

## A reliable non-standard finite difference scheme for solving nonlinear biochemical reaction model

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**Abstract.** In this paper, we present an efficient and accurate numerical scheme for the solution of a model biochemical reaction. The non-standard finite difference scheme based on Adomian decomposition method does not need to linearized or non-locally linearized for the nonlinear term of differential equation. The decomposition method is adopted to construct the numerical solutions. The results demonstrate reliability and efficiency of the algorithm developed.

**Keywords:** non-standard finite difference schemes, Adomian decomposition method, Biochemical reaction model.

### 1. Introduction

In recent times, the non-standard finite difference schemes by Mickens [1, 2, 3, 4, 5, 6] (in short NSFD) has developed as an alternative method for solving a wide range of problems whose mathematical models involve algebraic, differential, biological models, chaotic systems [5]. The technique has many advantages over the classical techniques [16], and provides an efficient numerical solution.

The well-known Michalis-Menten biochemical reaction model [14]



where  $E$  is the enzyme,  $A$  the substrate,  $Y$  the intermediate complex and  $X$  the product. The time evolution of scheme 26 can be determined from the solution

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of the system of coupled nonlinear *ODEs*[15]

$$(2) \quad \frac{dA}{dt} = -k_1EA + k_{-1}Y,$$

$$(3) \quad \frac{dE}{dt} = -k_1EA + (k_{-1} + k_2)Y,$$

$$(4) \quad \frac{dY}{dt} = k_1EA - (k_{-1} + k_2)Y,$$

$$(5) \quad \frac{dX}{dt} = k_2Y,$$

where the initial conditions

$$(6) \quad A(0) = A_0, \quad E(0) = E_0, \quad Y(0) = 0, \quad X(0) = 0,$$

and the parameters  $k_1$ ,  $k_{-1}$  and  $k_2$  are positive rate constants for each reaction.

The NSFD solution [8] for such differential equation of the form

$$(7) \quad \frac{dy}{dt} = f(t, y(t)),$$

where  $f(t, y(t))$  called the nonlinear term in the differential equation. Using finite difference method we have

$$(8) \quad \frac{dy}{dt} = \frac{y_{k+1} - \psi(h)y_k}{\phi(h)},$$

where  $\phi$  and  $\psi$  are functions of the step size  $h = \Delta t$ . The  $\psi$  and  $\phi$  have the following properties

$$(9) \quad \psi = 1 + o(h),$$

$$(10) \quad \phi(h, \lambda) = h + o(h^2),$$

$h \rightarrow 0$  and  $\lambda = \text{fixed}$ , the numerator function  $\psi$  is usually equal to one [13] unless the system has dissipation.

Examples of functions  $\phi(h, \lambda)$  that satisfy the previous condition are  $\phi(h) = h$ ,  $\sin(h)$ ,  $\sinh(h)$ ,  $e^h - 1$ ,  $\frac{1-e^{-\lambda h}}{\lambda}$ , etc.

Non linear terms can be in general be replaced by nonlocal discrete representations. For example,  $y^2 \approx y_k y_{k+1}$ ,  $y^3 \approx (\frac{y_{k+1} + y_{k-1}}{2})y_k^2$ . Set  $h = T/N$ ,  $t_n = nh$ ,  $n = 0, 1, \dots, N \in \mathbb{Z}^+$ . Then Eq.(7) can be discretized as follows,

$$(11) \quad y(t_{n+1}) = \psi(h)y(t_n) + \phi(h)f(t_{n+1}, y(t_{n+1}), y(t_n)),$$

where  $f(t_n, y(t_{n+1}), y(t_n))$  is come from the non-locally linearized of  $f(t_{n+1}, y(t_{n+1}))$ .

If we do not use the non-locally linearized the system the differential equation, a somewhat better method is chosen—the Newton iteration method—to numerically solve the algebraic equation. This requires that  $f(t, y(t))$  be smooth and that the inverse of the derivative operator  $f_y$  exists. For a system of equations, Newton method often needs a lot of time so it is not economical. Luckily, Adomian decomposition method (ADM) [10, 11, 12] can be used to solve this problem effectively.

