{n+\theta}\right)\right)-f\left(x_{n+\theta},\bar{y}_{n+\theta}\right)\right]+O\left(h^{k+3}\right). \qquad (6)$$

For some $\eta_{n+\theta}$ in the interval whose end are $\bar{y}_{n+\theta}$ and $y\left(x_{n+\theta}\right)$, we can write

$$f\left(x_{n+\theta},y\left(x_{n+s}\right)\right)-f\left(x_{n+\theta},\bar{y}_{n+\theta}\right)=\frac{\partial f}{\partial y}\left(x_{n+\theta},\eta_{n+\theta}\right)\left(y\left(x_{n+\theta}\right)-\bar{y}_{n+\theta}\right). \qquad (7)$$

Now, from (4-7) we have

$$\begin{aligned} y\left(x_{n+1}\right)-y_{n+1} &= h\frac{\partial f}{\partial y}\left(x_{n+\theta},\eta_{n+\theta}\right)\left(y\left(x_{n+\theta}\right)-\bar{y}_{n+\theta}\right)+Ch^{k+2}y^{(k+2)}\left(x_n\right)+O\left(h^{k+3}\right) \\ &= h\frac{\partial f}{\partial y}\left(x_{n+\theta},\eta_{n+\theta}\right)\left[C_1h^ky^{(k)}\left(x_n\right)+O\left(h^{k+1}\right)\right]+Ch^{k+2}y^{(k+2)}\left(x_n\right)+O\left(h^{k+3}\right) \\ &= h^{k+1}\left[\frac{\partial f}{\partial y}\left(x_{n+\theta},\eta_{n+\theta}\right)C_1y^{(k)}\left(x_n\right)+Cy^{(k+2)}\left(x_n\right)\right]+O\left(h^{k+3}\right). \end{aligned} \qquad (8)$$

It results from the above that order of new method (1-2) is k .

Consider the Dahlquist's test equation of form

$$y'=\lambda y, \qquad y\left(0\right)=y_0. \qquad (9)$$

Applying method (2-3) to this test equation results in getting equations of the form

$$y_{n+\theta}=\mu\bar{h}y_{n+1}+\sum_{j=0}^{k-2}\lambda_j y_{n+1-j}, \qquad (10)$$

$$y_{n+1}+\sum_{j=1}^{k}\alpha_j y_{n+1-j}=\bar{h}\beta_s y_{n+\theta}+\bar{h}^2\gamma y_{n+1}. \qquad (11)$$

where $\bar{h}=h\lambda$. Now, we substitute (10) to (11) and therefore we obtain

$$\sum_{j=0}^{k}c_j\left(\bar{h}\right)y_{n+1-j}=0, \qquad (12)$$

where

$$c_0 = 1 - \bar{h}^2 \ \beta_\theta \mu + \gamma \ - \bar{h}\beta_\theta \gamma_0,$$
$$c_j = \alpha_j - \bar{h}\beta_\theta \gamma_j, \quad j = 1, \dots, k-2,$$
$$c_{k-1} = \alpha_{k-1},$$
$$c_k = \alpha_k.$$

Therefore, the corresponding characteristic equation of k^{th} order difference equation of the method is

$$\pi \ \xi, \bar{h} \ = \sum_{j=0}^{k} c_j \xi^{1-j} = 0. \quad (13)$$

To obtain the region of absolute stability we use the boundary locus method. Thus, the stability regions given are not exact but are those which have been found using a numerical search. By collecting coefficients of different powers of $\bar{h}$ in (13), we obtain

$$A_2 \bar{h}^2 + A_1 \bar{h} + A_0 = 0, \quad (14)$$

Where A_0, A_1 and A_2 are functions of ξ. Inserting $\xi = e^{i\varphi}$,(14) gives us two roots $\bar{h} \ \varphi$, $i = 1, 2$, which describe the stability domain. Regions of A(α)-stability are given in Table 3 for A-EBDF, MEBDF, Enright methods and new methods. Tables 3 shows that regions of A(α)-stability for our new method is larger than those of the other mentioned methods.

Table 3. A(α)-stability for A-EBDF, MEBDF, Enright methods and new methods

k	1	2	3	4	5	6	7
A-EBDF							
Order	2	3	4	5	6	7	8
$\alpha(^\circ)$	90	90	90	88.85	84.2	75	61
MEBDF							
Order	2	3	4	5	6	7	8
$\alpha(^\circ)$	90	90	90	88.4	82.5	74.5	62
Enright methods							
Order	3	4	5	6	7	8	9
$\alpha(^\circ)$	90	90	87.88	82.03	73.10	59.95	37.61
New method							
Order	1	2	3	4	5	6	7
$\alpha(^\circ)$	90	90	90	90	89.11	73.46	61.05

Figure 1. The region of absolute stability of new method.

