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ORIGINAL ARTICLE

A new numerical algorithm for fractional model of Bloch equation in nuclear magnetic resonance

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Error analysis

Abstract This paper presents a new algorithm based on operational matrix of fractional integrations for fractional Bloch equation in Nuclear Magnetic Resonance (NMR). For construction of operational matrix Legendre scaling functions are used as a basis. Using this operational matrix in the equations, we obtain approximate solutions for fractional Bloch equation. Convergence as well as error of the proposed method is given. Results are also compared with known solution. Absolute errors graph are plotted to show the accuracy of proposed new algorithm.

1. Introduction

The Bloch equations, namely

$$\begin{aligned} \frac{dM_x(t)}{dt} &= \omega_0 M_y(t) - \frac{M_x(t)}{T_2}, \\ \frac{dM_y(t)}{dt} &= -\omega_0 M_x(t) - \frac{M_y(t)}{T_2}, \\ \frac{dM_z(t)}{dt} &= \frac{M_0 - M_z(t)}{T_1}, \end{aligned} \tag{1}$$

with initial conditions

$$M_x(0) = 0, \quad M_y(0) = 100 \text{ and } M_z(0) = 0.$$

are used in physics, chemistry, nuclear magnetic resonance (NMR), electron spin resonance (ESR) and magnetic resonance imaging (MRI).

Where $M_x(t), M_y(t)$ and $M_z(t)$ represent the system magnetisation in x, y and z component respectively, M_0 is the equilibrium magnetisation, ω_0 is the resonant frequency given by the Larmor relationship $\omega_0 = \gamma B_0$, where B_0 is the static magnetic field in z-component, T_1 is spin-lattice relaxation time, and T_2 is spin-spin relaxation time. Well posed-ness of this equation is known when derivatives are of integer order. The set of analytic solution of the system of Eq. (1) with initial conditions in Eq. (2) is given as

$$\begin{aligned} M_x(t) &= e^{-t/T_2}(M_x(0)\cos\omega_0 t + M_y(0)\sin\omega_0 t), \\ M_y(t) &= e^{-t/T_2}(M_y(0)\cos\omega_0 t - M_x(0)\sin\omega_0 t), \\ M_z(t) &= M_z(0)e^{-t/T_1} + M_0(1 - e^{-t/T_1}). \end{aligned} \tag{2}$$

The aim of this paper was to study Eq. (1) by replacing integer order time derivatives to fractional order derivatives because some physical quantity depends on the past so it is physically very important to study such systems. The fractional model of Bloch equation is given as follows:

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$$\frac{d^{\alpha}M_x(t)}{dt^{\alpha}} = \omega_0 M_y(t) - \frac{M_x(t)}{T_2},$$
$$\frac{d^{\beta}M_y(t)}{dt^{\beta}} = -\omega_0 M_x(t) - \frac{M_y(t)}{T_2}, \qquad (3)$$
$$\frac{d^{\gamma}M_z(t)}{dt^{\gamma}} = \frac{M_0 - M_z(t)}{T_1},$$

where $0 < \alpha, \beta, \gamma \leqslant 1$.

The fraction in time derivative suggests a modulation—or weighting—of system memory, and the assumption of fractional derivatives plays an important role affecting the spin dynamics described by the Bloch equations in Eq. (3), see [1,2]. In addition, it is known that fractional derivative is strongly dependent on the initial conditions; therefore, we should choose the fractional derivative most appropriate for handling the initial conditions of our physical problem. In NMR the initial state of the system is specified by the components of the magnetisation, and hence these need to be clearly recognised. The physical meaning of the fractional Bloch equations goes back to the basic formulation of the fractional Schrodinger equation in quantum mechanics.

There are several methods to obtain approximate solution for Bloch equation in NMR [3–10]. Recently some authors solve mathematical model of Bloch equation with fractional time derivative [11–13].