## 2. Adomian decomposition

Consider the general nonlinear equation [9]

$$u = N(u) + f,$$

where  $N$  is a nonlinear operator, and where  $f$  is supposed to be known. The decomposition method consists in looking for a solution having the series form

$$u = \sum_{i=0}^{\infty} u_i.$$

The nonlinear operator  $N$  is decomposed as

$$N(u) = \sum_{n=0}^{\infty} A_n,$$

where  $A_n$ 's are called Adomian's polynomials. In the first approach given by Adomian,  $A_n$ 's are obtained from the following equalities

$$\begin{aligned} v &= \sum_{i=0}^{\infty} \lambda^i u_i, \\ N(v) &= N\left(\sum_{i=0}^{\infty} \lambda^i u_i\right) = \sum_{n=0}^{\infty} \lambda^n A_n \end{aligned}$$

we remark that  $A_n$ 's are formally obtained from the relationship

$$A_n = \frac{1}{n!} \frac{d^n}{d\lambda^n} \left[ N\left(\sum_{i=0}^{\infty} \lambda^i u_i\right) \right]_{\lambda=0}.$$

The above process leads to the equality

$$\sum_{i=0}^{\infty} u_i = \sum_{n=0}^{\infty} A_n + f,$$

and the Adomian method consists in identifying  $u_i$  by means of the formula below

$$\begin{aligned} u_0 &= f, \\ u_1 &= A_0(u_0), \\ u_2 &= A_1(u_0, u_1), \\ &\vdots \\ u_n &= A_{n-1}(u_0, u_1, \dots, u_{n-1}). \end{aligned}$$

The solution  $u$  can be written as a series of functions  $u_i$  i.e.,

$$\sum_{i=0}^{\infty} |u_i| < +\infty.$$

**3. The numerical scheme**

Consider the nonlinear differential equation of the form

$$(12) \quad \frac{dy}{dt} = f(t, y(t)),$$

using the first derivatives of Mickens gives

$$(13) \quad \frac{y_{k+1} - y_k}{\phi(h)} = f(t_{k+1}, y_{k+1}),$$

solving Eq.13 for  $y_{k+1}$  gives

$$(14) \quad y_{k+1} = y_k + \phi(h)f(t_{k+1}, y_{k+1}).$$

For the nonlinear difference algebraic equations (14) using ADM to solve this kind of problems.

Suppose

$$(15) \quad y_{k+1} = \sum_{i=0}^{\infty} u_i,$$

where

$$(16) \quad u_0 = y_k,$$

$$(17) \quad u_1 = \phi(h)f(A_0),$$

$$(18) \quad u_2 = \phi(h)f(A_1),$$

⋮

$$(19) \quad u_n = \phi(h)f(A_{n-1}).$$

For the n-term of the ADM solution we have

$$(20) \quad y_{k+1} = \sum_{i=0}^{n-1} u_i.$$

**4. Application and results**

Systems (2)–(5) can be written as [15]

$$(21) \quad \frac{dx}{dt} = -x + (\beta - \alpha)y + xy,$$

$$(22) \quad \frac{dy}{dt} = \frac{1}{\epsilon}(x - \beta y - xy),$$

subject to the initial conditions

$$(23) \quad x(0) = 1, \quad y(0) = 0,$$

(24)

where  $\alpha$ ,  $\beta$  and  $\epsilon$  are dimensionless parameters. We will illustrate the ANSFD scheme to solve the system (21) and (22).

$$(25) \quad \frac{x_{k+1} - x_k}{\phi(h)} = -x_{k+1} + (\beta - \alpha)y_{k+1} + x_{k+1}y_{k+1},$$

$$(26) \quad \frac{y_{k+1} - y_k}{\phi(h)} = \frac{1}{\epsilon}(x_{k+1} - \beta y_{k+1} - x_{k+1}y_{k+1}),$$

where  $\phi(h) = \sin(h)$ . Solving (25) and (26) for  $x_{k+1}$  and  $y_{k+1}$  gives

$$(27) \quad x_{k+1} = x_k + \phi(h)(-x_{k+1} + (\beta - \alpha)y_{k+1} + x_{k+1}y_{k+1}),$$

$$(28) \quad y_{k+1} = y_k + \frac{\phi(h)}{\epsilon}(x_{k+1} - \beta y_{k+1} - x_{k+1}y_{k+1}).$$

Using the ADM to solve (27) and (28)

$$(29) \quad x_{k+1} = \sum_{i=0}^{n-1} v_i, \quad y_{k+1} = \sum_{i=0}^{n-1} u_i,$$

where

$$(30) \quad v_0 = x_k, \quad u_0 = y_k,$$

$$(31) \quad v_1 = \phi(h)[-v_0 + (\beta - \alpha)u_0 + v_0u_0], \quad v_1 = \frac{\phi(h)}{\epsilon}[v_0 - \beta u_0 - v_0u_0],$$

⋮

$$(32) \quad v_n = \phi(h)[-v_{n-1} + (\beta - \alpha)u_{n-1} + \sum_{i=0}^{n-1} v_j u_{n-1-j}],$$

$$(33) \quad u_n = \frac{\phi(h)}{\epsilon}[v_{n-1} - \beta u_{n-1} - \sum_{j=0}^{n-1} v_j u_{n-1-j}].$$

The biochemical reaction model (21) and (22) were numerically integrated using the ANSFD scheme is coded in the computer algebra package Maple and we employ the Maple's built-in fourth-order Runge-kutta procedure RK4. The Maple environment variable Digits controlling the number of significant Digits is set to 35 in all the calculations done in this paper we have set the dimensionless parameters  $\alpha = 0.375$ ,  $\beta = 1.0$  and  $\epsilon = 0.1$  with initial conditions  $x(0) = 1$ ,  $y(0) = 0$ . It is observed that the 4-term ANSFD solutions agree very well with the RK4 solution for time range  $t \in [0, 20]$ .

