Int. J. Adv. Appl. Math. and Mech. 2(1) (2014) 1 - 8
ISSN: 2347-2529
Available online at www.ijaamm.com

International Journal of Advances in **Applied Mathematics and Mechanics**

Solving time-fractional differential diffusion equation by theta-method

Research Article

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Received 11 July 2014; accepted (in revised version) 24 August 2014

Abstract: This paper proposes a numerical method to deal with the one-dimensional time-fractional diffusion equation defined by Caputo fractional derivative. The paper aims to present a general framework of the $\theta-$method for solving time-fractional diffusion differential equations for $(0 \leq \theta \leq 1)$. Consistency, stability and convergence analysis of the method is discussed. Finally, the obtained results reveal that the proposed technique is very effective, convenient and quite accurate to such considered problems.

MSC: 65M06 • 65N12 • 26A33

Keywords: Fractional PDE (FPDE) • Finite differences $\theta-$ method • Caputo fractional derivative • Von-Neumann stability analysis.

1. Introduction

Fractional order partial differential equations are generalizations of classical partial differential equations. Fractional derivatives are almost as old as their more familiar integer-order counterparts. Fractional calculus is one of the interest issues that attract many scientists, specially mathematicians and engineer scientists. Many natural phenomena can be present by fractional differential equations. Many authors in different fields such as chemical physics, fluid flows, electrical networks, viscoelasticity, try to modeling of these phenomena by fractional differential equations. Fractional calculus applied to model many meaningful things, such as fractional differential equation can model price volatility in finance [1, 2], model fast spreading of pollutants in hydrology [3], model the particle motions in a heterogeneous environment and long particle jumps of the anomalous diffusion in physics [4, 5]. The most common hydrologic and physics application of fractional calculus is the generation of fractional Brownian motion as a representation of aquifer material with long-range correlation structure [6, 7]. Other exact description of the applications of engineering, mechanics and mathematics *et al.*, the literature is made to [8–11]. Many cases of the real physical processes could be modeled in a reliable manner using fractional-order differential equations [12, 13]. Most fractional differential equations do not have exact analytic solutions, so approximation and numerical techniques must be used.
Fractional space derivatives are used to model anomalous diffusion or dispersion, where a particle plume spreads at a rate inconsistent with the classical Brownian motion model. When a fractional derivative replaces the second derivative in a diffusion or dispersion model, it leads to enhanced diffusion (also called superdiffusion).

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In this paper, we develop the basic theory of numerical solution for the time-fractional diffusion differential equation

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}=\frac{\partial^2 u(x,t)}{\partial x^2}+h(x,t), \qquad t\in[0,T]. \tag{1}$$

on a finite domain $x_L<x<x_R$. Here, we assume that $0<\alpha\le 1$ as the fractional order of the time derivative. Initial condition $u(x,0)=f(x)$ for $x_L<x<x_R$ and Dirichlet boundary conditions are as follows:
$u(x_L,t)=0$ and $u(x_R,t)=0$.
Published papers on the numerical solution of fractional partial differential equations are scarce. A different method for solving the fractional partial differential equation (1.1) is pursued in the recent paper of [12, 14–18]. The theta-method is generalization of implicit , explicit and Crank-Nicholson methods.

2. Preliminaries

For implementation of this method we need to the following definitions.(see [19, 20])

Definition 2.1 (Caputo fractional derivative).

Caputo fractional derivative $D_t^\alpha u(x,t)$ of order α with respect to time is defined as:

$$\begin{aligned} D_t^\alpha u(x,t)&=\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}\\ &=\frac{1}{\Gamma(n-\alpha)}\int_0^t \frac{1}{(t-\tau)^{\alpha-n+1}}.\frac{\partial^n u(x,\tau)}{\partial \tau^n}d\tau, \quad (n-1<\alpha<n)\end{aligned} \tag{2}$$

(where $\Gamma(.)$ is the Gamma function) and for $\alpha=n\in N$ defined as:

$$D_t^\alpha u(x,t)=\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}=\frac{\partial^n u(x,t)}{\partial t^n}$$

Remark 2.1.

Note that when $\alpha=1$, equation (1) is the clasical heat equation of the following form:

$$\frac{\partial u(x,t)}{\partial t}=\frac{\partial^2 u(x,t)}{\partial x^2},$$

Definition 2.2.