In this paper we present a new algorithm based on operational matrix of integration for the approximate solution of time fractional model of Bloch equation. Operational matrix has several applications in fractional calculus. For the construction of operational matrices and their applications in fractional calculus see [14–25]. Using operational matrix in Bloch model we obtain unknown coefficients for approximated parameter in model. Using these coefficients we obtain approximate solution for fractional model of Bloch equation in NMR. Convergence as well as error of the proposed method is given.

The present paper is organised as follows. In Section 2, we describe basic preliminaries. In Section 3, we construct operational matrix using Legendre scaling functions as basis. In Section 4, we describe the algorithm for the construction of approximate solutions. In Section 5, we show the convergence of approximate solution to the exact solution. In Section 6, we give error bound for the proposed method. In Section 7, we give numerical experiments and discussion for different cases of time derivative to show the effectiveness of the proposed method.

2. Preliminaries

There are several definitions of fractional order derivatives and integrals. These are not necessarily equivalent. In this paper, the fractional order differentiations and integrations are in well-known Caputo and Riemann-Liouville sense respectively [26,27].

The Legendre scaling functions $\{\phi_i(t)\}$ in one dimension are defined by

$$\phi_i(t) = \begin{cases} \sqrt{(2i+1)}P_i(2t-1), & \text{for } 0 \leqslant t < 1. \\ 0, & \textit{otherwise}, \end{cases}$$

where $P_i(t)$ is Legendre polynomials of order i on the interval $[-1, 1]$, given explicitly by the following formula:

$$P_i(t) = \sum_{k=0}^{i} (-1)^{i+k} \frac{(i+k)!}{(i-k)!} \frac{t^k}{(k!)^2}. \qquad (4)$$

Legendre scaling functions are constructed normalising the shifted Legendre polynomials. So the collection $\{\phi_i(t)\}$ forms an orthonormal basis for $L^2[0,1]$. The Legendre scaling function of degree i is given by

$$\phi_i(t) = (2i+1)^{\frac{1}{2}} \sum_{k=0}^{i} (-1)^{i+k} \frac{(i+k)!}{(i-k)!} \frac{t^k}{(k!)^2} \qquad (5)$$

A function $f \in L^2[0,1]$, with bounded second derivative $|f''(t)| \leqslant M$, expanded as infinite sum of Legendre scaling function and the series converges uniformly to the function $f(t)$,

$$f(t) = \lim_{n\to\infty} \sum_{i=0}^{n} c_i \phi_i(t), \qquad (6)$$

where $c_i = \langle f(t), \phi_i(t) \rangle$, and $\langle .,. \rangle$ is standard inner product on $L^2[0,1]$.

If the series is truncated at $n = m$, then we have

$$f \cong \sum_{i=0}^{m} c_i \phi_i = C^T \phi(t), \qquad (7)$$

where C and $\phi(t)$ are $(m+1) \times 1$ matrices given by

$C = [c_0, c_1, \ldots, c_m]^T$ and $\phi(t) = [\phi_0(t), \phi_1(t), \ldots, \phi_m(t)]^T$.

3. Operational matrix

Theorem 3.1. *Let* $\phi(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_n(x)]^T$, *be Legendre scaling vector and consider* $\alpha > 0$, *then*

$$I^{\alpha}\phi_i(x) = I^{(\alpha)}\phi(x), \qquad (8)$$

where $I^{(\alpha)} = (\omega(i,j))$, is $(n+1) \times (n+1)$ *operational matrix of fractional integral of order* α *and its* (i,j) *th entry is given by*

$$\omega(i,j) = (2i+1)^{1/2}(2j+1)^{1/2} \sum_{k=0}^{i}\sum_{l=0}^{j} (-1)^{i+j+k+l} \times \frac{(i+k)!(j+l)!}{(i-k)!(j-l)!(k)!(l!)^2(\alpha+k+l+1)\Gamma(\alpha+k+1)}$$
$$0 \leqslant i,j \leqslant n.$$

