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The New High Approximation of Stiff Systems of First Order IVPs Arising From Chemical Reactions by k-Step L-Stable Hybrid Methods

MOHAMMAD MEHDIZADEH KHALSARAEI•, ALI SHOKRI AND MARYAM MOLAYI

Department of Mathematics, Faculty of Sciences, University of Maragheh, Maragheh, Iran

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ABSTRACT

In this paper, we present a new class of hybrid methods for the numerical solution of first order ordinary differential equations (ODEs). The accuracy and stability properties of the new methods are investigated. In the final section, we apply new hybrid methods to solve two stiff chemical problems such as Robertson problem.

1. INTRODUCTION

Let us consider the system of ordinary differential equations

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

on the bounded interval $I = [x_0, X_N]$, where $y: I \to \boldsymbol{R}^m$ and $f: I \times \boldsymbol{R}^m \to \boldsymbol{R}^{m-1}$ is $N - 1$ times continuously differentiable function. The numerical integration of (1) has attracted a lot of attention in the past decades because several physical and chemical problems can be modeled by these equations. Several authors began explore and develop numerical approaches to integrate (1). These approaches are including Rung-Kutta method, linear multistep method, Taylor and extrapolation methods. Special multi-step methods based on numerical integration such as Adams-Bashforth methods, Adams-Moulton methods and methods based on numerical differentiation for solving first-order differential equations

•Corresponding Author: (Email address: mehdizadeh@maragheh.ac.ir)
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have been derived in Henrici [7] and Gear [5]. Several authors and researchers are focusing on the development of more efficient methods, e.g. general linear methods and general multistep methods [4, 5, 10–12, 18–23]. From discussion in some papers and books on the relative merits of linear multistep and Runge-Kutta methods, it emerged that the former class of methods, though generally the more efficient in terms of accuracy and week stability properties for a given number of functions evaluations per step, suffered the disadvantage of requiring additional starting values and special procedures for changing step length. For reducing these difficulties researchers have encouraged to seek other classes with low the step number of the linear multistep methods without reducing their order. Such formula which incorporates a function evaluation at on off-step point was proposed by Gear [5]. The k-step classical hybrid methods are as follows

$$\sum_{j=0}^{k} a_j y_{n+j} = h\sum_{j=0}^{k} b_j f_{n+j} + h\sum_{j=0}^{k} d_j f_{n+v_j} \tag{2}$$

where $\alpha_k = +1$, α_0 and b_0 are not both zero, $v_j \notin \{0,1,\dots,k\}$, and consistently with our previous usage, $f_{n+v_j} = f(x_{n+v_j}, y_{n+v_j})$. In order to implement such a formula, even when it is explicit (that is $b_k = 0$) a special predictor to estimate y_{n+v_j} is necessary. Thus a hybrid formula, unlike a linear multistep method, cannot be regarded as a method in its own right.

The paper is constructed as follows. In Section 2, we present a new method and explain how the coefficients of the method have obtained. We discuss in some detail the accuracy a stability region of the method. Numerical examples are given is Section 3.

2. CONSTRUCTION OF THE NEW HYBRID METHODS

For the numerical solution first of order initial value problems (1), we introduce the new hybrid methods of the form (2) with $k' = 1$, as follows:

$$\sum_{j=0}^{k} a_j y_{n+j} = h\sum_{j=0}^{k} b_j f_{n+j} + h\left(d_0 f_{n+v_0} + d_1 f_{n+v_1}\right) \tag{3}$$

where a_j, b_j, d_0, d_1 and $0 < v_0, v_1 < 1$ are $(2k+6)$ arbitrary parameters. For simplicity we assume that $v_1 = 1 - v_0$, so we have $(2k+5)$ free parameters, and (2) takes the form:

$$\sum_{j=0}^{k} a_j y_{n+j} = h\sum_{j=0}^{k} b_j f_{n+j} + h\left(d_0 f_{n+v_0} + d_1 f_{n+1-v_0}\right). \tag{4}$$

