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A FOURTH ORDER A-STABLE EXPLICIT ONE-STEP METHOD FOR SOLVING STIFF DIFFERENTIAL SYSTEMS ARISING IN CHEMICAL REACTIONS

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Abstract: In this paper, a new A-stable explicit one-step integration method is developed for numerically solving stiff differential systems which characterize several kinds of linear reactions and diffusion from biochemistry, physiology, etc. The method is based on deriving a nonlinear relation between the dependent variable and its derivatives from the well known Taylor expansion. The method can be classified as a rational method. The accuracy and stability properties of the method are investigated and shown to yield at least fourth-order and A-stable. Some differential systems arising in chemical reactions will be solved to illustrate the performance and accuracy of the method.

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1. Introduction

Stiff problem entails rapidly decaying transient solution, which arises naturally

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in wide variety of applications including the study of spring and damping system, the analysis of control system and problems in the chemical kinetics, see [1]. Stiff differential equations also occur in other kind of studies, such as biochemistry, biomedical system, weather prediction, mathematical biology and electronics. In chemical kinetics, stiffness is caused in the vast majority of cases merely by a great difference among the reaction rate constants. This problem is more likely to occur whenever we have a larger system or complicated models. The atmospheric phenomena as an example, involves transport with chemical reaction, thus stiffness can occur because of the time scales of the reactions are much smaller than times for movement over distances. Stiffness in heat transfer originates physically in one of two ways; sharp changes in the thermal environment of large differences in the rates which components of the system can transfer heat, see [2]. There is an equivalence between a subclass of stiff and singularly perturbed differential equations and some numerical methods are developed to treatment stiffness based on singular perturbation theory; see for example (see [12], [13], [14], [15], [16]). The classical fourth order Runge–Kutta (RK4) method and the implicit Adam–Bashforth–Moulton (ABM) predictor–corrector method have been widely used in order to solve the non-stiff problems numerically. If these two methods are used for solving stiff equations, they become very inefficient since the step size is controlled by stability rather than accuracy requirement, see [3]. The implicit methods work well with stiff problems but these methods require more work per step than the explicit methods (see [2], [9]). Although most of the numerical analysts were confident that the implicit methods work better in producing results for stiff problems, the explicit methods which recently was proven; see for example (see [4], [5], [6], [7], [8]); could also satisfy the stiff problems. Many phenomena of interest in physiology and biochemistry are characterized by reactions among several chemical species and diffusion in various mediums (see [10], [11]). In a closed system, both reactions and diffusion are governed by the following system of ordinary differential equations (ODEs)

$$y = My(t) \tag{1.a}$$

which guarantees conservation of the total amount of $y(t)$ for any $t > 0$. The aim of this paper is to present a new absolutely stable explicit one step method for numerically solving linear reaction system(1.a). The method is based on deriving a nonlinear relation between the dependent variable and its derivatives from the well known Taylor expansion. The method can be classified as a rational method. The accuracy and stability properties of the method are investigated and shown to yield at least fourth-order and A-stable. Some dif-

ferential systems will be solved to illustrate the performance and accuracy of the method.

2. Construction of the New Method

Consider the following system of ODEs

$$y' = f(y) = My(t),\ y(0) = y_0,\ t \in [0,b] \subset \mathbb{R},\ y(t) \in \mathbb{R}^n,\ M \in \mathbb{R}^{n\ x\ n} \quad (1.b)$$

The interval$[0,b]$ is divided into a number of subintervals$[t_j, t_{j+1}]$ with $t_0 = 0$ and $t_j = jh,\ j = 1,2,...,$ such that h is the step size. Suppose that we have solved numerically the IVP (1.b) up to a point t_j and have obtained a value y_j as an approximation of $y(t_j)$. Furthermore we are interested in obtaining y_{j+1}as an approximation of $y(t_{j+1})$. For that purpose, consider Taylor's expansions of y_{j+1} and y_{j-1}about t_j as follows

$$\Delta_{j+1} \equiv y_{j+1} - y_j = hy'_j + \frac{h^2}{2}y''_j + \frac{h^3}{6}y'''_j + \frac{h^4}{24}y^{(4)}_j + .. \quad (2)$$

$$\Delta_j \equiv y_j\ - y_{j-1} = hy'_j - \frac{h^2}{2}y''_j + \frac{h^3}{6}y'''_j - \frac{h^4}{24}y^{(4)} + ... \quad (3)$$