Proof. Using the Legendre scaling function of degree i, we get

$$I^{\alpha}\phi_i(x) = (2i+1)^{1/2} \sum_{k=0}^{i} (-1)^{i+k} \frac{(i+k)!}{(i-k)!} \frac{1}{(k!)^2} I^{\alpha} x^k$$
$$= (2i+1)^{1/2} \sum_{k=0}^{i} (-1)^{i+k} \frac{(i+k)!}{(i-k)!(k)!\Gamma(\alpha+k+1)} x^{\alpha+k}$$

using Legendre scaling function approximation for $x^{\alpha+k}$, we have

$$x^{\alpha+k} = \sum_{j=0}^{n} c_j \phi_j(x), \text{ where}$$
$$c_j = (2j+1)^{1/2} \sum_{l=0}^{j} (-1)^{l+j} \frac{(j+l)!}{(j-l)!} \frac{1}{(l!)^2} \frac{1}{(\alpha+k+l+1)}. \qquad (9)$$

Hence,

$$I^{\alpha}\phi_i(x)=\sum_{j=0}^{n}\omega(i,j)\phi_j(x), \tag{10}$$

where $\omega(i,j)$ is defined by

$$\omega(i,j)=(2i+1)^{1/2}(2j+1)^{1/2}\sum_{k=0}^{i}\sum_{l=0}^{j}(-1)^{i+j+k+l}\times\frac{(i+k)!(j+l)!}{(i-k)!(j-l)!(k)!(l!)^2(\alpha+k+l+1)\Gamma(\alpha+k+1)}. \tag{11}$$

Hence,

$$I^{\alpha}\phi_i(x)=[\omega(i,0),\omega(i,1),\omega(i,2),\ldots,\omega(i,n)]\Phi(x). \tag{12}$$

□

4. Method of solution

In this section, we describe the algorithm for the construction of approximate solution of the Bloch equation.

Let us consider

$$\frac{d^{\alpha}M_x(t)}{dt^{\alpha}}=C_1^T\phi(t),\ \frac{d^{\beta}M_y(t)}{dt^{\beta}}=C_2^T\phi(t),\ \frac{d^{\gamma}M_z(t)}{dt^{\gamma}}=C_3^T\phi(t), \tag{13}$$

from Eq. (13), we can write

$$M_x(t)=C_1^TI^{(\alpha)}\phi(t)+A^T\phi(t), \tag{14}$$

$$M_y(t)=C_2^TI^{(\beta)}\phi(t)+B^T\phi(t), \tag{15}$$

$$M_z(t)=C_3^TI^{(\gamma)}\phi(t)+D^T\phi(t), \tag{16}$$

where $M_x(0)=A^T\phi(t),\ M_y(0)=B^T\phi(t),\ M_z(0)=D^T\phi(t)$.

Using Eqs. (13)–(16) in Bloch model we obtain following equations

$$C_1^T\left(I+\frac{1}{T_2}I^{(\alpha)}\right)-\omega_0C_2^TI^{(\beta)}=\omega_0B^T-\frac{1}{T_2}A^T, \tag{17}$$

$$\omega_0C_1^TI^{(\alpha)}+C_2^T\left(I+\frac{1}{T_2}I^{(\beta)}\right)=-\omega_0A^T-\frac{1}{T_2}B^T, \tag{18}$$

$$C_3^T\left(I+\frac{1}{T_1}I^{(\gamma)}\right)=E^T-\frac{1}{T_1}D^T, \tag{19}$$

where $I^{(\alpha)}, I^{(\beta)}$ and $I^{(\gamma)}$ are operational matrices of fractional integration of order α,β and γ respectively. I is an identity matrix and $\frac{M_0}{T_1}=E^T\phi(t)$. Using following notations in Eqs. (17)–(19)

$$I_1=I+\frac{1}{T_2}I^{(\alpha)},\ I_2=I+\frac{1}{T_2}I^{(\beta)},\ I_3=I+\frac{1}{T_1}I^{(\gamma)},\ I_4=\omega_0I^{(\alpha)},\ I_5=\omega_0I^{(\beta)},$$
$$F_1=\omega_0B^T-\frac{1}{T_2}A^T,\ F_2=-\omega_0A^T-\frac{1}{T_2}B^T,\ F_3=E^T-\frac{1}{T_1}D^T, \tag{20}$$

we obtain,

$$C_1^TI_1-C_2^TI_5=F_1, \tag{21}$$

$$C_1^TI_4+C_2^TI_2=F_2, \tag{22}$$

$$C_3^TI_3=F_3, \tag{23}$$

$I_1, I_2, I_3, I_4, I_5, F_1, F_2$ and F_3 are known.

