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An Adaptive Step-Size Taylor Series Based Method and Application to Nonlinear Biochemical Reaction Model

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ABSTRACT

In this study, a Taylor series based method, which is the multi-step Differential Transform Method (DTM), is adapted to define a new adaptive step-size semi-analytical and numerical method. This new approach is applied to a nonlinear biochemical reaction model to obtain approximate analytical solutions in the form of piecewise convergent series with easily computable components. The numerical results obtained by using the present method are compared to those obtained by using the classical DTM, classical multi-step DTM and Runge-Kutta method. The present method gives a more accurate approximation with less computational effort than fixed step-size methods.

Key words: Taylor series, differential transformation method, adaptive algorithms, biochemical reaction models

INTRODUCTION

Nonlinear differential equations appear in mathematical models for many problems in applied science and engineering, especially in fluid mechanics, chemical engineering, biochemistry, solid state physics, plasma waves, optimal control, etc. Most of these real-life problems are still difficult to solve either analytically or numerically. Recently, numerical methods, which do not require discretization of space-time variables, perturbation or linearization, are introduced for finding analytical solutions of nonlinear problems. Differential Transform Method (DTM) is one of the most effective, convenient and accurate methods for both weakly and strongly nonlinear problems. DTM is a semi analytical-numerical method for solving a wide variety of differential equations and provides the solution in terms of Taylor series. There are also other methods based on Taylor series expansion such as Restricted Taylor series method (Gulsu and Ozis, 2005; Ismail *et al*., 2005) and Adomian decomposition method (Sen, 1988; Wazwaz, 1998; Hashim *et al*., 2006; El-Wakil and Abdou, 2007; Khalifa *et al*., 2008; Siddiqui *et al*., 2010). But DTM formulizes the Taylor series in a totally different manner. With this method, the given differential equation and related boundary conditions are transformed into a recurrence relation which leads to the solution of a system of algebraic equations as coefficients of a power series solution and is easily carried out in computer. Because of this property, the method is no need of linearization of the nonlinear problems and as a result avoids the large computational works and the round-off errors. Different applications of DTM can be found by Jang *et al*. (2000), Koksal and Herdem (2002),

Abdel-Halim Hassan (2002, 2008a, b), Ayaz (2004a, b), Arikoglu and Ozkol (2006), Liu and Song (2007), Momani and Odibat (2007), Chu and Chen (2008), El-Shahed (2008), Momani and Erturk (2008), Odibat (2008), Ravi Kanth and Aruna (2009), Kuo and Lo (2009), Al-Sawalha and Noorani (2009a, b), Ebaid (2010), Thongmoon and Pusjuso (2010), Kurulay and Bayram (2010), Alomari (2011), Demirdag and Yesilce (2011) Gupta (2011), Biazar *et al.* (2012) and Gokdogan *et al.* (2012a). Even if DTM is an effective tool for solving several linear and nonlinear problems arising in science and engineering, it also has some drawbacks. Since DTM gives a truncated Taylor series solution, it does not exhibit a good approximation in a large domain. To overcome the shortcoming, the multi-step DTM (MsDTM) was presented by Odibat *et al.* (2010), Keimanesh *et al.* (2011) Gokdogan *et al.* (2012b), Yildirim *et al.* (2012) and El-Zahar (2012) and succeeded in obtaining reliable approximate solutions for many problems. MsDTM is a reliable modification of DTM that provides the solution in terms of convergent series over a sequence of equal-length sub-intervals. However, for some important classes of problems and for the sake of accuracy and efficiency, it is necessary to allow variable-length step-size to be used (Lopeza *et al.*, 1997; Kobeissia and Kobeissia, 1988; Antohe and Gladwell, 2004; Celik Kizilkan and Aydin, 2006; Habib and El-Zahar, 2008 and Gu *et al.*,2011). In practical implementation of a numerical method for the solution of differential equations the use of variable-length step-size is a crucial point because it permits us to automatize the control of the error. Therefore, in this study, we adapted MsDTM to define a new adaptive step-size semi-analytical and numerical method. This new approach is applied directly to a nonlinear biochemical reaction model, without requiring linearization or perturbation and the analytical-numerical solutions of our model are obtained using piecewise convergent series with easily computable components over a sequence of variable-length sub-intervals. Then, a comparison between the present method, classical DTM, classical multi-step DTM and the Runge-Kutta method is presented. The present method gives a more accurate approximation with less computational effort than fixed step-size methods. The results demonstrate reliability and efficiency of the method developed for solving the considered problems.

