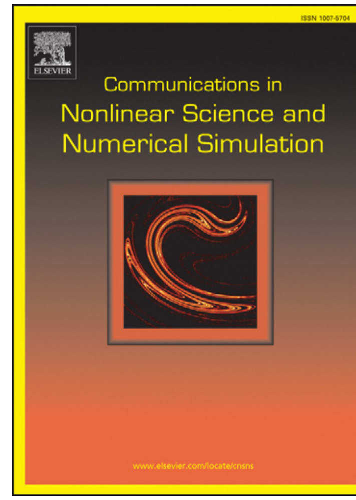

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On the numerical solutions for the fractional diffusion equation

M. M. Khader
Department of Mathematics, Faculty of Science, Benha University, Benha, Egypt
mohamedmbd@yahoo.com

Abstract

Fractional differential equations have recently been applied in various area of engineering, science, finance, applied mathematics, bio-engineering and others. However, many researchers remain unaware of this field. In this paper, an efficient numerical method for solving the fractional diffusion equation (F$\boldsymbol{D}$E) is considered. The fractional derivative is described in the Caputo sense. The method is based upon Chebyshev approximations. The properties of Chebyshev polynomials are utilized to reduce F$\boldsymbol{D}$E to a system of ordinary differential equations, which solved by the finite difference method. Numerical simulation of F$\boldsymbol{D}$E is presented and the results are compared with the exact solution and other methods.

Keywords: Finite difference method; Fractional diffusion equation; Chebyshev polynomials; Caputo derivative.

1. Introduction

Ordinary and partial fractional differential equations have been the focus of many studies due to their frequent appearance in various applications in fluid mechanics, viscoelasticity, biology, physics and engineering [1]. Consequently, considerable attention has been given to the solutions of fractional differential equations of physical interest. Most fractional differential equations do not have exact solutions, so approximation and numerical techniques ([2]-[5]), must be used. Recently, several numerical methods to solve the fractional differential equations have been given such as variational iteration method [6], homotopy perturbation method [15], Adomian's decomposition method [7], homotopy analysis method [4] and collocation method [12].
We describe some necessary definitions and mathematical preliminaries of the fractional calculus theory required for our subsequent development.

Definition 1.

The Caputo fractional derivative operator D^α of order α is defined in the following form:

$$D^\alpha f(x) = \frac{1}{\Gamma(m-\alpha)} \int_0^x \frac{f^{(m)}(t)}{(x-t)^{\alpha-m+1}} dt, \quad \alpha > 0,$$

where $m-1 < \alpha < m,\ m \in \mathbb{N},\ x > 0$.

Similar to integer-order differentiation, Caputo fractional derivative operator is a linear operation:

$$D^\alpha \left(\lambda\, f(x) + \mu\, g(x)\right) = \lambda\, D^\alpha\, f(x) + \mu\, D^\alpha\, g(x),$$

where λ and μ are constants.

For the Caputo's derivative we have [11]:

$$D^\alpha\, C = 0, \qquad \text{C is a constant,} \tag{1}$$

$$D^\alpha\, x^n = \begin{cases} 0, & \text{for} \quad n \in \mathbb{N}_0 \text{ and } n < \lceil \alpha \rceil; \\ \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)} x^{n-\alpha}, & \text{for} \quad n \in \mathbb{N}_0 \text{ and } n \geq \lceil \alpha \rceil. \end{cases} \tag{2}$$

We use the ceiling function $\lceil \alpha \rceil$ to denote the smallest integer greater than or equal to α. Also $\mathbb{N}_0 = \{0, 1, 2, ...\}$. Recall that for $\alpha \in \mathbb{N}$, the Caputo differential operator coincides with the usual differential operator of integer order.

For more details on fractional derivatives definitions and its properties see ([11], [13]).

The main goal in this article is concerned with the application of Chebyshev pseudospectral method to obtain the numerical solution of F$\boldsymbol{D}$E of the form:

$$\frac{\partial u(x,t)}{\partial t} = d(x,t) \frac{\partial^\alpha u(x,t)}{\partial x^\alpha} + s(x,t), \tag{3}$$

on a finite domain $a < x < b,\ 0 \leq t \leq T$ and the parameter α refers to the fractional order of spatial derivatives with $1 < \alpha \leq 2$. The function $s(x,t)$ is a source term.