Let the differential equation)1) has a unique solution $y(x)$ on $[a,b]$ and suppose that $y(x) \in C^{(p+1)}[a,b]$ for $p \geq 1$. Then the deference operator L for the method (2) can be written as

$$\begin{aligned} L[y(x),h] = {} & \sum_{j=0}^{k}\left[a_j y(x+jh) - hb_j y'(x+jh)\right] \\ & -h[d_0 y'(x+v_0 h) + d_1 y'(x+(1-v_0)h]. \end{aligned} \tag{5}$$

Definition 2.1. *For the method* (*2*)*, we define the functions* $\rho(\xi)$ *and* $\sigma(\xi)$ *as* $\rho(\xi) = \sum_{j=0}^{k} a_j \xi^j$, $\sigma(\xi) = \sum_{j=0}^{k} b_j \xi^j + d_0 \xi^{v_0} + d_1 \xi^{1-v_0}$ *and these functions are so called the first and second characteristic functions of the new method* (*2*)*, respectively*.

We can assume that the functions $\rho(\xi)$ and $\sigma(\xi)$ have no common factors since, otherwise, (2) can be reduced to anequation of lower order. In order that the difference equation (2) should be useful for numerical integration, it is necessary that (2) be satisfied with high accuracy by the solution of the differential equation $y' = f(x, y)$, when $h$is small for an arbitrary function $f(x, y)$. This imposes restrictions on the coefficients of (2). We assume that the function $y(x)$ has continuous derivatives of sufficiently high order. We firstly use the Taylor series expansion to determine all the coefficients of (2), which can be written as

$$L[y(x_n), h] = \sum_{j=0}^{k}\left[a_j \sum_{m=0}^{\infty} \frac{(jh)^m}{m!} y^{(m)}(x_n) - hb_j \sum_{m=0}^{\infty} \frac{(jh)^m}{m!} y^{(m-1)}(x_n) y^{(m)}(x_n)\right]$$
$$-h\sum_{m=0}^{\infty}\left(d_0 \frac{(v_0 h)^m}{m!} + d_1 \frac{((1-v_0)h)^m}{m!}\right) y^{(m-1)}(x_n)$$

Definition 2.2. *The linear k-step new hybrid method* (*2*) *are said to be of order p if* $C_0 = C_1 = C_2 = \cdots = C_p = 0$, $C_{p+1} \neq 0$. *Thus for any function* $y(x) \in C^{(p+2)}[a, b]$ *and for some nonzero constant* $C_{\{p+1\}}$, *we have*

$$L[y(x), h] = C_{p+1} h^{p+1} y^{(p+1)}(x_n) + O(h^{p+2}) ,$$

where C_{p+1} *is called the local truncation error constant*.

We know that the classical linear k-step methods are consistent if and only if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$. Of course these relations are hold if the mentioned methods have algebraic order $\rho \geq 1$. Hence the consistency will be achieved if at least we have $C_0 = C_1 = 0$, so in our new methods we must have $\sum_{j=0}^{k} a_j = 0$, $\sum_{j=0}^{k}(ja_j - b_j) - (d_0 + d_1) = 0$. Therefore, similar to the classical hybrid methods, our new hybrid methods (2), are consistent if and only if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$.

2.1. ONE-STEP NEW HYBRID METHODS

Upon choosing $k = 1$ in (2), we get

$$y_{n+1} - y_n = h(b_0 f_n + b_1 f_{n+1} + d_0 f_{n+v_0} + d_1 f_{n+1+v_0}), \qquad (6)$$

where b_j,d_j for $j = 0, 1$ and v_0 are five arbitrary parameters. Excluding v_0, there are four undetermined parameters b_0, b_1, d_0, d_1. As [9, 14–17], Taylor series expansion gives the following values for the parameters in (6)

$$b_0 = \frac{6v_0^2 - 6v_0 + 1}{12v_0(v_0 - 1)}, \quad b_1 = \frac{6v_0^2 - 6v_0 + 1}{12v_0(v_0 - 1)}$$
$$d_0 = -\frac{1}{12v_0(v_0 - 1)}, \quad d_1 = -\frac{1}{12v_0(v_0 - 1)}$$

where the local truncation error is

$$E_5 = \left(\frac{v_0^2}{144} - \frac{v_0}{144} + \frac{1}{720}\right) h^5 y^{(5)}(\xi).$$