First-order approximation method for the computation of Caputo's fractional derivative which is given by the expression:

$$D_t^\alpha u_i^n \cong g_{\alpha,k}\sum_{j=1}^{n} w_j^{(\alpha)}(u_i^{n-j+1}-u_i^{n-j}), \tag{3}$$

where:

$$g_{\alpha,k}=\frac{1}{\Gamma(1-\alpha)(1-\alpha)k^\alpha} \qquad and \qquad w_j^{(\alpha)}=j^{1-\alpha}-(j-1)^{1-\alpha}.$$

Definition 2.3.

θ -method, $(0\le\theta\le 1)$, is general finite-difference approximation to $\frac{\partial^2 u(x,t)}{\partial x^2}$ given by:

$$\frac{\partial^2 u(x,t)}{\partial x^2}\cong \theta\delta_{2,x}U_{i,j+1}+(1-\theta)\delta_{2,x}U_{i,j}, \tag{4}$$

such that we define:

$$\delta_{2,x}U_{i,j}=\frac{1}{(\Delta x)^2}(U_{i+1,j}-2U_{i,j}+U_{i-1,j}),$$

(where $h=\Delta x=\frac{x_R-x_L}{M}$ for x-axis and $U_{i,j}=U_i^j=U(x_i,t_j)$ represent the numerical approximation solution) In other words:

$$\frac{\partial^2 u(x,t)}{\partial x^2}\cong\frac{1}{h^2}\left\{\theta(U_{i+1}^{j+1}-2U_i^{j+1}+U_{i-1}^{j+1})+(1-\theta)(U_{i+1}^{j}-2U_i^{j}+U_{i-1}^{j})\right\},$$

Remark 2.2.

Note that $\theta=0$ gives the expilicit scheme, $\theta=\frac{1}{2}$ the Crank-Nicolson, and $\theta=1$ a fully implicit backward time-difference method.

3. Discretization of theta-method

Here, we assume $h=\Delta x=\frac{x_R-x_L}{M}$ for x-axis and $k=\Delta t=\frac{T}{K}$ for t-axis as grid size therefore we have: $x_i=x_L+ih; i=1,2,\dots,M$ and $t_j=jk; j=1,2,\dots,K$.
Without loss of generality we assume $h(x,t)=0$. Now, if $U_{i,j}=U(x_i,t_j)$ represent the numerical approximation solution with $\theta-$ method, with the discrete formula (3) is used to estimate the time-fractional derivative we have:

$$g_{\alpha,k}\sum_{j=1}^{n} w_j^{(\alpha)}(U_i^{n-j+1}-U_i^{n-j})+O(k)$$
$$=\frac{1}{h^2}\left\{\theta(U_{i+1}^{j+1}-2U_i^{j+1}+U_{i-1}^{j+1})+(1-\theta)(U_{i+1}^{j}-2U_i^{j}+U_{i-1}^{j})\right\}+O(h^2),$$

and we have:

$$g_{\alpha,k}\sum_{j=1}^{n} w_j^{(\alpha)}(U_i^{n-j+1}-U_i^{n-j})$$
$$=\frac{1}{h^2}\left\{\theta(U_{i+1}^{j+1}-2U_i^{j+1}+U_{i-1}^{j+1})+(1-\theta)(U_{i+1}^{j}-2U_i^{j}+U_{i-1}^{j})\right\}+T(x,t),$$

where $T(x,t)$ is the truncation term. Thus the numerical method is consistent.
The resulting finite difference equations are defined by:

$$g_{\alpha,k}\sum_{j=1}^{n} w_j^{(\alpha)}(U_i^{n-j+1}-U_i^{n-j})$$
$$=\frac{1}{h^2}\left\{\theta(U_{i+1}^{j+1}-2U_i^{j+1}+U_{i-1}^{j+1})+(1-\theta)(U_{i+1}^{j}-2U_i^{j}+U_{i-1}^{j})\right\},$$

or:

$$g_{\alpha,k}w_1^{(\alpha)}(U_i^{n}-U_i^{n-1})=-g_{\alpha,k}\sum_{j=2}^{n} w_j^{(\alpha)}(U_i^{n-j+1}-U_i^{n-j})$$
$$+\frac{1}{h^2}\left\{\theta(U_{i+1}^{j+1}-2U_i^{j+1}+U_{i-1}^{j+1})+(1-\theta)(U_{i+1}^{j}-2U_i^{j}+U_{i-1}^{j})\right\},$$