From(2) and(3) we have

$$\Delta_{j+1}\Delta_j \approx h^2(y'_j)^2 +\ h^4\left(\frac{1}{3}y'_j y'''_j - \frac{1}{4}(y''_j)^2\right) + O(h^6) \quad (4)$$

and from(2) and (4) we have the nonlinear relation

$$\Delta_{j+1} \cong \frac{h^2(y'_j)^2 +\ h^4\left(\frac{1}{3}y'_j y'''_j - \frac{1}{4}(y''_j)^2\right) + O(h^6)}{hy'_j - \frac{h^2}{2}y''_j + \frac{h^3}{6}y'''_j - \frac{h^4}{24}y^{(4)}_j + O(h^5)} \quad (5)$$

From (5) the numerical scheme is readily obtained, and can be written in the form

$$y_{j+1} = y_j + \frac{24h\ (y'_j)^2 + h^3\ \left(8y'_j\ y'''_j - 6(y''_j)^2\right)}{24y'_j - 12h\ y''_j + 4h^2y'''_j - h^3y^{(4)}_j} \quad (6)$$

or simply

$$y_{j+1} = y_j + \frac{24h\ (f_j)^2 + h^3\ \left(\ 8\ f_j\ f''_j - 6\ (\ f'_j)^2\ \right)}{24\,f_j - 12h\,f'_j + 4\,h^2\,f''_j - h^3\,f'''_j} \quad (7)$$

where $f_j = M\,y_j,\ f'_j = M\,f_j, f''_j = M\,f'_j, f'''_j = M\,f''_j$, and $24f_j - 12hf'_j + 4h^2f''_j - h^3f'''_j \neq 0$.

2.1. Local Truncation Error

Consider the functional given by

$$\ell(z(t),h) = z(t+h) - z(t) - \frac{24h\ z'(t)^2 + h^3\ \left(8z'(t)z'''(t) - 6z''(t)^2\right)}{24z'(t) - 12hz''(t) + 4h^2z'''(t) + h^3z^{(4)}(t)} \quad (8)$$

where $z(t)$ is an arbitrary function defined on$[0,b]$;and differentiable as often as we need, after expanding in Taylor series about t and collecting terms in h we obtain

$$\ell(z(x),h) = \frac{1}{15}\left(\frac{3z(t)z^{(5)}(t) - 15\,z''(t)z^{(4)}(t) + 10z'''(t)^2}{24z'(t) - 12hz''(t) + 4h^2z'''(t) - h^3z^{(4)}(t)}\right)h^5 + O(h^6) \quad (9)$$

which means that the method has at least fourth order of accuracy. The local truncation error of the method may be written as

$$T_{j+1} = \frac{1}{15}\left(\frac{3y_j'y_j^{(5)} - 15y_j''y_j^{(4)} + 10(y_j''')^2}{24y_j' - 12hy_j'' + 4h^2y_j''' - h^3y_j^{(4)}}\right)h^5 + O(h^6) \quad (10)$$

2.2. Consistency and Stability

Subtracting y_j from both sides of (6) and dividing the result by h, leads to

$$\frac{y_{j+1} - y_j}{h} = \frac{24(y_j')^2 + h^2\ \left(8y_j'y_j''' - 6(y_j'')^2\right)}{24y_j' - 12hy_j'' + 4h^2y_j''' - h^3y_j^{(4)}}, \quad y_j' \neq 0 \quad (11)$$

Taking limit as h tends to zero, on both sides of (11), we have

$$\lim_{h\to 0}\left(\frac{y_{j+1} - y_j}{h}\right) = y_j' = f(y_j). \quad (12)$$

Suggesting that the scheme defined by(6) is consistent.