On solving Eqs. (21) and (22) we get,

$$C_1^T=\left(F_1I_5^{-1}+F_2I_2^{-1}\right)\left(I_1I_5^{-1}+I_4I_2^{-1}\right)^{-1}, \tag{24}$$

$$C_2^T=\left\{\left(F_1I_5^{-1}+F_2I_2^{-1}\right)\left(I_1I_5^{-1}+I_4I_2^{-1}\right)^{-1}I_1-F_1\right\}I_5^{-1}, \tag{25}$$

From Eq. (23), we can write

$$C_3^T=F_3I_3^{-1}. \tag{26}$$

Using Eqs. (24)–(26) in Eqs. (14)–(16) respectively, we get approximate solution for Bloch equations in NMR.

5. Convergence analysis

Theorem 1. *Suppose that $y(x)\in L^2[0\,1]$ and $y_n(x)$ be the its nth approximation obtained by using (n + 1) elements of Legendre scaling vector. Suppose $|D^2y(x)|<K$, then $y_n(x)\to y(x)$ in the L^2 -sense with the following inequality:*

$$\|y(x)-y_n(x)\|_{L^2[0,1]}\leqslant\frac{K}{16}F_3\left(-\frac{1}{2}+n\right), \tag{27}$$

where $F_n(z)$ is Poly Gamma function.

Proof. Let,

$$y(x)=\sum_{i=0}^{\infty}c_i\phi_i(x), \tag{28}$$

Truncating series in Eq. (28),

$$y_n(x)=\sum_{i=0}^{n}c_i\phi_i(x). \tag{29}$$

Subtracting Eq. (29) from Eq. (28),

$$y(x)-y_n(x)=\sum_{i=n+1}^{\infty}c_i\phi_i(x), \tag{30}$$

From Eq. (30), we can write,

$$\|y(x)-y_n(x)\|^2_{L^2[0,1]}\leqslant\int_0^1\left(\sum_{i=n+1}^{\infty}c_i\phi_i(x)\right)^2, \tag{31}$$

Now Eq. (31), can be written as,

$$\|y(x)-y_n(x)\|^2_{L^2[0,1]}\leqslant\sum_{i=n+1}^{\infty}c_i^2, \tag{32}$$

Coefficients in the expansion given in Eq. (28), are given by,

$$c_i=\int_0^1y(x)\phi_i(x)dx=(2i+1)^{\frac{1}{2}}\int_0^1y(x)P_i(2x-1)dx, \tag{33}$$

substituting $2x-1=t$, in Eq. (33), we get,

$$c_i = \frac{(2i+1)^{\frac{1}{2}}}{2}\int_{-1}^{1} y\left(\frac{t+1}{2}\right)P_i(t)dt,$$
$$= \left(\frac{1}{2^2(2i+1)}\right)^{\frac{1}{2}}\int_{-1}^{1} y\left(\frac{t+1}{2}\right)d(P_{i+1}(t) - P_{i-1}(t))dt. \quad (34)$$

Now using integration part formula two times in Eq. (34), we get,

$$|c_i|^2 < \frac{k^2}{32(2i+1)(2i-1)^2(2i+3)^2} \times \left[\frac{2(2i-1)^2}{2i+5} + \frac{8(2i+1)^2}{2i+1} + \frac{2(2i+3)^2}{2i-3}\right],$$
$$|c_i|^2 < \frac{3K^2}{8(2i-3)^4}, \quad (35)$$

Using Eq. (35) in Eq. (32), we get,

$$\|y(x) - y_n(x)\|^2_{L^2[0,1]} \leqslant \frac{3}{8}\sum_{i=n+1}^{\infty}\frac{K^2}{(2i-3)^4}, \quad (36)$$