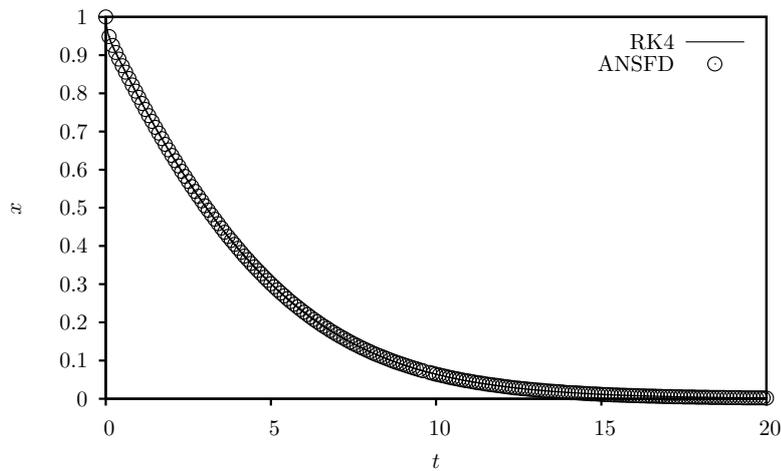
In Table 1 we present the absolute errors between RK4 solutions at time step  $\Delta t = 0.01$  and ANSFD solutions at time step  $\Delta t = 0.01$  and  $\Delta t = 0.01$ . Fig. 1 a and b show the solution for  $x$  and  $y$ , respectively, obtained by the 4-term ANSFD with  $\Delta t = 0.01$ . It is observed that the ANSFD solutions agree very well with the RK4 solutions for  $t$  upto  $t = 20$ .

### 5. Conclusion

In this paper, we derive a reliable algorithm based on Adomian decomposition for differential equations to solve a biochemical reaction model. The results obtained are in excellent agreement with those by (RK4) .

Table 1: Differences between 4-term ANSFD and RK4 solutions for the biochemical reaction model.

t	$\Delta =  \text{RK4}_{0.001} - \text{ANSFD}_{0.01} $		$\Delta =  \text{RK4}_{0.001} - \text{ANSFD}_{0.001} $	
	$\Delta x$	$\Delta y$	$\Delta x$	$\Delta y$
2	1.804E-04	6.406E-05	1.761E-05	6.249E-06
4	2.96E-04	1.493E-04	2.899E-05	1.462E-05
6	3.338E-04	2.213E-04	3.280E-05	2.174E-05
8	2.993E-04	2.4E-04	2.947E-05	2.364E-05
10	2.283E-04	2.06E-04	2.251E-05	2.032E-05
12	1.557E-04	1.502E-04	1.537E-05	1.483E-05
14	9.863E-05	9.858E-05	9.735E-06	9.731E-06
16	5.944E-05	6.050E-05	5.867E-06	5.972E-06
18	3.462E-05	3.556E-05	3.417E-06	3.510E-06
20	1.969E-05	2.032E-05	1.943E-06	2.005E-06



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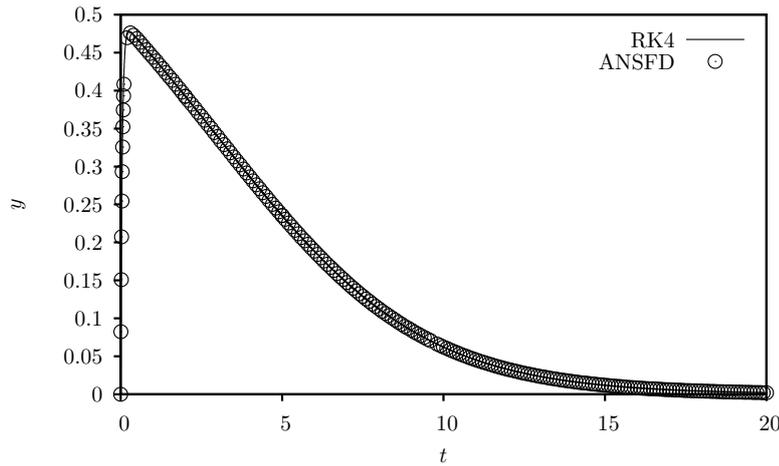


Figure 1: Solution of  $x$  and  $y$  using 4-term ANSFD ( $h = 0.01$ ) and RK4 ( $h = 0.001$ )

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