In order to examine the present method for the stability, let us consider the differential equation,

$$y' = \lambda y$$

where$\lambda$is a complex constant and $Re\ (\lambda) < 0$. For this equation, Eq(6) can be rewritten as

$$y_{j+1} = \frac{6 + 3(h\lambda) + (h\lambda)^2/2 + (h\lambda)^3/4}{6 - 3(h\lambda) + (h\lambda)^2/2 + (h\lambda)^3/4}y_j \quad (13)$$

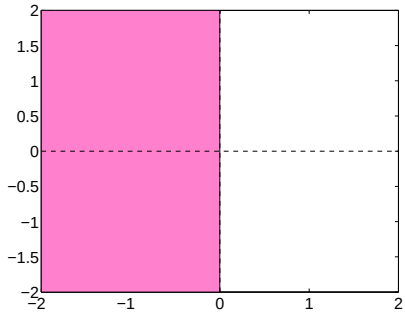

Figure 1: 2D stability region for the present method

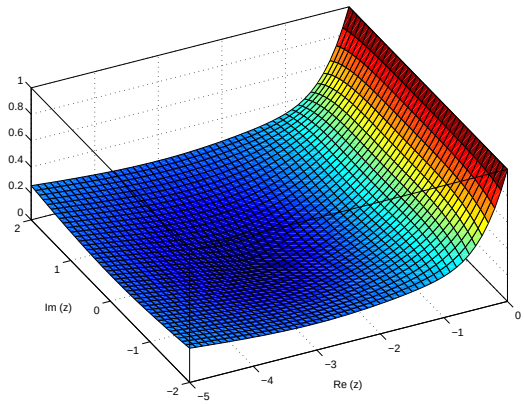

Figure 2: 3D stability region for the present method

Setting $z = \lambda h$ in the above equation, the amplification factor is therefore

$$R(z) = \frac{24 + 12z + 4z^2 + z^3}{24 - 12z + 4z^2 - z^3} \tag{14}$$

which has modulus less than one on the left-half complex plane, and thus the method is A-stable, see [5].

Using MATLAB we plot the stability region for the method and the region as given in Figure 1and Figure 2.

3. Numerical Results

In this section, we present numerical results which verify the theoretical results in the previous sections. Figure 3 describes a circular reaction with 3

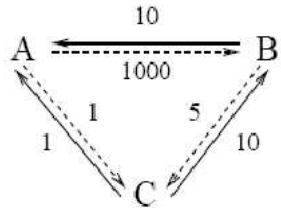

Figure 3: A circular reaction

substances$A$, B , C with initial values $A(0) = 1$, $B(0) = 2$ and $C(0) = 3$. The system of ODEs is as follows:

$$\frac{d}{dt}\begin{bmatrix} A(t) \\ B(t) \\ C(t) \end{bmatrix} = \begin{bmatrix} -1001 & 10 & 1 \\ 1000 & -15 & 10 \\ 1 & 5 & -11 \end{bmatrix} \begin{bmatrix} A(t) \\ B(t) \\ C(t) \end{bmatrix} = M \begin{bmatrix} A(t) \\ B(t) \\ C(t) \end{bmatrix} \quad (15)$$

For the stiff system(15), the drawback of explicit methods is more severe, where Euler's method for(15) is stable only if $h \leq 1.9782E - 03$, and RK4 method for(15) is stable only if $h \leq 2.9531E - 03$.

The problem has been integrated on the interval [0, 3] and the results are presented in Table 1 for different step size, h. The errors have been defined as the maximum of the absolute errors on the nodal points in the integration interval.

$$E_{\max} = \|\mathbf{y}(t_j) - \mathbf{y}_j\|_1$$

	Fourth order RK4 Method	New method
h		
1/128	-	5.8754e-001
1/256	-	1.3065e-001
1/512	1.8107e-001	2.2538e-002
1/1024	6.5021e-003	1.8633e-003
1/2048	2.6754e-004	1.1713e-004

Table 1: Maximum absolute errors for stiff system (15)

In Table 1, the maximum absolute errors generated by classical Rung-Kutta method show us that the numerical solutions do not approximate the true solutions of the stiff system correctly using 1/256 integration step size. We insert 2