BASIC CONCEPTS OF MULTI-STEP DIFFERENTIAL TRANSFORM METHOD

The MsDTM that has been developed for the analytical solution of the ODEs presented in this section for the systems of ODEs. For this purpose, we consider the following initial value problem for systems of ODEs:

$$\begin{aligned} x_1'(t) &= f_1(t, x_1, x_2, ..., x_n) \\ x_2'(t) &= f_2(t, x_1, x_2, ..., x_n) \\ &\vdots \\ x_n'(t) &= f_n(t, x_1, x_2, ..., x_n) \end{aligned} \tag{1}$$

subject to the initial conditions:

$$x_i(t_0) = c_i, \quad i = 1, 2, ..., n \tag{2}$$

Let $[t_0, T]$ be the interval over which we want to find the solution of the initial value problem Eq. (1-2). In actual applications of the DTM, the Nth-order approximate solution of the initial value problem (Eq. 1-2) can be expressed by the finite series:

$$x_i(t) = \sum_{k=0}^{N} X_i(k)(t-t_0)^k, \quad t \in [t_0, T], i = 1, 2, ..., n \tag{3}$$

where:

$$X_i(k) = \frac{1}{k!}\left[\frac{d^k x_i(t)}{dt^k}\right]_{t=t_0}, i = 1, 2, ..., n \tag{4}$$

Equations 3 and 4 imply that the concept of differential transformation is derived from the Taylor series expansion. From the basic definition of the differential transformation, one can obtain certain laws of transformational operations, some of these, are listed in Table 1. Using some fundamental operations of DTM, we have the following recurrence relation:

$$(k+1)X_i(k+1) = F_i(k, X_1, X_2, ..., X_n), X_i(0) = c_i, i = 1, 2, ..., n \tag{5}$$

where, $F_i(k, X_1, X_2, ..., X_n)$ is the differential transform of the function $f_i(t, x_1, x_2, ..., x_n)$ for i = 1, 2, ..., n.

The differential transform $X_i(k)$ of the unknown functions $x_i(t)$ can be obtained by solving the iterating algebraic system (Eq. 5). In order to speed up the convergence rate and to improve the accuracy of resulting solutions, the entire domain $[t_0, T]$ is usually split into sub-intervals and the algorithm of MsDTM is applied as follows:

Assume that the interval $[t_0, T]$ is divided into M sub-intervals $[t_{m-1}, t_m]$, m = 1, 2, ..., M of equal step-size $h = (T-t_0)/M$ by using the nodes $t_m = t_0+mh$. The main ideas of the MsDTM are as follows:

First, we apply the DTM to the initial value problem (Eq. 1-2) over the interval $[t_0, t_1]$, we will obtain the following approximate solution:

$$x_{i,1}(t) = \sum_{k=0}^{N} X_{i,1}(k)(t-t_0)^k \quad t \in [t_0, t_1] \tag{6}$$