If $v_0 \in (0,1) - \left\{\frac{5+\sqrt{5}}{10}, \frac{5-\sqrt{5}}{10}\right\}$, then error constant in E_5 is nonzero, and the method is of order 4, i.e. $\frac{v_0^2}{144} - \frac{v_0}{144} + \frac{1}{720} \neq 0$. If we take $v_0 = \left\{\frac{5+\sqrt{5}}{10}, \frac{5-\sqrt{5}}{10}\right\}$, then obviously $E_5 = 0$ and we get

$$E_6 = -\frac{(5v_0^2-5v_0+1)(5v_0^2-5v_0+4)}{1440} = 0.$$

For $v_0 = \frac{5+\sqrt{5}}{10}$, we have $b_0 = \frac{1}{12}$, $b_1 = \frac{1}{12}$, $b_2 = \frac{5}{12}$, $b_3 = \frac{5}{12}$ and the method is then

$$y_{n+1} - y_n = h\left(\frac{1}{12} f_n + \frac{1}{12} f_{n+1}\right) + h\left(\frac{5}{12} f_{n+\frac{5+\sqrt{5}}{10}} + \frac{5}{12} f_{n+\frac{5-\sqrt{5}}{10}}\right)$$

which is the implicit one-step method of order 6, and its local truncation error is

$$\boldsymbol{E_7 = \left(-\frac{(v_0^2-1)^6}{1728} - \frac{v_0^6}{1728} + \frac{1}{12096}\right) h^7 y^{(7)}(\xi) = -\frac{1}{1512000} h^7 y^{(7)}(\xi).}$$

Theorem2.3. *For every* $0 < v_0 < 1$, *the hybrid two off-step point method* (*6*) *is A-stable.*

.Proof By expanding y_{n+v_0} and y_{n+1+v_0} around x_{n+1} of order 3 and application of (6) to test problem $y' = \lambda y$ for which $y'' = \lambda^2 y$, we have $y_{n+1} + C(\bar{h}) y_n = 0$, where

$$C(\bar{h}) = \frac{-2(12v_0^2-12v_0+6\bar{h}v_0^2-6\bar{h}v_0+\bar{h})}{24v_0^2-24v_0-12\bar{h}v_0^2+12\bar{h}v_0+2\bar{h}-2\bar{h}^2+\bar{h}^3-2\bar{h}^3v_0+2\bar{h}^3v_0^2} \quad (7)$$

Therefore, the corresponding characteristic equation of first order difference equation of the methods is $\xi + C(\bar{h}) = 0$,where $\bar{h} = \lambda h$. Applying the necessary and sufficient condition for A-stability ($|C(\bar{h})| < 1, \ \forall \bar{h} \in (-\infty, 0)$) yields:

$$|C(\bar{h})| < 1 \leftrightarrow \bar{h} \in (-\infty, 0) \cup (1.99, +\infty), \ \forall 0 < v_0 < 1.$$

This concludes the A-stability. ■

The region of A-stability is plotted in Figure 1.

Theorem 2.4. *For every* $0 < v_0 < 1$, *the method* (*6*) *is L-stable.*

Proof. Since we have $\frac{y_{n+1}}{y_n} = -C(\bar{h})$, we observe that $\left|\frac{y_{n+1}}{y_n}\right| \to 0$ as $\bar{h} \to -\infty$, that means the method is L-stable. ■

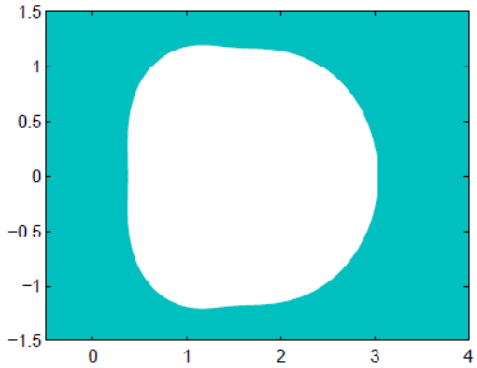

Figure 1. The region of absolute stability of (6).