Summing the above series we get,

$$\|y(x) - y_n(x)\|_{L^2[0,1]} \leqslant \frac{K}{16}F_3\left(-\frac{1}{2}+n\right).$$

From Eq. (36) as $n \to \infty$, $y_n(x) \to y(x)$ in the L^2 -sense. □

6. Error analysis

Theorem 2. *Let $(I_n^\alpha y)(x)$ be the nth approximation of Riemann-Liouville fractional integral operator $(I^\alpha y)(x)$ then we have the followings upper bounds of absolute error in its nth approximation*

$$\|(I^\alpha y)(x) - (I_n^\alpha y)(x)\|_{L^2[0,1]} \leqslant \frac{K}{16\sqrt{(\alpha+1)}}F_3\left(-\frac{1}{2}+n\right) \quad (37)$$

Proof. From the definition of Riemann-Liouville fractional integral operator, we can write

$$\|(I^\alpha y)(x) - (I_n^\alpha y)(x)\|_{L^2[0,1]} = \frac{1}{\sqrt{\alpha}}\int_0^x (x-\tau)^{\alpha-1}|y(\tau) - y_n(\tau)|d\tau. \quad (38)$$

Using Eq. (36) in (38), we get

$$\|(I^\alpha y)(x) - (I_n^\alpha y)(x)\|_{L^2[0,1]} \leqslant \frac{1}{\sqrt{\alpha}}\int_0^x (x-\tau)^{\alpha-1}\frac{K}{16}F_3\left(-\frac{1}{2}+n\right)d\tau$$
$$= \frac{K}{16\sqrt{\alpha}}F_3\left(-\frac{1}{2}+n\right)\int_0^x (x-\tau)^{\alpha-1}d\tau$$
$$\|(I^\alpha y)(x) - (I_n^\alpha y)(x)\|_{L^2[0,1]} \leqslant \frac{K}{16\sqrt{(\alpha+1)}}F_3\left(-\frac{1}{2}+n\right)x^\alpha. \quad (39)$$

Since $x \in [0, 1]$, Eq. (39) can be written as,

$$\|(I^\alpha y)(x) - (I_n^\alpha y)(x)\|_{L^2[0,1]} \leqslant \frac{K}{16\sqrt{(\alpha+1)}}F_3\left(-\frac{1}{2}+n\right).$$

□

7. Numerical results and discussion

In all the figures given below we have taken $\omega_0 = 1$, $T_1 = 1\,(s)^q$ and $T_2 = 20\,(ms)^q$. In Figs. 4–6, absolute errors are denoted by E_1, E_2, E_3 for n = 3,7 and 11 respectively. In these respective figures E_2, E_3 are multiplied by 10^5.

Figs. 1–3, represent approximate and exact solution for $M_x(t), M_y(t)$ and $M_z(t)$ respectively. These figures show accuracy of the proposed method.

Figs. 4–6, show the behaviour of absolute errors of integer order Bloch equation for different values of n = 3,7 and 11. From Figs. 4–6, it is observed that absolute error decreases with the increasing n. Similarly as we increase the dimension of basis function, we obtain more accurate numerical solution.

Figs. 7–9, show the behaviour of solutions with time for different values of α, β and γ. It is clear that the solution varies continuously for Bloch equation in NMR and for $\alpha = \beta = \gamma = 1$ solution for standard Bloch equation is obtained. From Figs. 7 and 9 it is clear that the approximate solution for $M_x(t)$ and $M_z(t)$ increases with the increase in time for different values of $\alpha = \gamma = 0.7, 0.8, 0.9$ and 1. But in Fig. 8 the approximate solution for $M_y(t)$ decreases with the increase in time for different values of $\beta = 0.7, 0.8, 0.9$ and 1.

In Table 1, we have compared our results from the Homotopy Perturbation Method (HPM) [11], iterative method [13] and exact solution.