We also assume an initial condition:

$$u(x,0) = u^0(x), \quad a < x < b, \tag{4}$$

and the following Dirichlet boundary conditions:

$$u(a,t) = u(b,t) = 0. \tag{5}$$

Note that $\alpha = 2$, Eq.(3) is the classical diffusion equation:

$$\frac{\partial u(x,t)}{\partial t} = d(x,t) \frac{\partial^2 u(x,t)}{\partial x^2} + s(x,t).$$

The main idea of this work is to apply the Chebyshev collocation method to discretize (3) to get a linear system of ordinary differential equations thus greatly simplifying the problem, and use the finite difference method (FDM) ([8]-[10], [16]) to solve the resulting system.
Chebyshev polynomials are a well known family of orthogonal polynomials on the interval $[-1, 1]$ that have many applications [14]. They are widely used because of their good properties in the approximation of functions. However, with our best knowledge, very little work was done to adapt this polynomials to the solution of fractional differential equations.

The organization of this paper is as follows. In the next section, the approximation of fractional derivative $D^{\alpha}y(x)$ is obtained. Section 3 summarizes the application of Chebyshev collocation method to solve (3). As a result, a system of ordinary differential equations is formed and the solution of the considered problem is introduced. In section 4, some comparisons and numerical results are given to clarify the method. Also a conclusion is given in section 5. Note that we have computed the numerical results using Matlab programming.

2. Derivation an approximate formula for fractional derivatives using Chebyshev series expansion

The well known Chebyshev polynomials [14] are defined on the interval $[-1, 1]$ and can be determined with the aid of the following recurrence formula:

$$T_{n+1}(z) = 2\,z\,T_n(z) - T_{n-1}(z), \qquad T_0(z) = 1, \quad T_1(z) = z \qquad n = 1, 2, \ldots .$$

The analytic form of the Chebyshev polynomials $T_n(z)$ of degree n is given by:

$$T_n(z) = \sum_{i=0}^{[\frac{n}{2}]} (-1)^i \, 2^{n-2\,i-1} \, \frac{n\,(n-i-1)!}{(i)!\,(n-2\,i)!} \, z^{n-2\,i}. \tag{6}$$

Where $[n/2]$ denotes the integral part of $n/2$. The orthogonality condition is:

$$\int_{-1}^{1} \frac{T_i(z)\,T_j(z)}{\sqrt{1-z^2}}\,dz = \begin{cases} \pi, & \text{for} \quad i = j = 0; \\ \frac{\pi}{2}, & \text{for} \quad i = j \neq 0; \\ 0, & \text{for} \quad i \neq j. \end{cases} \tag{7}$$

In order to use these polynomials on the interval $x \in [0, 1]$ we define the so called shifted Chebyshev polynomials by introducing the change of variable $z = 2x - 1$.
The shifted Chebyshev polynomials is defined as: $T_n^*(x) = T_n(2x-1) = T_{2n}(\sqrt{x})$.

The analytic form of the shifted Chebyshev polynomial $T_n^*(x)$ of degree n is given by:

$$T_n^*(x) = \sum_{i=0}^{n} (-1)^i \; 2^{2\,n-2\,i} \; \frac{n\,(2\,n-i-1)!}{(i)!\,(2\,n-2\,i)!} \, x^{n-i}. \tag{8}$$

The function $y(x)$, square integrable in $[0,1]$, may be expressed in terms of shifted Chebyshev polynomials as:

$$y(x) = \sum_{i=0}^{\infty} c_i \, T_i^*(x),$$

where the coefficients c_i, $i = 1, 2, ...$ are given by:

$$c_0 = \frac{1}{\pi} \int_{-1}^{1} \frac{y(0.5\,x+0.5)\,T_0(x)}{\sqrt{1-x^2}} \, dx, \qquad c_i = \frac{2}{\pi} \int_{-1}^{1} \frac{y(0.5\,x+0.5)\,T_i(x)}{\sqrt{1-x^2}}, \, dx. \tag{9}$$