By every $0 < v_0 < 1$, we derive one-step A-stable and L-stable hybrid two off-step method which is of order ≥ 5, and so is appropriate for solving stiff first-order initial value problem. For example, let $v_0 = \frac{1}{3}$, and so we have

$$y_{n+1} - y_n = \frac{h}{8}\left(f_n + f_{n+1} + 3f_{n+\frac{1}{3}} + 3f_{n+\frac{2}{3}}\right) \tag{8}$$

which will be used for the numerical solution of examples in Section 3.

2.2. Two-Step New Hybrid Methods

Upon choosing $k = 2$ in (2), we get

$$a_2 y_{n+2} + a_1 y_{n+1} + a_0 y_n = h(b_0 f_n + b_1 f_{n+1} + b_2 f_{n+2}) + h\left(d_0 f_{n+v_0} + d_1 f_{n+1+v_0}\right) \tag{9}$$

where $a_2 = +1$, b_j for $j = 0,1,2$, $a_j$and $d_j$for$j = 0,1$ and v_0 are five arbitrary parameters. Excluding v_0, there are eight undetermined parameters. In order to implement such a formula, we suppose that v_0 is free parameter and by substituting $C_i = 0, i = 0,1, \ldots ,6$, we have

$$a_0 = -\frac{15v_0^2 - 15v_0 - 13}{3(5v_0^2 - 5v_0 + 1)}, \qquad a_1 = -\frac{16}{3(5v_0^2 - 5v_0 + 1)},$$

$$b_0 = \frac{15v_0^4 - 30v_0^3 + 4v_0^2 + 11v_0 - 2}{9(5v_0^2 - 5v_0 + 1)(v_0 - 1)v_0}, \quad b_1 = \frac{4(15v_0^4 - 30v_0^3 + 7v_0^2 + 8v_0 - 2)}{9(5v_0^2 - 5v_0 + 1)(v_0 - 1)v_0},$$

$$b_2 = \frac{3v_0^2 - 3v_0 - 4}{9(v_0 + 1)(v_0 - 2)}, d_0 = -\frac{4(3v_0^2 - 1)}{9v_0(v_0 - 1)(v_0 - 2)(2v_0 - 1)(5v_0^2 - 5v_0 + 1)},$$

$$d_1 = -\frac{4(3v_0^2 - 6v_0 + 2)}{9v_0(v_0 - 1)(v_0 + 1)(2v_0 - 1)(5v_0^2 - 5v_0 + 1)},$$

and its local truncation error is

$$E_7 = \frac{1}{11340}\left(\frac{21v_0^4 - 42v_0^3 + 5v_0^2 + 16v_0 - 4}{5v_0^2 - 5v_0 + 1}\right) h^7 y^{(7)}(\xi).$$

Therefore if

$$v_0 \notin (0,2) - \left\{\frac{21-(\sqrt{37}-4)\sqrt{21}}{42}, \frac{21+(\sqrt{37}-4)\sqrt{21}}{42}, \frac{21+(\sqrt{37}+4)\sqrt{21}}{42}\right\},$$

(and also $v_0 \neq 0,1,2$), then the error constant of E_7 is nonzero and hence the order of new two-step method is 6. Now if we select a value for v_0 from $\left\{\frac{21-(\sqrt{37}-4)\sqrt{21}}{42}, \frac{21+(\sqrt{37}-4)\sqrt{21}}{42}, \frac{21+(\sqrt{37}+4)\sqrt{21}}{42}\right\}$, then we have $E_7 = 0$ and $E_8 \neq 0$, this means that the order ofour two-step method is 7. For example by choosing $v_0 = \frac{1}{3}$, we have

$$a_0 = -49, \quad a_1 = 48, \quad b_0 = \frac{16}{3}, \quad b_1 = \frac{28}{3}, \quad b_2 = \frac{7}{30}, \quad d_0 = \frac{108}{5}, \quad d_1 = \frac{27}{2}.$$