From the table it is observed that the accuracy by our method (n = 4) is better than the method in [11] for n = 4 and the iterative method in [13] in which we have taken thousands of iterations.

8. Conclusions and future works

Our numerical algorithm is easy in comparison with existing methods for the approximate solution of fractional Bloch equation in NMR because construction of operational matrix is very easy. Better accuracy is attained because we are approximating time derivative first. It is shown that how the approximate solution varies continuously for different values of α, β

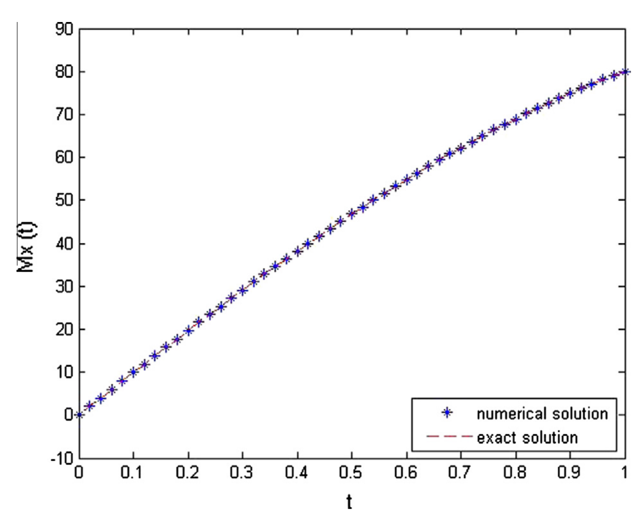

Figure 1 Comparison of exact and approximate solution for $M_x(t)$.

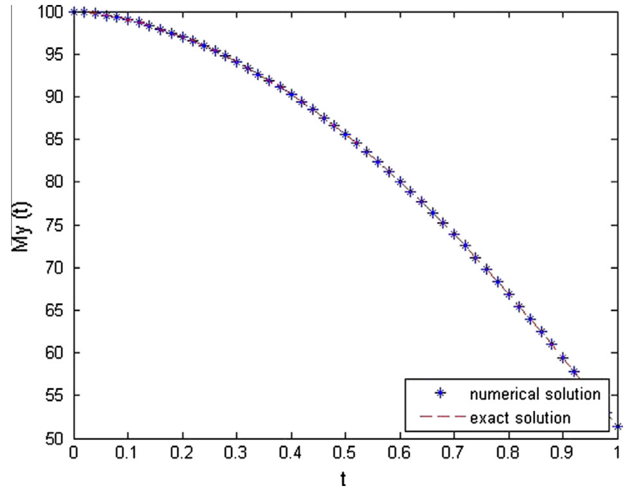

Figure 2 Comparison of exact and approximate solution for $M_y(t)$.

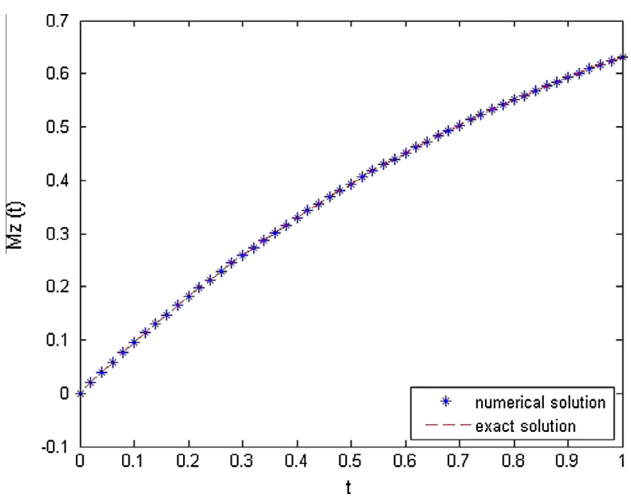

Figure 3 Comparison of exact and approximate solution for $M_z(t)$.