Also, if we consider $r=\frac{1}{h^2}$ then with reordering we have:
i) for $n=1$, $i=1,2,\dots,N-1$:

$$-r\theta U_{i-1}^1+(g_{\alpha,k}+2r\theta)U_i^1-r\theta U_{i+1}^1=(g_{\alpha,k}+2r(1-\theta))U_i^0+r(1-\theta)(U_{i+1}^0+U_{i-1}^0)$$

ii) for $n\geq 2$, $i=1,2,\dots,N-1$:

$$-r\theta U_{i-1}^n+(g_{\alpha,k}+2r\theta)U_i^n-r\theta U_{i+1}^n=(g_{\alpha,k}+2r(1-\theta))U_i^{n-1}$$
$$+r(1-\theta)(U_{i+1}^{n-1}+U_{i-1}^{n-1})-g_{\alpha,k}\sum_{j=2}^{n} w_j^{(\alpha)}(U_i^{n-j+1}-U_i^{n-j}) \quad (5)$$

with boundary conditions: $U_0^n=U_N^n=0$, $n=1,2,\dots,$
and initial conditions: $U_i^0=f_i=f(x_i)$, $i=1,2,\dots,N-1$, cases (i)and (ii) requires, at each time step, to solve a tridiagonal system of linear equations.

4. Analysis of stability, consistency and convergence

For stability analysis we will use Von-Neumann's method (Fourier series method).(see [21]) In special case for $\theta=\frac{1}{2}$ (Crank-Nicolson Method) we have following theorem.

Theorem 4.1.
The fractional discretization ($\theta=\frac{1}{2}$) for the time-fractional diffusion equation is unconditionally stable for $0\leq\alpha\leq 1$

Proof. To study the stability of the method, we look for a solution of the form $u_j^n = \zeta_n e^{iwjh}, i = \sqrt{-1}$, w real.Therefore (5) becomes:

$$
\begin{aligned}
&-r\zeta_n e^{iw(j-1)h} + (g_{\alpha,k}+2r)\zeta_n e^{iwjh} - r\zeta_n e^{iw(j+1)h} \\
&\quad = (g_{\alpha,k}-2r)\zeta_{n-1} e^{iwjh} + r(\zeta_{n-1} e^{iw(j+1)h} + \zeta_{n-1} e^{iw(j-1)h}) \\
&\quad - g_{\alpha,k}\sum_{j=2}^{n} w_j^{(\alpha)}(\zeta_{n-j+1} e^{iwjh} - \zeta_{n-j} e^{iwjh})
\end{aligned}
$$

with simplifying and reordering we have:

$$
\begin{aligned}
&(1+\frac{2r}{g_{\alpha,k}}(1-cos(wh)))\zeta_n \\
&\quad = (1-\frac{2r}{g_{\alpha,k}})\zeta_{n-1} + \frac{2r}{g_{\alpha,k}}\zeta_{n-1} cos(wh) - \sum_{j=2}^{n} w_j^{(\alpha)}(\zeta_{n-j+1} - \zeta_{n-j})
\end{aligned}
$$

this can be reduced to:

$$
\zeta_n = \frac{(1-\frac{2r}{g_{\alpha,k}})\zeta_{n-1} + \frac{2r}{g_{\alpha,k}}\zeta_{n-1} cos(wh) - \sum_{j=2}^{n} w_j^{(\alpha)}(\zeta_{n-j+1} - \zeta_{n-j})}{(1+\frac{2r}{g_{\alpha,k}}(1-cos(wh)))} \tag{6}
$$

From (6),since

$$
(1+\frac{2r}{g_{\alpha,k}}(1-cos(wh))) \geq 1
$$

for all α, n, w, h, k we have:

$$
\zeta_1 \leq \zeta_0(1-\frac{2r}{g_{\alpha,k}}(1-cos(wh))), \tag{7}
$$

and

$$
\zeta_n \leq \zeta_{n-1}(1-\frac{2r}{g_{\alpha,k}}(1-cos(wh))) - \sum_{j=2}^{n} w_j^{(\alpha)}(\zeta_{n-j+1} - \zeta_{n-j}) \tag{8}
$$

Thus, for $n = 2$; the last inequality implies:

$$
\zeta_2 \leq \zeta_1(1-\frac{2r}{g_{\alpha,k}}(1-cos(wh))) - w_2^{(\alpha)}(\zeta_1 - \zeta_0) \tag{9}
$$

Repeating the process until

$$
\zeta_j \leq \zeta_{j-1}, \qquad j = 1, 2, \ldots, n-1,
$$

we finally have:

$$
\zeta_n \leq \zeta_{n-1}(1-\frac{2r}{g_{\alpha,k}}(1-cos(wh))) - \sum_{j=2}^{n} w_j^{(\alpha)}(\zeta_{n-j+1} - \zeta_{n-j}) \leq \zeta_{n-j}
$$

since each term in the summation is negative. This shows that the inequalities (7) and (8) imply

$$
\zeta_n \leq \zeta_{n-1} \leq \zeta_{n-2} \leq \ldots \leq \zeta_1 \leq \zeta_0
$$

Thus, $\quad \zeta_n = |U_j^n| \leq \zeta_0 = |U_j^0| = |f_j|, \quad$ which entails $||U_j^n|| \leq ||f_j||, \quad$ and we have stability. □

Remark 4.1.
If U be an approximated solution and u be exact solution and $F_{i,j}(U) = 0$ represent approximated difference equation of FPDE at mesh point (x_i, t_j). By substitution U with u value $F_{i,j}(u) = T_{i,j}$ represented local truncation error (LTE) at mesh point (x_i, t_j).

