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A NEW CLASS OF L-STABLE HYBRID ONE-STEP METHODS FOR THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

MOHAMMAD MEHDIZADEH[1] AND MARYAM MOLAYI

Abstract. In this paper, a class of one-step hybrid methods for the numerical solution of ordinary differential equations (ODEs) are considered. The accuracy and stability properties of these methods are investigated. By judicious choice of the coefficients in these formulae a class of method is derived which is shown to be L-stable and so is appropriate for the solution of certain ordinary differential and stiff differential equations. We apply the new method for numerical integration of some famous stiff chemical problems such chemical Akzo-Nobel problem, ROBER problem (suggested by Robertson) and some others which are very popular in numerical studies.

1. Introduction

Consider the system of ordinary differential equations of the form

$$\frac{dy}{dx} = f(x, y), \qquad y(0) = y_0, \tag{1.1}$$

where $x \in [0, X]$, $y \in R^m$ and $f \in R^{m+1}$.

In [6] Dahlquist defines A-stability as follows:

Definition 1.1. *A numerical method applied to test equation $y' = \lambda y$ (λ is complex constant with $Re\lambda < 0$) with fixed positive h, is said to be A-stable if its region of absolute stability contains the whole of the left-hand half-plane $Re\lambda h < 0$.*

He then established that the trapezoidal rule

$$y_{n+1} = y_n + \frac{h}{2}\left(f_n + f_{n+1}\right).$$

is the most accurate linear multistep method satisfying his A-stability requirement.
The search for higher order A-stable multistep methods was carried out in the two main directions:

- use higher derivatives of the solutions ,
- throw in additional stages, off-step points, super-future points and like .

This leads into the large field general linear methods [3]-[16].

In this paper, we construct a new class of A-stable hybrid one-step method which improves the computational efficiency and stability aspects. By using one off-step point in first derivative of the solution $y(x)$ and appropriate choice of the coefficients, a class of method is derived which has higher order of accuracy and good stability characteristics. The proposed method is L-stable and so is appropriate for the solution of certain ordinary differential and stiff differential equations. Following [5] a formal definition for L-stability is as follows:

Definition 1.2. *A one-step numerical method is said to be L-stable if it is A-stable and, in addition, when applied to the scalar test equation $y' = \lambda y$, it yields $y_{n+1} = R(\lambda h)y_n$, where $|R(\lambda h)| \to 0$ as $Re\lambda h \to -\infty$. R is the stability polynomial of the method.*

The paper is constructed as follows. In Section 2, we present the new scheme, we explain how the coefficients of the method has obtained. In Section 3, we discuss in some details the accuracy and stability region of the method. Numerical examples are given in Section 4 and a comparison is made with existing methods for results to show the efficiency of the new method.

2. The new method

For the numerical solution of (1.1), we introduce a class of hybrid methods with one off-step points as

[1] *corresponding author*
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follows:

(2.1)
$$\bar{y}_{n+\theta} = (\theta-1)^2 y_n + \theta(2-\theta)y_{n+1} + \theta(\theta-1)hf_{n+1},$$

(2.2)
$$y_{n+1} - y_n = h(\beta_0 f_n + \beta_1 f_{n+1} + \beta_2 \bar{f}_{n+\theta}),$$

where

$$f_{n+1} = f(x_{n+1}, y_{n+1}), \quad \bar{f}_{n+\theta} = f(x_{n+\theta}, \bar{y}_{n+\theta}),$$
$$x_{n+\theta} = x_n + \theta h,\ 0 < \theta < 1.$$

$\beta_i, i = 0, 1, 2$ and θ, are four arbitrary parameters. Now, as in [5] with the difference equation (2.2), we can associate the difference operator L as follows:

$$L[y(x), h] = y(x+h) - y(x) - h(\beta_0 y'(x) +$$
$$\beta_1 y'(x+h) + \beta_2 y'(x+\theta h)), \tag{2.3}$$

where the function $y(x)$ has continuous derivatives at least of order 4. Expanding the test function $y(x+ih)$ and its derivatives $y'(x+ih)$ and $y'(x+\theta h)$ as Taylor series around x, and collecting terms in (2.3) gives:

$$L[y(x), h] = C_0 y(x) + C_1 h y'(x) + \ldots$$
$$+ C_q h^q y^{(q)}(x) + \ldots. \tag{2.4}$$