Table 1: Fundamental operations of differential transform method

Original function	Transformed function
$x(t) = \beta(u(t) \pm v(t))$	$X(k) = \beta U(k) \pm \beta V(k)$
$x(t) = u(t)\,v(t)$	$X(k) = \sum_{\ell=0}^{k} U(\ell)V(k-\ell)$
$x(t) = \frac{d^m u(t)}{dt^m}$	$X(k) = \frac{(k+m)!}{k!}U(k+m)$
$x(t) = (\beta+t)^m$	$X(k) = \begin{cases} 1 & , \text{if } k = m \\ \frac{m!}{k!(m-k)!}(\beta+t_0)^{m-k} & , \text{if } k < m \\ 0 & , \text{if } k > m \end{cases}$
$x(t) = e^{\lambda t}$	$X(k) = \frac{\lambda^k}{k!}e^{\lambda t_0}$
$x(t) = \sin(\omega t+\beta)$	$X(k) = \frac{\omega^k}{k!}\sin(\omega t_0+\beta+\frac{k\pi}{2})$
$x(t) = \cos(\omega t+\beta)$	$X(k) = \frac{\omega^k}{k!}\cos(\omega t_0+\beta+\frac{k\pi}{2})$

using the initial conditions $x_i(t_0) = c_i$. For $m \geq 2$ and at each sub-interval $[t_{m-1}, t_m]$, we will use the initial conditions $x_{i,m}(t_{m-1}) = x_{i,m-1}(t_{m-1})$ and apply the DTM to the initial value problem (Eq. 1-2) over the interval $[t_{m-1}, t_m]$. The process is repeated and generates a sequence of the approximate solutions $x_{i,m}(t)$, m = 1,....., M, i = 1, 2, ..., n for the solutions $x_i(t)$:

$$x_{i,m}(t) = \sum_{k=0}^{N} X_{i,m}(k)(t - t_{m-1})^k \quad t \in [t_{m-1}, t_m] \tag{7}$$

Finally, the MsDTM assumes the following solution:

$$x_i(t) = \begin{cases} x_{i,1}(t) & , \quad t \in [t_0, t_1], \\ x_{i,2}(t) & , \quad t \in [t_1, t_2], \\ \vdots & \\ x_{i,M}(t) & , \quad t \in [t_{M-1}, t_M]. \end{cases} \quad ,i = 1, 2, ..., n \tag{8}$$

ADAPTIVE STEP-SIZE ERROR CONTROL ALGORITHM

Here, we present an adaptive step-size error control algorithm based on discussing some properties of the MsDTM.

MsDTM has several advantageous properties over the widely used classical methods. One of the advantages of the MsDTM is that the approximate solution is given as a piecewise polynomial function defined on the sub-intervals of the whole interval and the local error of this solution, at the interior points of the sub-interval, is less than that one at the end point. This property offers a different facility for adaptive error control. Another advantage of the MsDTM is that the truncated Taylor's series solution is obtained in explicit form in every sub-interval. This property facilitates to investigate several properties of the approximate solution such as the local error of approximate solution for each component because the main term of the local error is known in the form of $|X_{i,m}(N)|\tau^N$ where τ is the local time variable in a sub-interval $[t_m, t]$. The series term $|X_{i,m}(N)|\tau^N$ can be viewed as a local error estimate for the series of degree N-1, which is then applied to the more accurate series of degree N. Generally, the local error should not be calculated from the next series term, $|X_{i,m}(N+1)\tau^{N+1}$, due to the extra computation required and the fact that it is not a reliable error estimate (Corliss and Lowery, 1977).

So without any further calculation one can estimate the admissible step-size to ensure the prescribed local error by use just one coefficient of our obtained series solution. Using this technique while we apply MsDTM we get an automatic step-size control algorithm too. One simple step-size control algorithm could be the following.