In practice, only the first $(m+1)$-terms shifted Chebyshev polynomials are considered. Then we have:

$$y_m(x) = \sum_{i=0}^{m} c_i \, T_i^*(x). \tag{10}$$

Theorem 1. *(Chebyshev truncation theorem)*

The error in approximating $y(x)$ by the sum of its first m terms is bounded by the sum of the absolute values of all the neglected coefficients. If

$$y_m(x) = \sum_{k=0}^{m} c_k \, T_k(x), \tag{11}$$

then

$$E_T(m) \equiv |y(x) - y_m(x)| \leq \sum_{k=m+1}^{\infty} |c_k|, \tag{12}$$

for all $y(x)$, all m, and all $x \in [-1, 1]$.

Proof. The Chebyshev polynomials are bounded by one, that is, $|T_k(x)| \leq 1$ for all $x \in [-1, 1]$ and for all k. This implies that the k-th term is bounded by $|c_k|$. Subtracting the truncated series from the infinite series, bounding each term in the difference, and summing the bounds gives the theorem. $\square$

The main approximate formula of the fractional derivative of $y(x)$ is given in the following theorem.

Theorem 2.

Let $y(x)$ be approximated by Chebyshev polynomials as (10) and also suppose $\alpha > 0$ then:

$$D^{\alpha}(y_m(x)) = \sum_{i=\lceil\alpha\rceil}^{m} \sum_{k=0}^{i-\lceil\alpha\rceil} c_i \, w_{i,k}^{(\alpha)} \, x^{i-k-\alpha}, \tag{13}$$

where $w_{i,k}^{(\alpha)}$ is given by:

$$w_{i,k}^{(\alpha)} = (-1)^k \; 2^{2\,i-2\,k} \frac{i\,(2\,i-k-1)!\,(i-k)!}{(k)!\,(2\,i-2\,k)!\,\Gamma(i-k+1-\alpha)}. \tag{14}$$

Proof. Since the Caputo's fractional differentiation is a linear operation we have:

$$D^{\alpha}(y_m(x)) = \sum_{i=0}^{m} c_i \, D^{\alpha}(T_i^*(x)). \tag{15}$$

Employing Eqs. (1)-(2) we have:

$$D^{\alpha}\, T_i^*(x) = 0, \qquad i = 0, 1, ..., \lceil\alpha\rceil - 1, \quad \alpha > 0. \tag{16}$$

Also, for $i = \lceil\alpha\rceil, ..., m$, by using Eqs.(1)-(2), we get:

$$\begin{aligned} D^{\alpha}\, T_i^*(x) &= \sum_{k=0}^{i} (-1)^k \; 2^{2\,i-2\,k} \frac{i\,(2\,i-k-1)!}{(k)!\,(2\,i-2\,k)!} \, D^{\alpha}\, x^{i-k} \\ &= \sum_{k=0}^{i-\lceil\alpha\rceil} (-1)^k \; 2^{2\,i-2\,k} \frac{i\,(2\,i-k-1)!\,(i-k)!}{(k)!\,(2\,i-2\,k)!\,\Gamma(i-k+1-\alpha)} \, x^{i-k-\alpha}. \end{aligned} \tag{17}$$

A combination of Eqs. (15), (16) and (17) leads to the desired result.

Test example:

Consider the function $y(x) = x^2$ with $m = 3$ and $\alpha = 1.5$, the Chebyshev series of x^2 is:

$$x^2 = \frac{3}{8}\, T_0^*(x) + \frac{4}{8}\, T_1^*(x) + \frac{1}{8}\, T_2^*(x).$$