Definition 2.1. [5] *The difference operator (2.3) and the associate difference equation (2.2) are said to be of order p if, in (2.4) it holds:*

$$C_0 = C_1 = \ldots = C_p = 0,\ C_{p+1} \neq 0\,.$$

Excluding θ, there are three undetermined parameters $\beta_0, \beta_1, \beta_2$. Using Taylor series expansion gives the following values for the parameters in (2.2):

$$\beta_0 = \frac{3\theta - 1}{6\theta}, \quad \beta_1 = \frac{3\theta - 2}{6(\theta - 1)}, \quad \beta_2 = -\frac{1}{6\theta(\theta - 1)}$$

The local truncation error is:

$$E_4 = (\frac{\theta}{36} - \frac{1}{72})h^4 y^{(4)}(\zeta).$$

If we take $\theta = \frac{1}{2}$ then obviously $E_4 = 0$, and we have

$$\beta_0 = \frac{1}{6}, \quad \beta_1 = \frac{1}{6}, \quad \beta_2 = -\frac{2}{3},$$

and the method is then

$$y_{n+1} - y_n = h(\frac{1}{6}f_n + \frac{1}{6}f_{n+1} - \frac{2}{3}\bar{f}_{n+\theta}),$$

which is the implicit one-step method of order 4, and its local truncation error is

$$E_5 = (\frac{\theta^2}{144} + \frac{\theta}{144} - \frac{1}{180})h^5 y^{(5)}(\zeta) = -\frac{1}{2880}h^5 y^{(5)}(\zeta)\,.$$

To get formula (2.1) (evaluation the value of $y_{n+\theta}$ at off-step point, i.e. $x_{n+\theta}$) Newton's interpolation formula for nodes x_{n+1} (double node), $x_n, x_{n-1}, \cdots, x_{n-k+1}$ (simple nodes) has been used. For more details see [3].

3. Accuracy and stability analysis

We now prove the following lemma regarding the order of accuracy of (2.2) used in the way described by stages (2.1) and (2.2).

Theorem 3.1. *Let:*

(i) *formula (2.1) is of order 2,*
(ii) *formula (2.2) is of order 3,*

and they are solved using an iteration scheme iterated to convergence. Then scheme (2.1)-(2.2) has order 3.

Proof. The local truncation error for (2.1) of order 2 is

$$y(x_{n+\theta}) - \bar{y}_{n+\theta} = C_1 h^3 y^{(3)}(x_n) + o(h^4), \tag{3.1}$$

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 (2.2) of order 4 is

$$y(x_{n+1}) - y_{n+1} = C_2 h^4 y^{(4)}(x_n) + O(h^5), \tag{3.2}$$

where $C_2 = \frac{\theta}{36} - \frac{1}{72}$ is the error constant of the method (2.2). Assuming that y_n, be exact, then from (2.1) and (2.2) the difference operator associated with method (2.2) is

$$y(x_{n+1}) - y_{n+1} = C_2 h^4 y^{(4)}(x_n) + h\beta_2 \Big[f\big(x_{n+\theta}, y(x_{n+\theta})\big)$$
$$- f(x_{n+\theta}, \bar{y}_{n+\theta}) \Big] + O(h^5). \tag{3.3}$$

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

$$f\big(x_{n+\theta}, y(x_{n+\theta})\big) - f(x_{n+\theta}, \bar{y}_{n+\theta}) = \frac{\partial f}{\partial y}\big(x_{n+\theta}, \eta_{n+\theta}\big)$$
$$\big(y(x_{n+\theta}) - \bar{y}_{n+\theta}\big). \tag{3.4}$$

Now, from (3.1)-(3.4) we have

$$\begin{aligned} y(x_{n+1}) - y_{n+1} &= h\frac{\partial f}{\partial y}(x_{n+\theta}, \eta_{n+\theta})\big(y(x_{n+\theta}) - \bar{y}_{n+\theta}\big) \\ &\quad + C_2 h^4 y^{(4)}(x_n) + O(h^5) \\ &= h\frac{\partial f}{\partial y}(x_{n+\theta}, \eta_{n+\theta})\big[C_1 h^3 y^{(3)}(x_n) + o(h^4)\big] \\ &\quad + C_2 h^4 y^{(4)}(x_n) + O(h^5) \\ &= h^4\big[\frac{\partial f}{\partial y}(x_{n+\theta}, \eta_{n+\theta}) C_1 y^{(3)}(x_n) + C_2 y^{(4)}(x_n)\big] \\ &\quad + O(h^5). \end{aligned}$$