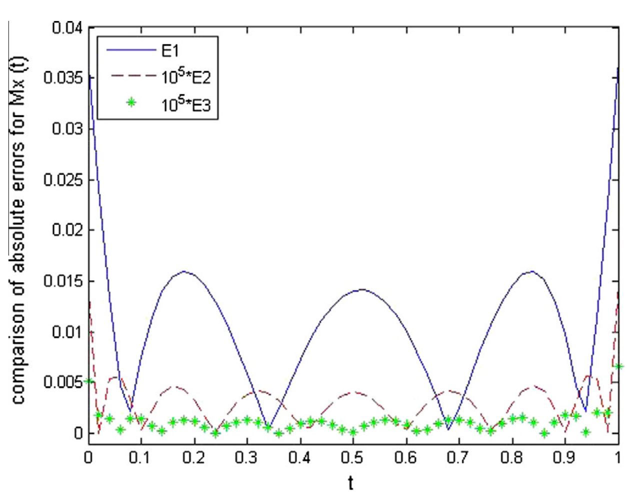

Figure 4 Comparison of absolute errors for $M_x(t)$ at different values of n = 3, 7 and 11.

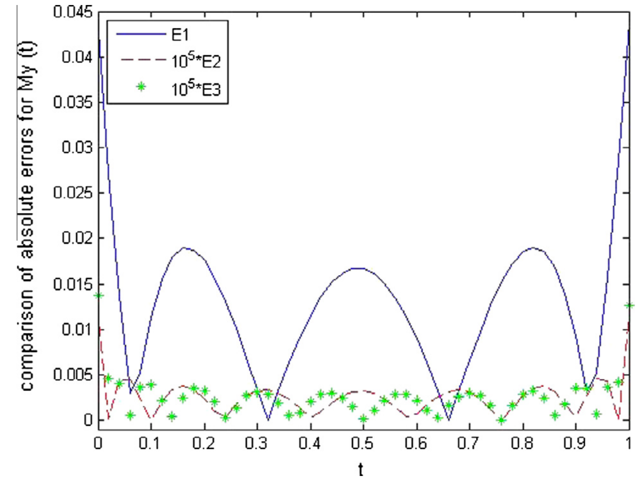

Figure 5 Comparison of absolute errors for $M_y(t)$ at different values of n = 3, 7 and 11.

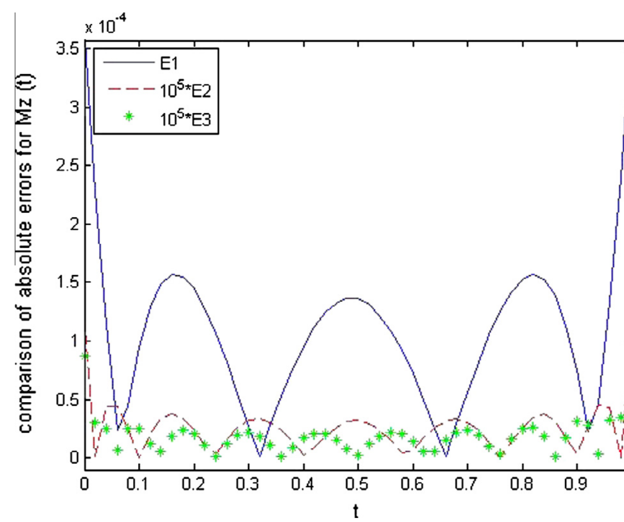

Figure 6 Comparison of absolute errors for $M_z(t)$ at different values of n = 3, 7 and 11.

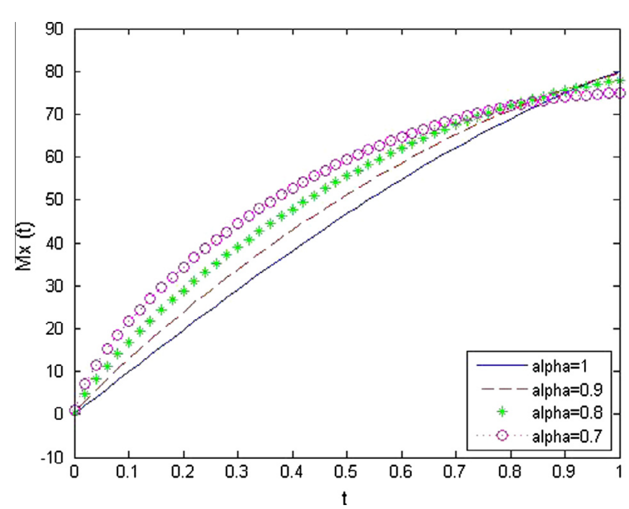

Figure 7 Approximate solution for $M_x(t)$ at different values of α.