So the method is

$$y_{n+2} + 48y_{n-1} - 49y_n = \frac{h}{30}(7f_{n-2} + 280f_{n-1} + 160f_n) + \frac{h}{10}\left(216f_{n+\frac{1}{3}} + 135f_{n+\frac{2}{3}}\right) \qquad (10)$$

that is the implicit two-step method of order 6 and its local truncation is $E_7 = -\frac{4}{8505}h^7y^7(\xi)$. If we set $v_0 = \frac{21+(\sqrt{37}+4)\sqrt{21}}{42}$, then we have

$$a_0 = \frac{973 - 160\sqrt{37}}{3}, \quad a_1 = \frac{-976 + 160\sqrt{37}}{3}, \quad b_0 = \frac{-79 + 13\sqrt{37}}{3},$$

$$b_1 = -24 + 4\sqrt{37}, \quad b_2 = \frac{19-\sqrt{37}}{108}, d_0 = \frac{(-83\sqrt{37}+605)\sqrt{21}}{1512} + \frac{4861\sqrt{37}-29503}{216},$$

$$d_1 = \frac{(83\sqrt{37} - 605)\sqrt{21}}{1512} + \frac{4861\sqrt{37} - 29503}{216}.$$

By these coefficients we have an implicit two-step method of order 7 with local truncation error $E_8 = \frac{2\sqrt{37}-13}{158760}h^8y^{(8)}(\xi)$.

Theorem 2.5. *Any two-step hybrid methods derived from* (9)*, with* $0 < v_0 < 2$ *and* $v_0 \neq 1$ *are L-stable.*

Proof. Note that (for simplicity) the third order approximation of y_{n+v_0} and y_{n+1+v_0} around x_{n+2} enough for provingthe L-stability of new method (9). Therefore by expanding y_{n+v_0} and y_{n+v_0+1} around x_{n+2} of order 3 and application of (6) to test problem $y^{(k)} = \lambda^k y$ for $k = 1,2,3$, we have $P_2(z)y_{n+2} + P_1(z)y_{n+1} + P_0(z)y_n = 0$, where $z = \lambda h$, and $P_0(z) = -zb_0 + a_0$, $P_1(z) = -zb_1 + a_1$ and

$$P_2(z) = 1 - b_2z - (d_0 + d_1)z + \left(d_0(v_0 - 2) - d_1(v_0 + 1)\right)z^2$$
$$-\frac{1}{2}\left((d_0 + d_1)v_0^2 + (-4d_0 + d_1)v_0 + 4d_0 + d_1\right)z^3$$
$$-\frac{1}{6}(d_0(v_0 - 2)^3 - d_1(v_0 + 1)^3)z^4.$$

If we assume that $\xi = \frac{1+z}{1-z}$, then by simple calculation and by using Hurwitz theorem, we see that the new method (9), are A-stable for any $0 < v_0 < 2$ and $v_0 \neq 1$.

Furthermore, the new derived A-stable methods (9), are also L-stable because we have $\lim_{z\to-\infty}\frac{P_0(z)}{P_2(z)} = 0$ and $\lim_{z\to-\infty}\frac{P_1(z)}{P_2(z)} = 0$. ■

3. 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 the new method for a given fixed step size 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 v_0 is $\frac{1}{3}$ and $\frac{2}{3}$ to get new method which can take the form

$$\bar{y}_{n+\frac{1}{3}} = y_{n+1} - \frac{2h}{3}f_{n+1} + \frac{4h^2}{18}f'_{n+1}, \tag{11}$$

$$\bar{y}_{n+\frac{2}{3}} = y_{n+1} - \frac{h}{3}f_{n+1} + \frac{h^2}{18}f'_{n+1}, \tag{12}$$

$$y_{n+1} - y_n = \frac{1}{8}\left(f_n + f_{n+1} + 3\left(\bar{f}_{n+\frac{1}{3}} + \bar{f}_{n+\frac{2}{3}}\right)\right), \tag{13}$$

However before we solve the presented test problems, we are going to make some remarks about implementation of the new scheme. Suppose that the following iteration

$$\bar{y}^{[m]}_{n+\frac{1}{3}} = y^{[m]}_{n+1} - \frac{2h}{3}f^{[m]}_{n+1} + \frac{4h^2}{18}f'^{[m]}_{n+1} \tag{14}$$

$$\bar{y}^{[m]}_{n+\frac{2}{3}} = y^{[m]}_{n+1} - \frac{h}{3}f^{[m]}_{n+1} + \frac{h^2}{18}f'^{[m]}_{n+1} \tag{15}$$