Now, by using (13), we obtain:

$$D^{\frac{3}{2}}\, x^2 = \sum_{i=2}^{3} \sum_{k=0}^{i-2} c_i \, w_{i,k}^{(\frac{3}{2})} \, x^{i-k-\frac{3}{2}}, \qquad \text{where,} \quad w_{2,0}^{(\frac{3}{2})} = \frac{16}{\Gamma(\frac{3}{2})}, \quad w_{3,0}^{(\frac{3}{2})} = \frac{192}{\Gamma(\frac{5}{2})}, \quad w_{3,1}^{(\frac{3}{2})} = \frac{-96}{\Gamma(\frac{3}{2})},$$

therefore:

$$D^{\frac{3}{2}}\, x^2 = c_2\, w_{2,0}^{(\frac{3}{2})}\, x^{\frac{1}{2}} + c_3\, w_{3,0}^{(\frac{3}{2})}\, x^{\frac{3}{2}} + c_3\, w_{3,1}^{(\frac{3}{2})}\, x^{\frac{1}{2}} = \frac{2}{\Gamma(\frac{3}{2})}\, x^{\frac{1}{2}}.$$

3. Procedure of solution for the fractional diffusion equation

Consider the F$\boldsymbol{D}$E of type given in Eq.(3). In order to use Chebyshev collocation method, we first approximate $u(x,t)$ as:

$$u_m(x,t) = \sum_{i=0}^{m} u_i(t)\, T_i^*(x). \tag{18}$$

From Eqs. (3), (18) and Theorem 1 we have:

$$\sum_{i=0}^{m} \frac{d\,u_i(t)}{dt}\, T_i^*(x) = d(x,t) \sum_{i=\lceil\alpha\rceil}^{m} \sum_{k=0}^{i-\lceil\alpha\rceil} u_i(t)\, w_{i,\,k}^{(\alpha)}\, x^{i-k-\alpha} + s(x,t), \tag{19}$$

we now collocate Eq.(19) at $(m+1-\lceil\alpha\rceil)$ points x_p as:

$$\sum_{i=0}^{m} \dot{u}_i(t) T_i^*(x_p) = d(x_p,t) \sum_{i=\lceil\alpha\rceil}^{m} \sum_{k=0}^{i-\lceil\alpha\rceil} u_i(t)\, w_{i,\,k}^{(\alpha)}\ x_p^{i-k-\alpha} + s(x_p,t), \qquad p = 0,1,...,m-\lceil\alpha\rceil. \tag{20}$$

For suitable collocation points we use roots of shifted Chebyshev polynomial $T_{m+1-\lceil\alpha\rceil}^*(x)$. Also, by substituting Eqs.(18) and (13) in the initial conditions or boundary conditions we can find $\lceil\alpha\rceil$ equations. For example by substituting Eqs.(18) and (13) in boundary conditions (5) we obtain:

$$\sum_{i=0}^{m} (-1)^i\, u_i(t) = 0, \qquad \sum_{i=0}^{m} u_i(t) = 0. \tag{21}$$

Equation (20), together with $\lceil\alpha\rceil$ equations of the boundary conditions (21), give $(m+1)$ ordinary differential equations which can be solved, for the unknown $u_i, i = 0,...,m$, using FDM, as described in the following section.

4. Numerical simulation and comparison

In this section, we implement the proposed method to solve F$\boldsymbol{D}$E (3) with different two cases through the introduced examples. Also, a comparison with method in [10], which is based on the FDM of fractional derivative is given.

Example 1:

In this example, we consider (3) with $\alpha = 1.8$, of the form:

$$\frac{\partial\, u(x,t)}{\partial\, t} = d(x,t)\frac{\partial^{1.8} u(x,t)}{\partial x^{1.8}} + s(x,t), \quad 0 < x < 1, quadt > 0,$$

with the coefficient function: $d(x,t) = \Gamma(1.2)x^{1.8}$, and the source function: $s(x,t) = 3x^2(2x-1)e^{-t}$, with initial condition: $u(x,0) = x^2(1-x)$, and zero Dirichlet conditions.