4. NUMERICAL RESULTS

In this section we present four numerical results to compare the performance of our new methods. We have programmed these methods in MATLAB.

Example 1. The first test problem which we consider is

$$y_1' = -0.1y_1 - 49.9y_2, \quad y_1(0) = 2,$$
$$y_2' = -50y_2, \quad y_2(0) = 1,$$
$$y_3' = 70y_2 - 120y_3, \quad y_3(0) = 2,$$

with theoretical solution

$$y_1 = e^{-0.1x} + e^{-50x}, \quad y_2 = e^{-50x}, \quad y_3 = e^{-50x} + e^{-120x},$$

and the results are tabulated in Table 4 at different values of x. We have obtained slightly better results than those of HBDF[4].

Table 4. Results for Example 1.

x	y	Error in the new method	Error in HBDF [3]
40	y_1	5.88E-15	2.5E-10
	y_2	9.45E-23	6.96E-24
	y_3	8.05E-19	6.96E-24
10^2	y_1	4.0E-15	4.02E-11
	y_2	1.88E-24	1.09E-24
	y_3	1.88E-24	1.09E-24
10^3	y_1	5.08E-14	4.06E-13
	y_2	1.23E-29	1.07E-26
	y_3	1.23E-29	1.07E-26

Example 2. The second test problem which we consider is

$$y_1' = -21y_1 + 19y_2 - 20y_3, \quad y_1(0) = 1,$$
$$y_2' = 19y_1 - 21y_2 + 20y_3, \quad y_2(0) = 0,$$
$$y_3' = 40y_1 - 40y_2 - 40y_3, \quad y_3(0) = -1,$$

with theoretical solution

$$y_1 = \frac{1}{2}e^{-2x} + \frac{1}{2}e^{-40x}\left(\cos 40x + \sin 40x\right),$$
$$y_2 = \frac{1}{2}e^{-2x} - \frac{1}{2}e^{-40x}\left(\cos 40x + \sin 40x\right),$$
$$y_3 = -e^{-40x}\left(\cos 40x - \sin 40x\right),$$

The results of the numerical integration at 10^2 and 10^3 are presented in Table 5 solving with the method of order four and fixed stepsize $h = 0.001$.

Table 5. Results for Example 2.

x	y	Error in the new method
10^2	y_1	1.65E-12
	y_2	1.65E-12
	y_3	2.02E-18
10^3	y_1	2.91E-16
	y_2	2.91E-16
	y_3	6.05E-18

Example 3. Consider the stiff system of initial value problems

$$y_1' = -0.1y_1 - 49.9y_2,$$
$$y_2' = -50y_2,$$
$$y_3' = 70y_2 - 120y_3,$$

with initial value $y(0) = (1, 0, 0)^T$ whose exact solution is

$$y_1 = e^{-0.1x} + e^{-50x},$$
$$y_2 = e^{-50x},$$
$$y_3 = e^{-50x} + e^{-120x}. \qquad (10)$$

The numerical results are illustrated in following Table 6.

Table 6. The results for Example 3

x	y	Error in the new method	Error in the BDF[12]
0.1	y_1	2.41E-08	1.75E-07
	y_2	3.54E-11	3.59E-08
	y_3	6.93E-9	3.72E-08
0.18	y_1	1.78E-08	1.64E-05
	y_2	3.88E-07	2.79E-07
	y_3	9.17E-07	2.79E-07

Example 4. Let us consider the following stiff problem

$$y_1' = -0.04y_1 + 10^4 y_2 y_3,$$
$$y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3\times 10^7 y_2{}^2,$$
$$y_1' = 3\times 10^7 y_2{}^2,$$

with initial value $y(0) = (1,0,0)^T$. This is a chemistry problem suggested by Robertson. The results of the numerical integration at $X = 0.4, 40$ and 400 are presented in Table 7 solving with (7) and fixed stepsize $h = 0.001$.

Table 7. Numerical results for Example 4

x	y	The new method
0.4	y_1	9.85172113863285E-1
	y_2	3.38639537890963E-5
	y_3	1.47940221854871E-2
40	y_1	7.15827068718903E-1
	y_2	9.1855347645673E-6
	y_3	2.84163745746394E-1
400	y_1	4.50548668477070E-1
	y_2	3.22290144170159E-6
	y_3	5.49478108624731E-1

5. DISCUSSION

HSDMMs which are based on the second derivative of solution and off-step points, are A(α)-stable of order up to 10. Therefore, they are appropriate for the solution of certain ordinary differential and stiff differential equations.

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