$$y^{[m+1]}_{n+1} = y_n + \frac{1}{8}\left(f_n + f_{n+1} + 3\left(\bar{f}^{[m]}_{n+\frac{1}{3}} + \bar{f}^{[m]}_{n+\frac{2}{3}}\right)\right), \tag{16}$$

is being used to solve nonlinear (11–13). More precisely, suppose $y_1 = y(0)$, which is the initial value in anytest problem. By using an explicit method, we make an initial guess for $y_2^{[0]}$. This value is substituted into (14) to evaluate $\bar{y}^{[0]}_{1+\frac{1}{3}}$ and $\bar{y}^{[0]}_{1+\frac{2}{3}}$. So, we can obtain an improved approximation $y_2^{[1]}$ by substituting $\bar{y}^{[0]}_{1+\frac{1}{3}}$ and $\bar{y}^{[0]}_{1+\frac{2}{3}}$ into (16). This value is then substituted into (14) to get $\bar{y}^{[1]}_{1+\frac{1}{3}}$ and $\bar{y}^{[0]}_{1+\frac{2}{3}}$. Then, the process will go on.

In this section, we have used several multistep methods for the numerical integration of the three test problems. These methods are:

SDMM: The second derivative two-step method developed by Ismail and Ibrahim [13]. Consider the SDMM of the form

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h\beta_k(f_{n+k} - \beta^* f_{n+k-1}) + h^2\gamma_k(g_{n+k} - \gamma^* g_{n+k-1}),$$

where $g(x, y) = y'' = f_x + f f_y$, α_i, β_k and γ_k are parameters to be determined. They were established the mentioned SDMMs with k -step and other k+1 until order 10 with two free parameters β^* and γ^* which take some values to get larger stability regions than the others. The coefficients of these methods are represented in Table 1a and b in [11].

MEBDF: Suppose the value y_{n+k} at the points x_{n+j}, $0 \le j \le k-1$ are computed.

Stage 1. Using the k-step BDF scheme evaluate $\bar{y}_{n+k}$

$$y_{n+k} - h\hat{\beta}_k f_{n+k} = -\sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j}.$$

Stage 2. Compute $\bar{y}_{n+k+1}$ by solving the following algebraic equation:

$$y_{n+k+1} - h\hat{\beta}_k f_{n+k+1} = -\hat{\alpha}_{k-1}\hat{y}_{n+k} - \sum_{j=0}^{k-2} \hat{\alpha}_j y_{n+j+1}.$$

Stage 3. Evaluate

$$\bar{f}_{n+k} = f(t_{n+k}, \bar{y}_{n+k}), \qquad \bar{f}_{n+k+1} = f(t_{n+k+1}, \bar{y}_{n+k+1}).$$

Stage 4. Compute y_{n+k} as the solution of

$$y_{n+k} - h\hat{\beta}_k f_{n+k} = -\sum_{j=0}^{k-1} \bar{\alpha}_j y_{n+j} + h(\bar{\beta}_k - \hat{\beta}_k)\bar{f}_{n+k} + h\bar{\beta}_{k+1}\bar{f}_{n+k+1}$$

The formula coefficients $\bar{\beta}_i, \hat{\beta}_i, \bar{\alpha}_i$ and $\hat{\alpha}_i$, are defined by Cash [3].

LSODE: A BDF code of Hindmarsh [8].

Example 3.1 (Robertson Problem)

3.1. GENERAL INFORMATION

The problem consists of a stiff system of 3 non-linear ordinary differential equations. It was proposed by H.H. Robertson in 1966 [18]. The name ROBER was given by Hairer and Wanner [6]. The INdAM-Bari Test Set group contributed this problem to the testset. The software part of the problem is in the file roberf available at [13].

3.2. MATHEMATICAL DESCRIPTION OF THE PROBLEM

The problem is of the form

$$\frac{dy}{dt} = f(y), \quad y(0) = y_0 ,$$

with $y \in \boldsymbol{R}^3$, $t \in [0, T]$ and the function f is defined by $f = (f_1, f_2, f_3)^T$ where

$$f_1 = -0.04y_1 + 10^4 y_2 y_3,$$
$$f_2 = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2,$$
$$f_3 = 3 \times 10^7 y_2^2,$$

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

1.	A	$\xrightarrow{k_1}$	B
2.	$B+B$	$\xrightarrow{k_2}$	$C+B$
3.	$B+C$	$\xrightarrow{k_3}$	$A+C$

Figure 2. Reaction scheme for problem ROBER.