- One gives the admissible local error $\delta > 0$ and chooses the order N of the MsDTM
- From calculation, the values $|X_{i,m}(N)|$ i = 1, 2,...,n, are known for every solution component i
- At the grid point t_m we calculate the value $E_N = \max(|X_{i,m}(N)|)$, i = 1, 2, ..., n
- We select such step-size h_m for which $h_m = (\delta/E_N)^{1/(N)}$ and $t_{m+1} = t_m + h_m$

Another step-size selection may be just to use the last two coefficients of our series solution instead of only one, as mentioned above and imposing that both sets of coefficients are lower than the admissible local error that is:

$$h_m = \min\left(\left(\frac{\delta}{\mathbf{E}_{N-1}}\right)^{1/(N-1)}, \left(\frac{\delta}{\mathbf{E}_N}\right)^{1/(N)}\right) \tag{9}$$

The step selection methods above performed very similarly in the current study. Both methods provided stable, accurate solutions and used approximately the same number of time steps in head-to-head calculations.

We can conclude that for the present step-size control algorithm, there is no need for further calculations contrary to the Richardson extrapolation or embedded R-K algorithms. We have to remark that the step size control by Richardson extrapolation require 12 further function evaluation for a fourth order Rung-Kutta method. Also, there is no rejected step as occurs in any variable step formulation for Rung-Kutta or multistep methods because we choose the step-size once the series approximations are generated in order to obtain a required precision level.

Now, the present adaptive step-size error control algorithm is applied with MsDTM to obtain approximate analytical-numerical solutions of a nonlinear biochemical reaction system. We call this technique as adaptive step-size multi-step DTM (AsDTM).

APPLICATION TO NONLINEAR BIOCHEMICAL REACTION MODEL

Consider the well-known Michaelis–Menten biochemical reaction model (Schnell and Mendoza, 1997), i.e., the single enzyme substrate reaction scheme:

$$E + A \rightleftharpoons Y \rightarrow E + X \tag{10}$$

where, E is the enzyme, A the substrate, Y the intermediate complex and X the product. The time evolution of scheme (10) can be determined from the solution of the system of coupled nonlinear ODEs (Sen, 1988):

$$\begin{aligned}
\frac{dA}{dt} &= -k_1 E A + k_{-1} Y,\\
\frac{dE}{dt} &= -k_1 E A + (k_{-1} + k_2) Y,\\
\frac{dY}{dt} &= k_1 E A - (k_{-1} + k_2) Y,\\
\frac{dX}{dt} &= k_2 Y,
\end{aligned} \tag{11}$$

subject to the initial conditions:

$$A(0) = A_0,\ E(0) = E_0,\ Y(0) = 0,\ X(0) = 0 \tag{12}$$

where, the parameters k_1, k_{-1} and k_2 are positive rate constants for each reaction. Systems (Eq. 10-12) can be reduced to only two equations for A and Y. And in dimensionless form of concentrations of substrate, x and intermediate complex between enzyme and substrate, y, are given by Sen (1988):

$$\begin{aligned}\frac{dx}{dt} &= -x + (\beta-\alpha)y + xy\\ \frac{dy}{dt} &= \frac{1}{\varepsilon}(x - \beta y - xy)\end{aligned} \tag{13}$$

subject to the initial conditions x(0) = 1 and y(0) = 0, where α, β and ε are dimensionless parameters. For small value of ε, Eq. 13 becomes much stiffer or singularly perturbed and requires special numerical treatments to solve it (El-Zahar and E-Kabeir, 2013). By using the fundamental operations of DTM in Table 1, we obtained the following recurrence relation to the Eq. 13:

$$\begin{aligned}&X_m(k+1)=\left(-X_m(k)+(\beta-\alpha)\,Y_m(k)+\sum_{\ell=0}^{k}X_m(\ell)X_m(k-\ell)\right)\Big/(k+1)\\ &Y_m(k+1)=\left(X_m(k)-\beta Y_m(k)-\sum_{\ell=0}^{k}X_m(\ell)X_m(k-\ell)\right)\Big/(\varepsilon k+\varepsilon)\\ &X_0(0)=1,\quad Y_0(0)=0,\quad X_m(0)=x_{m-1}(t_m),\quad Y_m(0)=y_{m-1}(t_m),\qquad m=1,2,.....\end{aligned} \tag{14}$$