Note that the exact solution to this problem is: $u(x,t) = x^2(1-x)e^{-t}$,
which can be verified by applying the fractional differential formula (2).
We apply the suggested method with $m = 3$, and approximate the solution $u(x,t)$ as follows:

$$u_3(x,t) = \sum_{i=0}^{3} u_i(t)\, T_i^*(x). \tag{22}$$

Using Eq.(20) we have:

$$\sum_{i=0}^{3} \dot{u}_i(t) T_i^*(x_p) = d(x_p,t) \sum_{i=2}^{3} \sum_{k=0}^{i-2} u_i(t)\, w_{i,k}^{(1.8)}\, x_p^{i-k-1.8} + s(x_p,t), \qquad p = 0,1, \tag{23}$$

where x_p are roots of the shifted Chebyshev polynomial $T_2^*(x)$, i.e.,

$$x_0 = 0.146447, \qquad x_1 = 0.8872983.$$

By using Eqs.(23) and (21) we obtain the following system of ordinary differential equations:

$$\dot{u}_0(t) + k_1\, \dot{u}_1(t) + k_2\, \dot{u}_3(t) = R_1\, u_2(t) + R_2\, u_3(t) + s_0(t), \tag{24}$$

$$\dot{u}_0(t) + k_{11}\, \dot{u}_1(t) + k_{22}\, \dot{u}_3(t) = R_{11}\, u_2(t) + R_{22}\, u_3(t) + s_1(t), \tag{25}$$

$$u_0(t) - u_1(t) + u_2(t) - u_3(t) = 0, \tag{26}$$

$$u_0(t) + u_1(t) + u_2(t) + u_3(t) = 0, \tag{27}$$

where:

$$k_1 = T_1^*(x_0), \qquad k_2 = T_3^*(x_0), \qquad k_{11} = T_1^*(x_1), \qquad k_{22} = T_3^*(x_1),$$
$$R_1 = d(x_0,t)\, w_{2,0}^{(\alpha)}\, x_0^{2-\alpha}, \qquad R_2 = d(x_0,t)\, [w_{3,0}^{(\alpha)}\, x_0^{3-\alpha} + w_{3,1}^{(\alpha)}\, x_0^{2-\alpha}],$$
$$R_{11} = d(x_1,t)\, w_{2,0}^{(\alpha)}\, x_1^{2-\alpha}, \qquad R_{22} = d(x_1,t)\, [w_{3,0}^{(\alpha)}\, x_1^{3-\alpha} + w_{3,1}^{(\alpha)}\, x_1^{2-\alpha}].$$

Now, we use FDM to solve the system (24)-(27). We will use the following notations: $t_i = i\,\Delta t$ to be the integration time $0 \le t_i \le T$, $\Delta t = \tau = T/N$, for $i = 0, 1, ..., N$. Define $u_i^n = u_i(t_n)$, $s_i^n = s_i(t_n)$. Then the system (24)-(27), is discretize in time and take the following form:

$$\frac{u_0^n - u_0^{n-1}}{\Delta t} + k_1\, \frac{u_1^n - u_1^{n-1}}{\Delta t} + k_2\, \frac{u_3^n - u_3^{n-1}}{\Delta t} = R_1\, u_2^n + R_2\, u_3^n + s_0^n, \tag{28}$$

$$\frac{u_0^n - u_0^{n-1}}{\Delta t} + k_{11}\, \frac{u_1^n - u_1^{n-1}}{\Delta t} + k_{22}\, \frac{u_3^n - u_3^{n-1}}{\Delta t} = R_{11}\, u_2^n + R_{22}\, u_3^n + s_0^n, \tag{29}$$

$$u_0^n - u_1^n + u_2^n - u_3^n = 0, \tag{30}$$

$$u_0^n + u_1^n + u_2^n + u_3^n = 0. \tag{31}$$

We can write the above system (28)-(31) in the following matrix form as follows:

$$\begin{pmatrix} 1 & k_1 & -\tau\, R_1 & k_2 - \tau\, R_2 \\ 1 & k_{11} & -\tau\, R_{11} & k_{22} - \tau\, R_{22} \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{pmatrix}^n = \begin{pmatrix} 1 & k_1 & 0 & k_2 \\ 1 & k_{11} & 0 & k_{22} \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{pmatrix}^{n-1} + \begin{pmatrix} s_0 \\ s_1 \\ 0 \\ 0 \end{pmatrix}^n \tag{32}$$