It results from the above that order of new method (2.1)-(2.2) is 3. □

Theorem 3.2. *For every $0 < \theta < 1$, the method (2.2) is A-stable.*

Proof. Applying method (2.1)-(2.2) to test problem $y' = \lambda y$, results

$$\bar{y}_{n+\theta} = (\theta-1)^2 y_n + \theta(2-\theta)y_{n+1} + \theta(\theta-1)\bar{h}y_{n+1}, \tag{3.5}$$

$$y_{n+1} - y_n = \bar{h}(\beta_0 y_n + \beta_1 y_{n+1} + \beta_2 \bar{y}_{n+\theta}) \tag{3.6}$$

where $\bar{h} = h\lambda$. Now, we substitute (3.5) into (3.6) and therefor we obtain

$$\begin{aligned} y_{n+1} - y_n = \bar{h}(&\beta_0 y_n + \beta_1 y_{n+1} + \beta_2((\theta-1)^2 y_n \\ &+ \theta(2-\theta)y_{n+1} + \theta(\theta-1)\bar{h}y_{n+1})). \end{aligned} \tag{3.7}$$

By substituting the value of $\beta_0, \beta_1, \beta_2$ in (3.7), we have

$$y_{n+1} = \underbrace{\frac{1+\frac{1}{3}\bar{h}}{1-\frac{2}{3}\bar{h}+\frac{1}{6}\bar{h}^2}}_{R(\bar{h})} y_n. \tag{3.8}$$

Therefor, the corresponding characteristic equation of first order difference equation of the methods is

$$\xi + R(\bar{h}) = 0.$$

Applying the necessary and sufficient condition for A-stability ($|R(\bar{h})| < 1, \forall \bar{h} \in (-\infty, 0)$) yields:

$$|R(\bar{h})| < 1 \Longleftrightarrow \bar{h} \in (-\infty, 0), \forall\, 0 < \theta < 1.$$

This concludes the A-stability. The region of A-stability is plotted in Fig.1. □

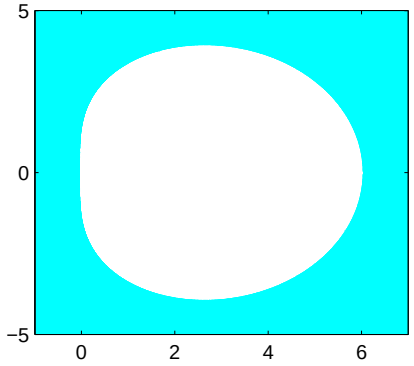

Figure 1: The region of absolute stability of (2.2).

Theorem 3.3. *For every $0 < \theta < 1$, the method (2.2) is L-stable.*

Proof. From (3.8) we observe that $|R(\lambda h)| \to 0$ as $\bar{h} \to \infty$, that means the method is L-stable. □

4. Numerical results

In this section we present some numerical results to compare the performance of our new class of methods with that of other numerical methods. What we shall be attempting to do, is to show the superior performance of new method for a given fixed stepsize over some special methods for a small selection of examples. We do not claim that our numerical results demonstrate the superiority of our approach over any of existing approaches. However, we do feel that our results indicate that a properly implemented version of our algorithm should be useful for the numerical integration of stiff differential systems. We have programmed these methods in MATLAB. Assume that the value of θ is $\frac{2}{3}$ to get new method which can take the form

$$\bar{y}_{n+\frac{2}{3}} = \frac{1}{9}y_n + \frac{8}{9}y_{n+1} - \frac{2}{9}hf_{n+1}, \tag{4.1}$$

$$y_{n+1} - y_n = \frac{1}{4}(f_n + 3\bar{f}_{n+\frac{2}{3}}). \tag{4.2}$$

However before we solve presented test problems, we are going to make some remarks about implementation of (4.1)-(4.2). Suppose that the following iteration

$$\bar{y}^{[m]}_{n+\frac{2}{3}} = -\frac{2}{9}hf^{[m]}_{n+1} + \frac{8}{9}y^{[m]}_{n+1} + \frac{1}{9}y_n, \tag{4.3}$$

$$y^{[m+1]}_{n+1} = y_n + \frac{1}{4}(f_n + 3\bar{f}^{[m]}_{n+\frac{2}{3}}). \tag{4.4}$$

is being used to solve nonlinear (4.1)-(4.2). More precisely, suppose $y_1 = y(0)$, which is the initial value in any test problem. By using an explicit method, we make an initial guess for $y^{[0]}_2$. This value together with initial condition y_1 are substituted into (4.3) to evaluate $\bar{y}^{[0]}_{1+\frac{2}{3}}$. So, we can obtain an improved approximation $y^{[1]}_2$ by substituting $\bar{y}^{[0]}_{1+\frac{2}{3}}$ into (4.4). This value is then substituted into (4.3) to get $\bar{y}^{[1]}_{1+\frac{2}{3}}$. Then, the process will go on.