The approximate solutions of the system (13) for ε = 0.1, α = 0.375, β = 1.0 and tϵ[0.0, 0.4], using the AsDTM with N = 6 and δ = 0.001 are given as follows:

$$x(t)=\begin{cases}1-t+8.625t^2-63.083t^3+373.18t^4-1979.4t^5+10156\,t^6, & t\in[0.0,0.0453],\\ 0.96783-0.50115(t-0.0453)+3.2934(t-0.0453)^2-22.811(t-0.0453)^3\\ +123.18(t-0.0453)^4-565.27(t-0.0453)^5+2375.4(t-0.0453)^6, & t\in[0.0453,0.1027],\\ 0.94667-0.2794(t-0.1027)+1.0249(t-0.1027)^2-6.8583(t-0.1027)^3\\ +35.256(t-0.1027)^4-148.61(t-0.1027)^5+544.13(t-0.1027)^6, & t\in[0.1027,0.1757],\\ 0.92983-0.20069(t-0.1757)+0.24633(t-0.1757)^2-1.5782(t-0.1757)^3\\ +7.9295(t-0.1757)^4-32.172(t-0.1757)^5+110.33(t-0.1757)^6, & t\in[0.1757,0.2708],\\ 0.91209-0.17906(t-0.2708)+0.048537(t-0.2708)^2-0.25941(t-0.2708)^3\\ +1.2878(t-0.2708)^4-5.1375(t-0.2708)^5+17.183(t-0.2708)^6, & t\in[0.2708,\ 0.4000].\end{cases}$$

$$y(t)=\begin{cases}10.0t-105.0t^2+762.08t^3-4446.2t^4+23128t^5-1.1602E5\ t^6, & t\in[0,0.0453],\\ 0.29298+3.9128(t-0.0453)-40.271(t-0.0453)^2+278.45(t-0.0453)^3\\ -1492.8(t-0.0453)^4+6772.3(t-0.0453)^5-27987(t-0.0453)^6, & t\in[0.0453,0.1027],\\ 0.42456+1.2019(t-0.1027)-12.502(t-0.1027)^2+84.210(t-0.1027)^3\\ -431.50(t-0.1027)^4+1809.7(t-0.1027)^5-6572.4(t-0.1027)^6, & t\in[0.1027,0.1757],\\ 0.46895(t-0.1757)+\ 0.24832(t-0.1757)^2-2.9289(t-0.1757)^3+19.443(t-0.1757)^3\\ -97.523(t-0.1757)^4+394.86(t-0.1757)^5-1350.1(t-0.1757)^6, & t\in[0.1757,0.2708],\\ 0.47690-0.0022168(t-0.2708)-0.48952(t-0.2708)^2+3.2060(t-0.2708)^3\\ -15.884(t-0.2708)^4+63.288(t-0.2708)^5-211.38(t-0.2708)^6, & t\in[0.2708,\ 0.4000].\end{cases}$$

Figure 1 shows the obtained solutions of (13) for ε = 0.1, α = 0.375, β = 1.0 over a narrow region, t ϵ[0, 0.4], containing the boundary layer region, using DTM, MsDTM (N = 6, h = 0.1), AsDTM (N = 6, δ = 0.001) and RK4 (h = 0.00001). We can see in Fig. 1 that the solutions obtained by DTM have a small interval of convergence and deviates much from AsDTM solution and the numerical RK4 solution, while the solutions obtained by AsDTM have wide intervals of convergence and agree