3.3. ORIGIN OF THE PROBLEM

The ROBER problem describes the kinetics of an auto catalyticreaction given by Robertson (1966) [18]. The structure of thereactions is given in Figure 2, where k_1, k_2 and k_3 are the rate constants and A, B and C are the chemical species involved. Under some idealized conditions [1] and the assumption thatthe mass action law is applied for the rate functions, the following mathematical model consisting of a set of three ODEs can be set up

$$\begin{pmatrix} y'_1 \\ y'_2 \\ y'_3 \end{pmatrix} = \begin{pmatrix} -k_1 y_1 + k_3 y_2 y_3 \\ k_1 y_1 - k_2 y_2^2 - k_3 y_2 y_3 \\ k_2 y_2^2 \end{pmatrix}$$

with $(y_1(0), y_2(0), y_3(0))^T = (y_{01}, y_{02}, y_{03})^T$, where y_1, y_2 and y_3 denote the concentrations of *A, B* and *C,* respectively and y_{01}, y_{02} and y_{03} are the concentrations at time $t = 0$. The ROBER problem is very popular innumerical studies [3] and it is often used as a test problem in the stiff integrators comparisons. The numerical values of the rate constants used in the test problem are $k_1 = 0.04$, $k_2 = 3 \times 10^7$ and $k_3 = 10^4$ and the initial concentrations $y_{01} = 1$, $y_{02} = 0$ and $y_{03} = 0$. The large difference amongthe reaction rate constants is the reason for stiffness. As is typical for problems arising in chemical kinetics this special system has a small very quick initial transient. This phase is followed by a very smooth variation of the components where a large step size would be appropriate for a numerical method.

3.4. NUMERICAL SOLUTION OF THE PROBLEM

The system of ODEs is integrated for $t \in [0, 4000]$. In Figure 3, we present the behavior of the components of the solution over $[0, 10^{11}]$, respectively. The results of the numerical integration of this problem at $x = 0.4$, 40 and 4000 using the new method, MEBDF and those obtained by LSODE taken from Shampine [19] are presented in Table 1, solving with the method of order four and fixed step size $h = 0.001$.