We will use the notation for the above system:

$$A\, U^n = B\, U^{n-1} + S^n, \qquad \text{or} \quad U^n = A^{-1} B\, U^{n-1} + A^{-1}\, S^n, \tag{33}$$

where: $U^n = (u_0^n,\, u_1^n,\, u_2^n,\, u_3^n)^T$, $S^n = (s_0^n,\, s_1^n,\, 0, 0)^T$. For $n = 1$, the initial solution U^0, can obtain from the initial condition of the problem, $u(x, 0)$ and using Eq.(9).

The obtained numerical results by means of the proposed method are shown in table 1 and figures 1 and 2. In the table 1, the absolute errors between the exact solution u_{ex} and the approximate solution u_{approx}, at $m = 3$, $m = 5$ and $m = 7$ with the final time $T = 2$ are given. But, in the figures 1 and 2, comparison between the exact solution u_{exact}, the numerical solution using [10], u_{FDM}; and the approximate solution using our proposed method u_{Cheb}, at $T = 1$ with time step $\tau = 0.0025$, with $m = 9$ and $m = 11$ respectively. From table 1, it is evident that the overall errors can be made smaller by adding new terms from the series (22).

Table 1: The absolute error between the exact and approximate solutions at $m = 3,\ m = 5$ and $m = 7$ and $T = 2$.

x	$\lvert u_{ex} - u_{approx.}\rvert$ at $m = 3$	$\lvert u_{ex} - u_{approx.}\rvert$ at $m = 5$	$\lvert u_{ex} - u_{approx.}\rvert$ at $m = 7$
0.0	0.170849 e-03	0.274260 e-04	0.300045 e-05
0.1	0.021094 e-03	0.420794 e-04	0.417836 e-05
0.2	0.176609 e-03	0.376716 e-04	0.544655 e-05
0.3	0.301420 e-03	0.844125 e-04	0.617664 e-05
0.4	0.404138 e-03	0.327010 e-04	0.648973 e-05
0.5	0.489044 e-03	0.361133 e-04	0.639512 e-05
0.6	0.563305 e-03	0.194954 e-04	0.595329 e-05
0.7	0.633367 e-03	0.295780 e-04	0.531930 e-05
0.8	0.705677 e-03	0.492488 e-04	0.459538 e-05
0.9	0.786679 e-03	0.283224 e-04	0.379345 e-05
1.0	0.882821 e-03	0.773238 e-04	0.300045 e-05

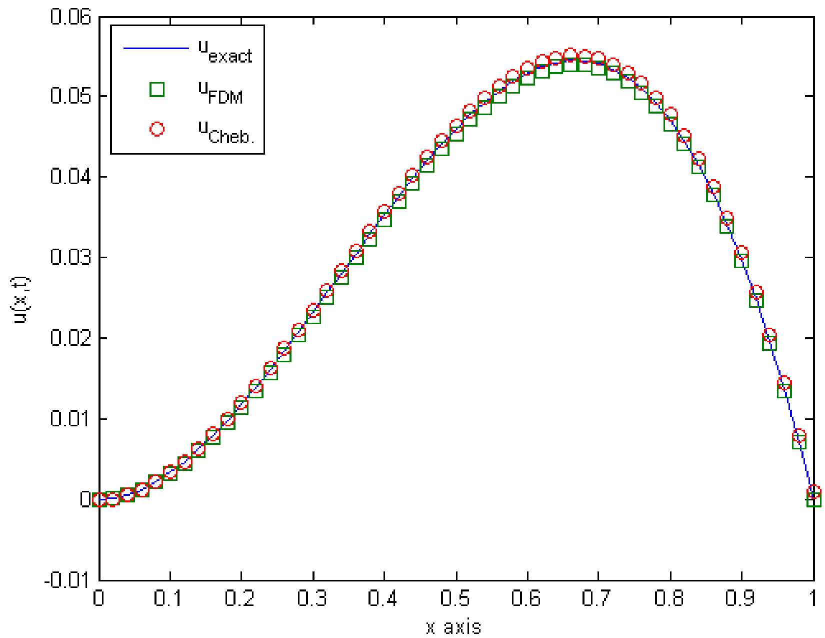

Figure 1. Comparison between the exact solution, the numerical solution using [10] and approximate solution using our proposed method at $T = 1$ with $\tau = 0.0025,\ m = 9$.