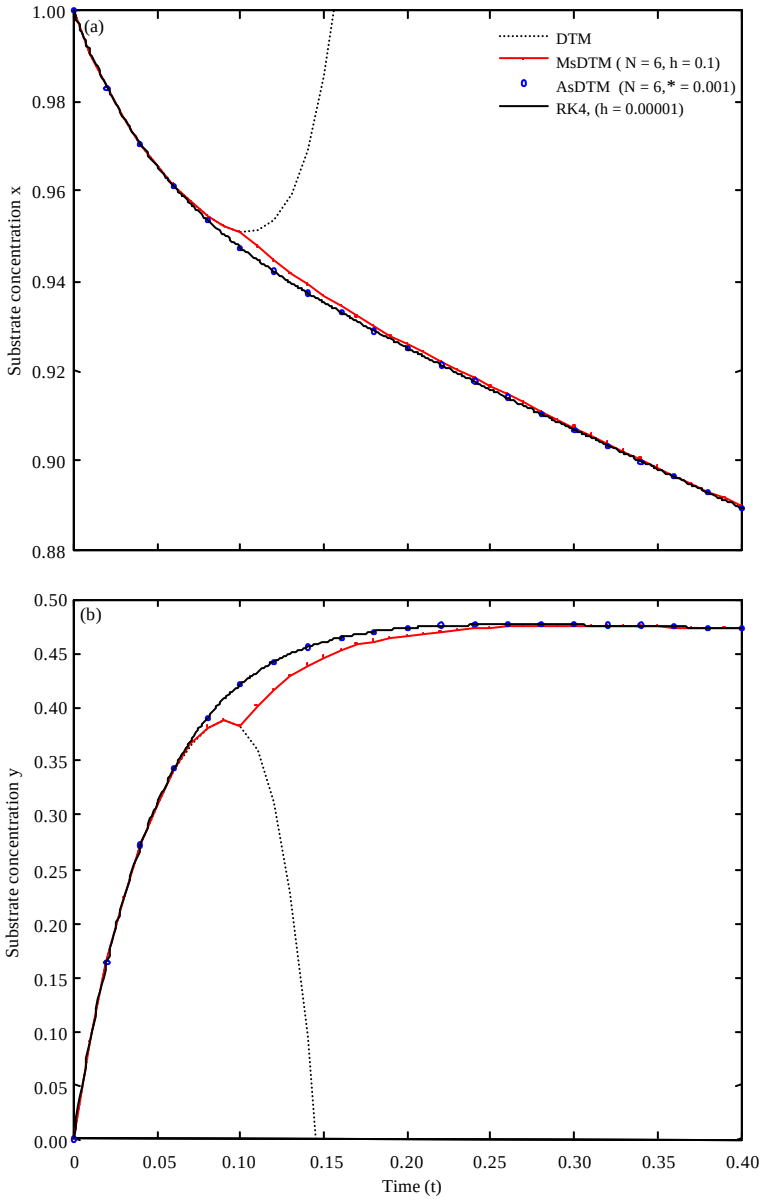

Fig. 1a-b: Comparison of the solutions of (a) substrate x and (b) substrate y, obtained by the DTM, MsDTM, AsDTM and RK4 method

very well with RK4 solution. For the solutions obtained by MsDTM, the step size h = 0.1 is not sufficient to approximate the solution over the boundary layer region where MsDTM needs step size h<0.0453 to achieve the given admissible local error δ.

Figure 2 shows the obtained solutions of Eq. 13 using the AsDTM (N = 6, δ = 0.001) and the RK4 (h = 0.00001) for $t \in [0, 5.0]$. We can observe the high agreement between the solution obtained using the AsDTM and the one obtained using RK4 over a large interval.

The results obtained and shown in Fig. 1 and 2 confirm that the new approach, AsDTM, increases the interval of convergence for the series solution.