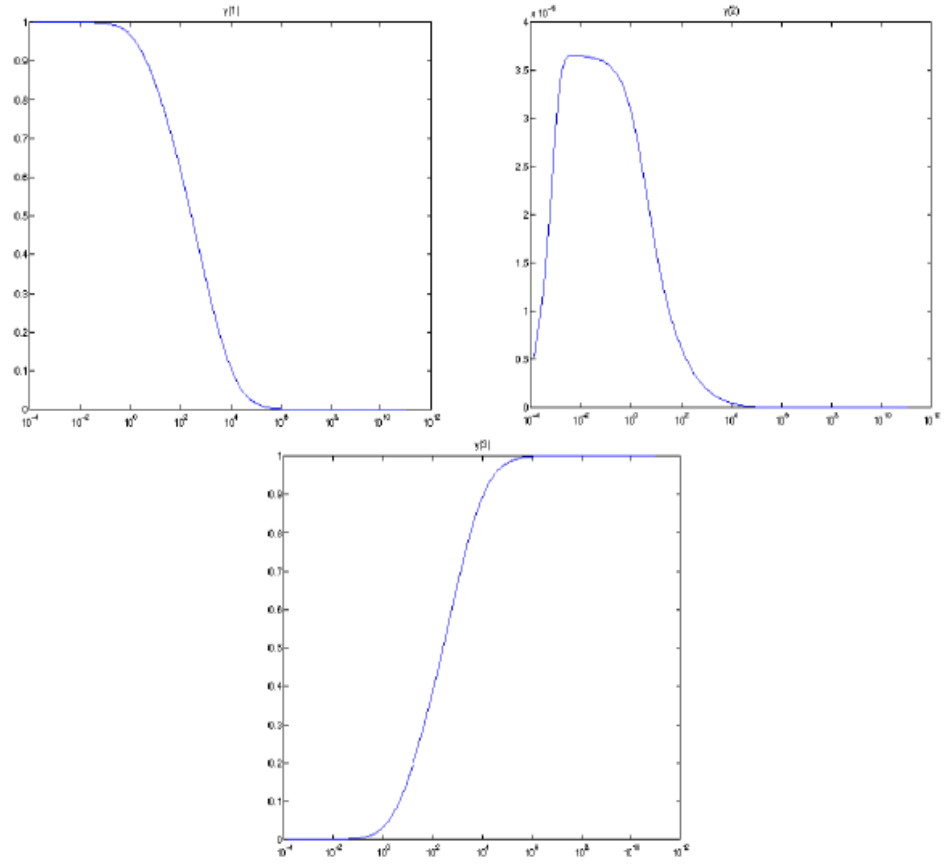

Figure 3. Behavior of the solution on $[0, 10^{11}]$.

Table 1. The results of Example 3.1.

x	y_i	The new method	MEBDF	LSODE
0.4	y_1	9.85172113863231E-1	9.85172113861E-01	9.8517E-01
	y_2	3.38639537890947E-5	3.38639737897E-05	3.3864E-05
	y_3	1.47940221854882E-2	1.47940221854E-02	1.4794E-02
40	y_1	7.15827068718994E-1	7.15827068782E-01	7.1582E-01
	y_2	9.18553476456752E-6	9.18553476564E-06	9.1851E-06
	y_3	2.84163745746361E-1	2.84163745733E-01	2.8417E-01
4000	y_1	1.83202041873152E-1	1.83202281848E-01	1.8320E-01
	y_2	8.94235840002591E-7	9.94237268115E-07	8.9423E-07
	y_3	8.16797063891367E-1	8.16794145152E-01	8.1680E-01

Example 3.2. *The second chemical problem which we consider is*

$$y'_1 = -0.013y_2 - 1000y_1y_2 - 2500y_1y_3,$$

$$y'_2 = -0.013y_2 - 1000y_1y_2,$$
$$y'_3 = -2500y_1y_3,$$

with $y_1(0) = 0, y_2(0) = 1$and $y_3(0) = 1$. This problem was integrated using the (11) and the results obtained at the end point of the range of integration. In Table 2, we list the results obtained for this integration. The true solution was obtained using an explicit fourth order Runge-Kutta method with a very small value of $h = 0.0001$.

Table 2. The results for Example 3.2.

X	y_i	Exact solution	New method	SDMM	MEBDF	LSODE
2.0	y_1	-0.36169E-5	0.3E-14	0.82E-10	0.61E-09	0.47E-7
	y_2	0.99815	0.2E-9	0.61E-05	0.23E-06	0.64E-5
	y_3	1.01849	0.5E-9	0.57E-05	0.18E-06	0.41E-5

Eexample 3.3. *As our next example, consider the Van der Pol's equation*

$$y'_1 = y_2,$$
$$y'_2 = \mu^2\left((1 - y_1^2)y_2 - y_1\right),$$

with initial value $y(0) = (2,0)^T$. In Table 3, we have shown the numerical results by choosing $\mu = 500$.

Table 3. The results for Example 3.3.

x	y_i	The new method	MEBDF	SDMM
1	y_1	-1.865095092042	-1.865095088625	-1.865095087315
	y_2	0.7524845332338	0.7524845321936	0.7524845321726
5	y_1	1.8985234562308	1.8985234559231	1.8985234558247
	y_2	&-0.7289532569877	-0.7289532563817	-0.7289532562558
10	y_1	1.7865365203243	1.7865365202446	1.7865365201649
	y_2	-0.8156276589356	-0.8156276585412	-0.8156276584317
20	y_1	1.5075643289291	1.5075643283014	1.5075643282181
	y_2	-1.1911230034566	-1.1911230029201	-1.1911230027615

4. CONCLUSION

In the present paper we have developed a new k-step hybrid methods for the numerical solution of stiff systems of first order initial value problems arising from chemical reactions such as Robertson problem. For stiff systems, because of the stability condition, the time step restriction becomes severe, especially when they have to be integrated over long periods of time. According to the numerical results and theorems, high order accuracy, wide stability region and low implementation cost of the new hybrid methods make them to be successful in applying on large stiff systems of initial value problems arising from chemical reactions.

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