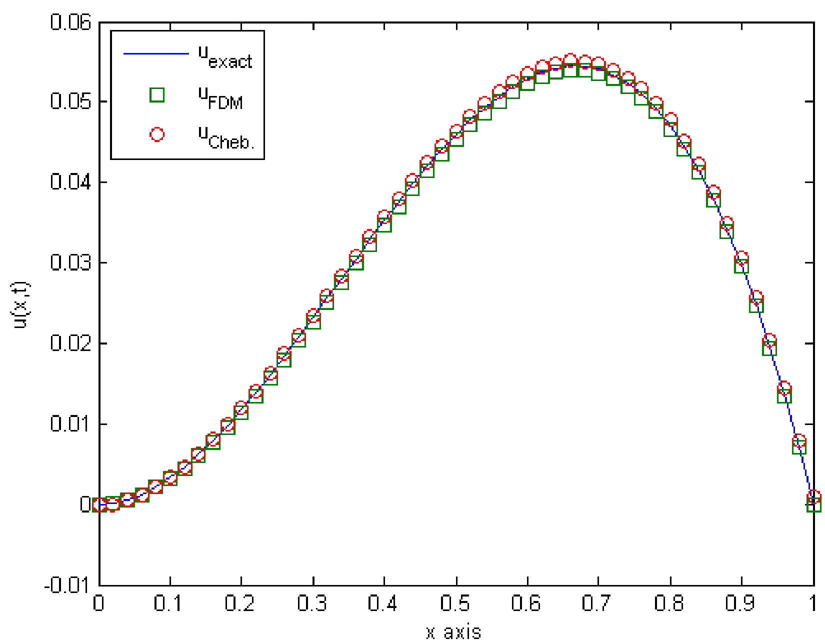

Figure 2. Comparison between the exact solution, the numerical solution using [10] and approximate solution using our proposed method at $T = 1$ with $\tau = 0.0025,\ m = 11$.

Example 2:

In this example, we consider (3) with the following functions:
The initial condition: $u(x;0) = \sin(\pi x) - 0.5x^2(1-x), \quad 0 < x < 1,$
and Dirichlet conditions: $u(0,t) = u(1,t) = 0$.
Note that the exact solution to this problem (in the case $\alpha = 2$) is:

$$u(x,t) = e^{-\pi^2 t}\sin(\pi x) - 0.5x^2(1-x).$$

We apply the suggested method with different values of m. By the same procedure in the first example, we can obtain the approximate solution. In this example we will compare our results with those obtained by the finite difference method (FDM) [10].

The obtained numerical results by means of the proposed method u_{Cheb}, FDM, u_{FDM} and exact solution u_{exact} are shown in figure 3, with the final time $T = 2$ and the time step $\tau = 0.0025$, with $m = 5$ and $\alpha = 2$. Also, the obtained numerical results by means of the proposed method u_{Cheb} and FDM, u_{FDM} are shown in figure 4, with the final time $T = 2$ and the time step $\tau = 0.0025$, with $m = 7$ and $\alpha = 1.5$.