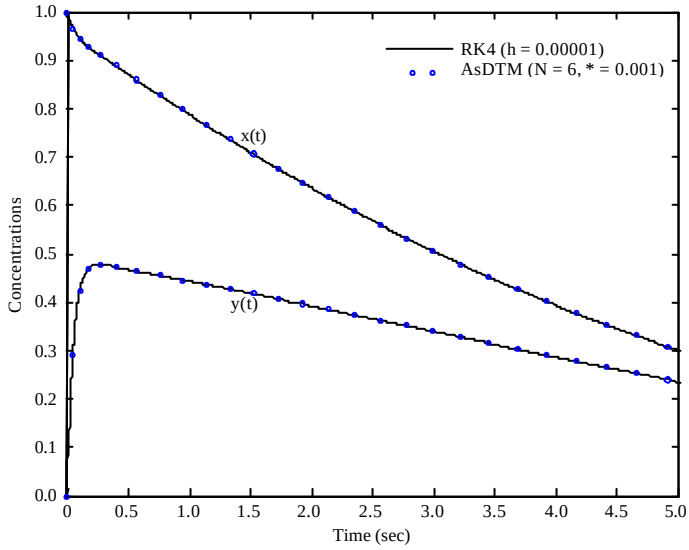

Fig. 2: Approximate solutions of the Eq. 13 by AsDTM and RK4 method

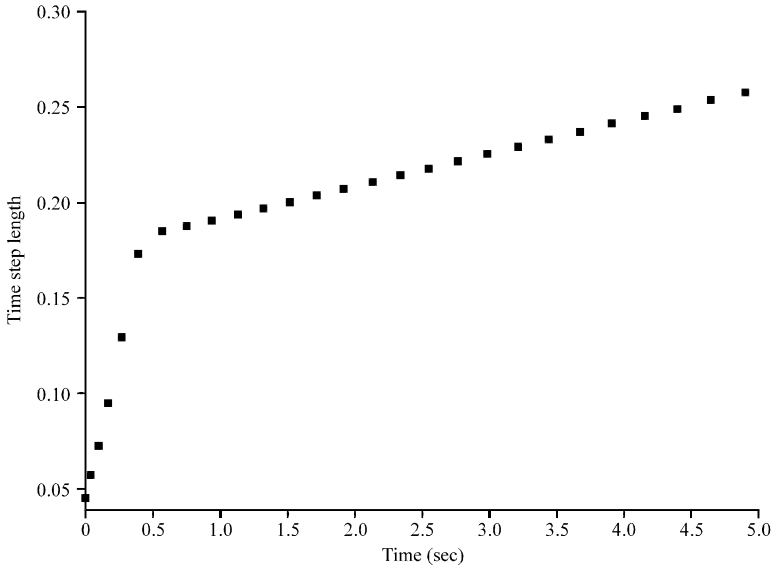

Fig. 3: Time-step length used by AsDTM in solution of Eq. 13

Figure 3 shows the time-step length used for solving Eq. 13 by the AsDTM. We can observe that the given admissible local error $\delta = 0.001$, is achieved by the AsDTM using 27 time-step, while the MsDTM needs step size $h<0.0453$ to achieve the given admissible local error δ and consequently needs at least 111 time-step.

The difference between the AsDTM solutions and the numerical RK4 solutions are given in Fig. 4 for different values of ε and δ where, $E_y(t) | y(t)-y_{RK4} |$ and $E_x(t) | x(t)-x_{RK4} |$. We can observe that the solutions obtained using the AsDTM and the RK4 method are in high agreement for different values of ε and δ.