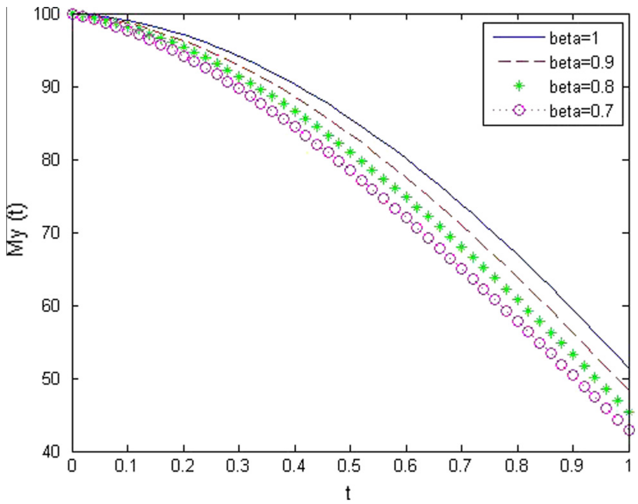

Figure 8 Approximate solution for $M_y(t)$ at different values of β.

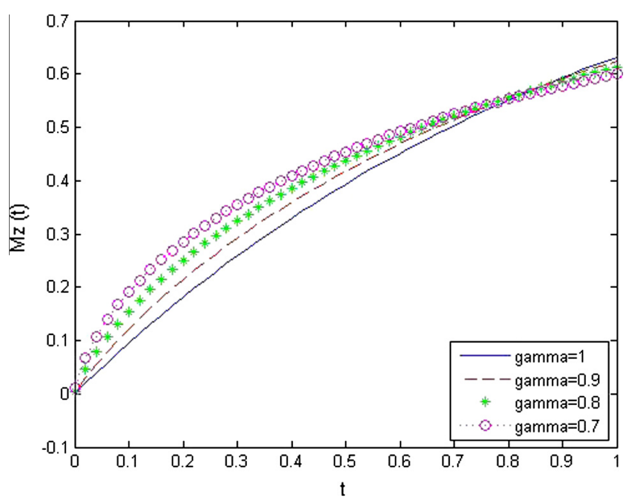

Figure 9 Approximate solution for $M_z(t)$ at different values of γ.

Table 1 Comparison among the approximate solutions of exiting methods, present method and exact solution of Mx, My and Mz for alpha = 1.

M	t	Exact solution	Present method	Method in [11]	Method in [13]
$M_x(t)$	0.2	19.6693	19.6693	19.6677	19.6597
	0.4	38.1707	38.1707	38.1413	38.1621
	0.6	54.7955	54.7955	54.6270	54.7803
	0.8	68.9228	68.9228	68.3307	68.9168
	1.0	80.0432	80.0433	78.4583	80.0388
$M_y(t)$	0.2	97.0315	97.0315	97.0783	97.0329
	0.4	90.2823	90.2823	90.3399	90.2846
	0.6	80.0943	80.0943	79.8246	80.1033
	0.8	66.9388	66.9389	65.5723	66.9425
	1.0	51.3951	51.3952	47.6269	51.3992
$M_z(t)$	0.2	0.1813	0.1813	0.1813	0.1812
	0.4	0.3297	0.3297	0.3297	0.3296
	0.6	0.4512	0.4512	0.4512	0.4511
	0.8	0.5507	0.5507	0.5507	0.5506
	1.0	0.6321	0.6321	0.6321	0.6321

and γ. For future work we can use operational matrices of different orthonormal polynomials to achieve better accuracy.

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