Theorem 4.2.
The truncation error $T(x,t)$ of the fractional finite difference $\theta-$scheme is: $\qquad T(x,t) = O(k) + O(h^2)$.

Proof.

$$T(x,t) = g_{\alpha,k}\sum_{j=1}^{n} w_j^{(\alpha)}(U_i^{n-j+1} - U_i^{n-j}) - \frac{1}{h^2}\left[\theta\left(U_{i+1}^{j+1} - 2U_i^{j+1} + U_{i-1}^{j+1}\right) + (1-\theta)\left(U_{i+1}^{j} - 2U_i^{j} + U_{i-1}^{j}\right)\right],$$

that with Taylor expansion we can write:

$$T(x,t) = g_{\alpha,k}\sum_{j=1}^{n} w_j^{(\alpha)}\left[\left(u_i^n + (k-1)\frac{\partial u}{\partial t} + \frac{(k-1)^2}{2}\frac{\partial^2 u}{\partial t^2} + \ldots\right) - \left(u_i^n - k\frac{\partial u}{\partial t} + \frac{k^2}{2}\frac{\partial^2 u}{\partial t^2} + \ldots\right)\right] + O(k)$$
$$- \frac{\theta}{h^2}\left[\left(u_i^n - h\frac{\partial u}{\partial x} + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2} + \ldots\right) - 2u_i^n + \left(u_i^n + h\frac{\partial u}{\partial x} + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2} + \ldots\right)\right]$$
$$- \frac{(1-\theta)}{h^2}\left[\left(u_i^{n-1} - h\frac{\partial u}{\partial x} + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2} + \ldots\right) - 2u_i^{n-1} + \left(u_i^{n-1} + h\frac{\partial u}{\partial x} + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2} + \ldots\right)\right],$$

Finally:

$$T(x,t) = O(k) + O(h^2).$$

□

Corollary 4.1.
This theorem shows that this method is consistent , because for $h \to 0$ and $\Delta t \to 0$, LTE tend to zero.

Corollary 4.2.
According to stability analysis and consistency of this method, now from Lax-Richtmyer's equivalence theorem (see [21]), this method is convergence.

5. Numerical Examples

Now, we implement two examples for (1) to comparing exact and numerical solutions.

Example 5.1.
Consider equation (1) as

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2}, \qquad t \in [0,T].$$

on $\Omega = \{(x,t)|0 < x < 1, 0 \le t \le T\}$ with initial conditions:

$$u(x,0) = sin(\pi x), \quad 0 < x < 1$$

and boundary conditions:

$$u(0,t) = 0, \quad u(1,t) = 0, \quad t \ge 0$$

We can show that exact solution for $\alpha = 1$ is:

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

The approximated and exact solutions shown in Figure 1 verify the reliability of presented method. The maximum absolute error value for some different values of $\theta, \alpha, \Delta x, \Delta t$ are given in Table 1.

Example 5.2.
Consider equation (1) as

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} + h(x,t), \qquad t \in [0,T].$$

on $\Omega = \{(x,t)|0 < x < 1, 0 \le t \le T\}$ with initial conditions:

$$u(x,0) = x(1-x), \quad 0 < x < 1$$

Table 1. Max. absolute Error of Example 5.1 for different θ at time $T = 1$.

h=Δx	k=Δt	θ	Max.Error
0.1	0.1	0.5	0.001514
		0.6	0.001378
		0.7	0.001424
		0.8	0.001645
		0.9	0.001698
0.05	0.05	0.5	4.2319 e-04
		0.6	4.1875 e-04
		0.7	4.3217 e-04
		0.8	4.3987 e-04
		0.9	4.4598 e-04