Example 4.1. *Consider the initial value problem*

$$\begin{aligned} y' &= -5xy^2 + \frac{5}{x} - \frac{1}{x^2}, \\ y(1) &= 1. \end{aligned}$$

with the exact solution $y(x) = \frac{1}{x}$.

We compare the results of method (4.2) and Runge-Kutta method of 4 stage (RK_4) with $h = 0.1$ and $h = 0.025$.

The results for Example 4.1

x_i	h	RK_4	Error with method (2.2)
1.0	0.1	0	0
2.2		-0.001373	2.72E-06
3.4		-0.000321	4.25E-07
4.6		0.000121	1.2E-07
5.8		0.000058	4.66E-08
7.0		0.000033	2.16E-08
⋮		⋮	
25.0		0.000001	1.24E-10
1.0	0.025	0	0
2.2		-0.0002156	4.8E-08
3.4		-0.0000632	7.5E-09
4.6		0.0000021	2.12E-09
5.8		0.0000062	8.18E-10
7.0		0.0000003	3.78E-10
⋮		⋮	
25.0		0.0000008	2.18E-12

Example 4.2. *Consider the stiff system of initial value problem*

$$y_1{}' = -1002y_1 + 1000y_2^2,$$
$$y_2{}' = y_1 - y_2(1 + y_2),$$
$$y_1(0) = 1, \quad y_2(0) = 1.$$

with the exact solution

$$y_1 = e^{-2x},$$
$$y_2 = e^{-x}.$$

We have solved this problem at $X = 50$ and compared the results with those of Wu's method [2]. A stepsize $h = 0.05$ has been used here. One can also use the smaller stepsize to get significantly more accurate than this result. For the numerical result see Table 2.

The results for Example 4.2

X	h	Y	Error with method (2.2)	Error in [2]
50	0.05	y_1	4.13E-25	2.3E-21
		y_2	1.29E-22	1.4E-18

Example 4.3. *Consider the non-linear system of differential equations:*

$$y_1' = \lambda y_1 + y_2^2,$$

$$y_2' = -y_2,$$

where $\lambda = 10000$. *The exact solution is:*

$$y_1(x) = \frac{-e^{-2x}}{(\lambda+2)},$$

$$y_2(x) = e^{-x},$$

and the results are tabulated in Table 3 for $h = 0.0001$ *at different values of* X.

The results for Example 4.3

X	y_i	Error with method (2.2)
3	y_1	1.778769E-20
	y_2	2.078539E-12
5	y_1	2.493147E-19
	y_2	4.664012E-13
10	y_1	5.743522E-20
	y_2	6.345662E-12

Example 4.4. *Let us consider the following stiff problem*

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

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 4 solving with (4.2) and fixed stepsize $h = 0.001$.

The results for Example 4.4

X	y_i	method (2.2)
0.4	y_1	9.851712513470 07E-1
	y_2	3.386395543179683E-5
	y_3	1.479401090987736E-2
40	y_1	7.158270697983733 2E-1
	y_2	9.185534805990503E-6
	y_3	2.841637446676256E-1
400	y_1	4.505186352465841E-1
	y_2	3.22290144176527E-6
	y_3	5.494781086256178E-1

Example 4.5. *Consider the following stiff system arose from a chemistry problem*

$$\begin{aligned} {y_1}' &= -0.013y_2 - 1000y_1y_2 - 2500y_1y_3, \\ {y_2}' &= -0.013y_2 - 1000y_1y_2, \\ {y_3}' &= -2500y_1y_3, \end{aligned}$$

with initial value $y(0) = (0, 1, 1)^T$.

In Table 5 we give the results obtained for the integration of this problem at $X = 2.0$. A stepsize $h = 0.001$ has been used here. Comparison with the formulas in [1] and [4], the new formula gives more accurate results.

The results for Example 4.5

X	y_i	Exact solution	Error with (2.2)
2.0	y_1	-0.3616933169289E-5	7.7632E-17
	y_2	0.99815029984230	4.1714E-11
	y_3	01.018493388244	4.1908E-11
		Error in [1]	Error in [4]
2.0	y_1	0.82E-10	0.31E-08
	y_2	0.61E-05	0.18E-05
	y_3	0.57E-05	0.57E-05

Example 4.6. *As our last test equation, we consider chemical Akzo Nobel problem. This IVP is a stiff system of 6 non-linear differential equations. It has been taken from* [11, 16].