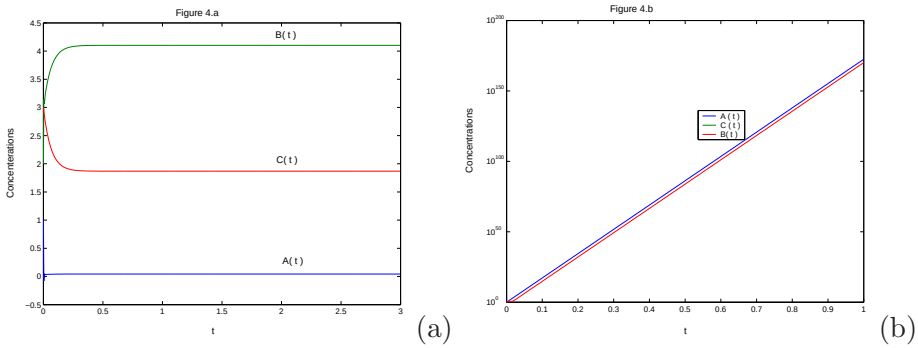

Figure 4: Stable solutions obtained using the present method (**a**) and the unstable solutions using RK4 method (**b**) at $h = 1/256$

dashes (-) to indicate this phenomenon. This is because RK4 method is not A-stable methods, which cause it to suffer some stability restrictions. Obviously, 1/256 integration step size is not enough to meet the stability restrictions. Therefore, there is a need to increase the number of integration steps in order to obtain the accurate numerical solutions while the new method performs better even for small size of step size.

Next, we consider the conserved system

$$\frac{d}{dt}\begin{bmatrix} A(t) \\ B(t) \\ C(t) \end{bmatrix} = \begin{bmatrix} -10 & 0.5 & 0 \\ 1 & -1 & 0 \\ 9 & 0.5 & 0 \end{bmatrix} \begin{bmatrix} A(t) \\ B(t) \\ C(t) \end{bmatrix} \tag{16}$$

where $A(0) = 1$and $B(0) = 10$ and $C(0) = 0$. The problem has been integrated on the interval [0, 10] and the results are presented in Table 2.

h	$E_{\max}$	order
1/8	5.8564e-003	
1/16	4.0824e-004	3.8425
1/32	2.6646e-005	3.9374
1/64	1.6957e-006	3.9374
1/128	1.0683e-007	3.9885
1/256	6.7019e-009	3.9946
1/512	4.1961e-010	3.9974
1/1024	2.6292e-011	3.9974

Table 2: Numerical results for system (15)

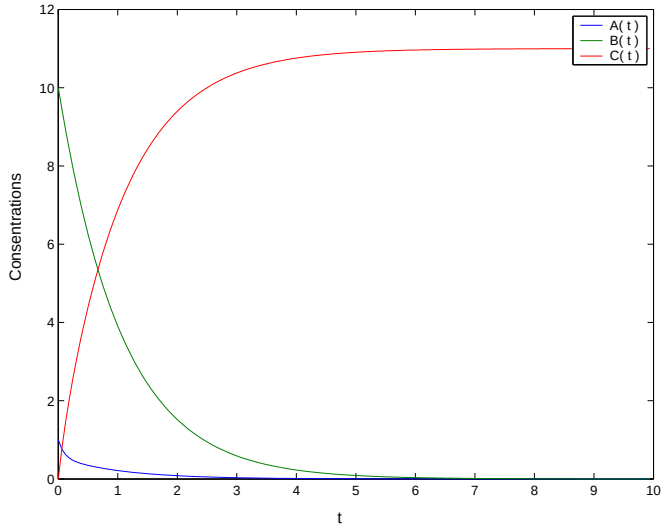

Figure 5: Stable solutions of (16) using the present method at $h = 1/8$.

4. Conclusion

We have proposed a new fourth order one-step explicit method for numerically solving stiff differential systems characterizing several kinds of linear reactions and diffusion from biochemistry, physiology, etc. Unlike most of explicit methods, the new method is absolutely stable in spite of its explicitness. In addition to the method is of high order allowing large step sizes with stiff systems. The method can be classified as a rational method. We have applied the method on two stiff systems arising in chemical reactions and presented the numerical results in tables and figures. It can be observed that the numerical results verify the theoretical ones and the present method approximates the solution very well.

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