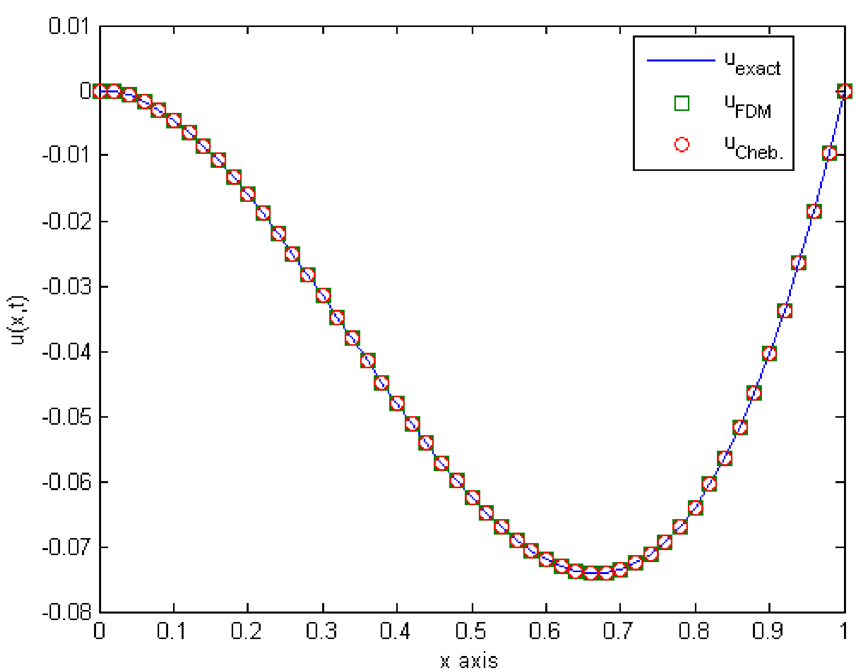

Figure 3. Comparison between the exact solution, the numerical solution using [10] and approximate solution using our proposed method at $T = 2$ with $\tau = 0.0025,\ m = 5$.

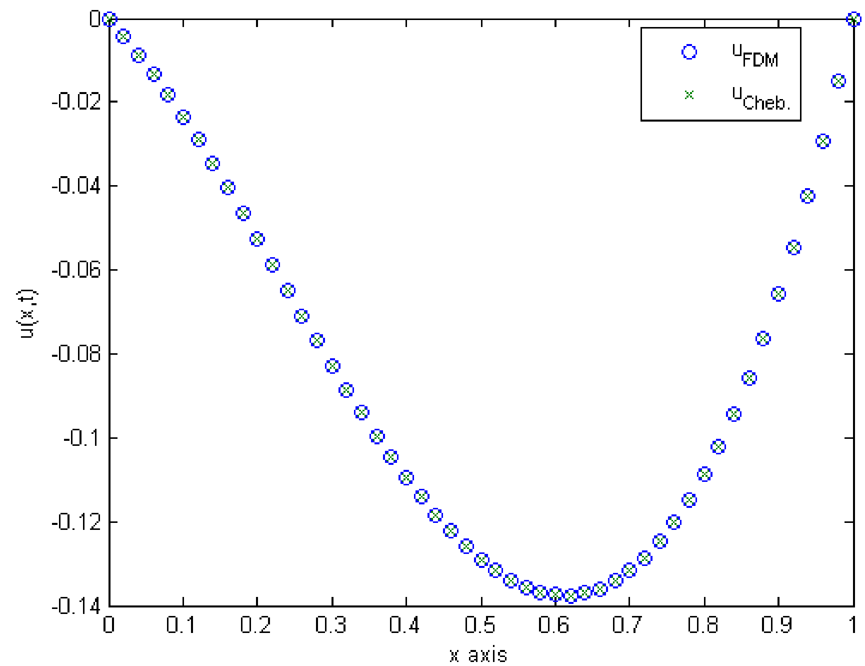

Figure 4. Comparison between, the numerical solution using [10] and the approximate solution using our proposed method at $T = 2$ with $\tau = 0.0025$, $m = 7$ and $\alpha = 1.5$.

5. Conclusion

The properties of the Chebyshev polynomials are used to reduce the fractional diffusion equation to the solution of system of ordinary differential equations. The fractional derivative is considered in the Caputo sense. From the solutions obtained using the suggested method we can conclude that these solutions are in excellent agreement with the already existing ones and show that this approach can be solve the problem effectively. It is evident that the overall errors can be made smaller by adding new terms from the series (22). Comparisons are made between approximate solutions and exact solutions and other methods to illustrate the validity and the great potential of the technique. All numerical results are obtained using Matlab 7.1.

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