Mathematical description of the problem: The problem is of the form:

$$\frac{dy}{dx} = f(y), \quad y(0) = y_0, \quad y \in \mathbb{R}^6, \quad 0 \le x \le 180,$$

and the function f is defined by

$$f = \begin{pmatrix} -2r_1 + r_2 - r_3 - r_4 \\ -\frac{1}{2}r_1 - r_4 - \frac{1}{2}r_5 + F_{in} \\ r_1 - r_2 + r_3 \\ -r_2 + r_3 - 2r_4 \\ r_2 - r_3 + r_5 \\ -r_5 \end{pmatrix}$$

where the r_i and F_{in} are auxiliary variables, given by

$$\begin{aligned} r_1 &= k_1 y_1^4 y_2^{\frac{1}{2}}, \quad k_1 = 18.7, \\ r_2 &= k_2 y_3 y_4, \quad k_2 = 0.58, \\ r_3 &= \frac{k_2}{K} y_3 y_5, \quad K = 34.4, \\ r_4 &= k_3 y_1 y_4^2, \quad k_3 = 0.09, \\ r_5 &= k_4 y_6^2 y_2^{\frac{1}{2}}, \quad k_4 = 0.42, \\ F_{in} &= klA \left(\frac{p(O_2)}{H} - y_2 \right), \\ klA &= 3.3, \ p(O_2) = 0.9, \ H = 737. \end{aligned}$$

Finally the initial vector y_0 is given by
$y_0 = (0.437, 0.00123, 0, 0, 0, 0.367)^T$.

Origin of the problem: The problem originates from Akzo Nobel Central Research in Arnhem, The Netherlands. It describes a chemical process, in which 2 species, MBT and CHA, are mixed, while oxygen is continuously added. The resulting species of importance is CBS. The reaction equations, as given by Akzo Nobel, are the last equation describes an equilibrium

$$Ks^1 = \frac{[MBT \cdot CHA]}{[MBT] \cdot [CHA]},$$

while the others describe reactions, whose velocities are given by

$$\begin{aligned} r_1 &= k_1 [MBT]^4 \cdot [O_2]^{\frac{1}{2}}, \\ r_2 &= k_2 [MBTS] \cdot [CHA], \\ r_3 &= \frac{k_2}{K} [MBT] \cdot [CBS], \\ r_4 &= k_3 [MBT] \cdot [CHA]^2, \\ r_5 &= k_4 [MBT \cdot CHA]^2 [O_2]^{\frac{1}{2}}, \end{aligned}$$

respectively. Here the square brackets '[ ]' denote concentrations. The inflow of oxygen per volume unit is denoted by F_{in}, and satisfies

$$F_{in} = klA \left(\frac{p(O_2)}{H} - [O_2] \right),$$

where klA is the mass transfer coefficient, H is the Henry constant and $P(O_2)$ is the partial oxygen pressure. $P(O_2)$ is assumed to be independent of $[O_2]$. The parameters $k_1, k_2, k_3, k_4, K, klA, H$ and $P(O_2)$ are given constants. The process is started by mixing 0.437 mol/L $[MBT]$ with 0.367 mol/L $[MBT.CHA]$ The concentration of oxygen at the beginning is 0.00123 mol/L. Initially, no other species are present. The simulation is performed on the time interval [0 180 min]. Identifying the concentrations $[MBT], [O_2], [MBTS], [CHA], [CBS], [MBT.CHA]$ with $y_1, \cdots, y_6$, respectively, one easily arrives at the

mathematical formulation of the preceding subsection. Solution of this problem at $t = 180$ using new method is reported in Table 6.

The results for Example 4.6

t	y_i	method (2.2)
180	y_1	1.161625832012301E-1
	y_2	1.119412194091551E-3
	y_3	1.621250677283227E-1
	y_4	3.395915545576541E-3
	y_5	1.646185137343564E-1
	y_6	1.989543899632128E-1

5. Conclusions

We have derived a class of methods that, as it has been shown in section 2, has extensive region of stability and in particular is L-stable up to order 4. This property, let us to apply the new method for numerical solution of stiff systems of ODEs with high accuracy. We do not claim that our numerical results demonstrate the superiority of our approach over any of the more conventional approaches. However, we do feel that our results indicate that a properly implemented version of our algorithm should be useful for the numerical integration of stiff differential systems.

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Faculty of Mathematical Science
University of Maragheh
Maragheh, Iran
E-mail address: mehdizadeh@maragheh.ac.ir

Faculty of Mathematical Science
University of Maragheh
Maragheh, Iran
E-mail address: m.molayi.66@gmail.com