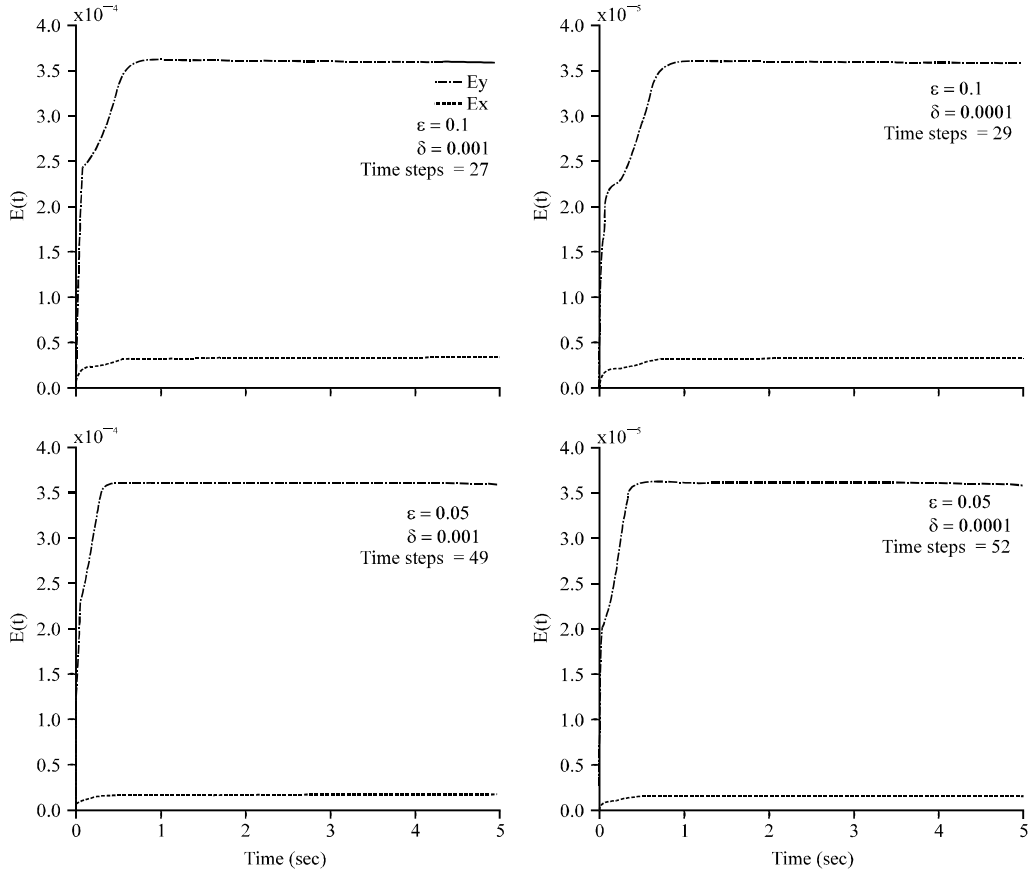

Fig. 4: Difference between the AsDTM solutions and numerical RK4 solutions at different values of ε and δ

Table 2: Comparison of processing time and time-step at different values of δ and ε

		MsDTM		AsDTM	
ε	δ	Time-step	Processing time (sec)	Time-step	Processing time (sec)
0.1	0.0010	111	0.0799	27	0.0131
	0.0001	163	0.0811	29	0.0131
0.05	0.0010	207	1.0503	49	0.0210
	0.0001	303	1.2450	52	0.0211

Table 2 presents a comparison of processing time and time-step used in solving the system (13) by MsDTM and AsDTM to achieve a specific tolerance, δ, for different values of ε, where all calculations are carried out by MAPLE 14 software in a PC with a Pentium 2 GHz and 512 MB of RAM. We can observe that the AsDTM is a fast and effective tool for solving the considered problems using fewer time steps.

CONCLUSION

In this study, we adapted the multi-step DTM to define a new adaptive step-size semi-analytical and numerical method. This new approach provides analytical solutions in the form of piecewise convergent series with easily computable components over a sequence of variable-length

sub-intervals. This approach is simple in applicability as it does not require linearization or perturbation like other numerical and approximate methods. We have applied it to the well-known Michaelis-Menten nonlinear biochemical reaction system and the obtained piecewise series solutions are presented. Numerical results are presented in figures and tables at different values of the tolerance δ and the perturbation parameter ε. The results confirm that the proposed method is a very accurate and efficient method compared with classical DTM, classical MsDTM, and RK4 method. The method works successfully in handling the biochemical reaction system with a minimum size of computations and a wide interval of convergence for the series solutions. This emphasizes the fact that the present method is applicable to many other nonlinear systems and it is reliable and promising when compared with the existing methods.

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