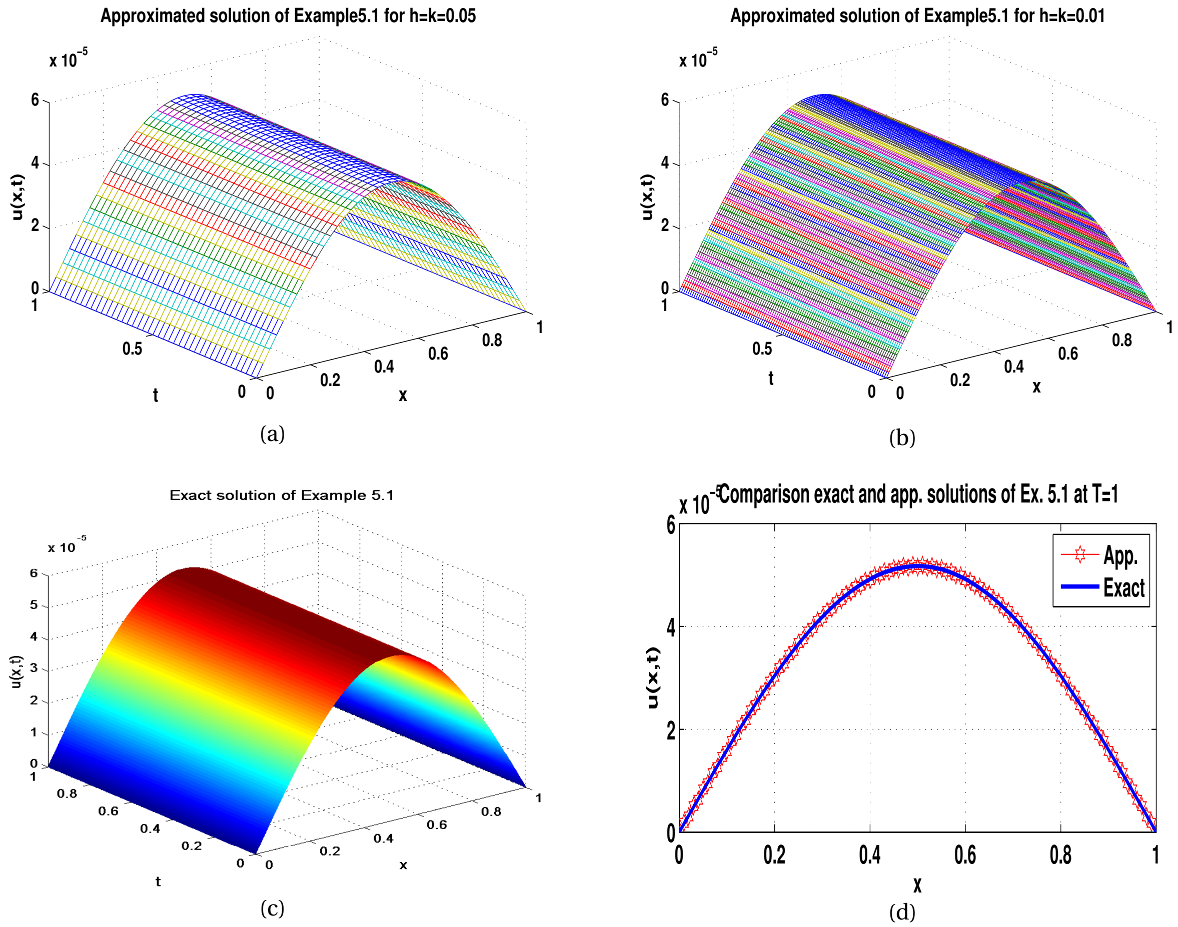

Fig. 1. Comparison between exact and numerical solutions for the Example 5.1 with $\alpha = 1$

and boundary conditions: $u(0,t) = 0, \quad u(1,t) = 0, \quad t \geq 0$
We can show that exact solution is:

$$u(x,t) = x(1-x)cos(x+t),$$

when

$$h(x,t) = x(1-x)cos(x+t+\frac{\alpha\pi}{2}) - (1-2x)cos(x+t) + x(1-x)sin(x+t),$$

The approximated and exact solutions shown in Fig. 2 verify the reliability of presented method. The maximum absolute error value for some different values of $\theta, \alpha, \Delta x, \Delta t$ are given in Table 2.

Table 2. Max. absolute Error of Example 5.2 for different α, θ at time $T = 1$.

h=Δx	k=Δt	α	θ	Max.Error
0.1	0.1	0.5	0.5	0.001471
			0.6	0.001394
			0.7	0.001462
			0.8	0.001524
			0.9	0.001602
0.05	0.05	0.75	0.5	2.1124 e-04
			0.6	2.0915 e-04
			0.7	2.1231 e-04
			0.8	2.1301 e-04
			0.9	2.1386 e-04

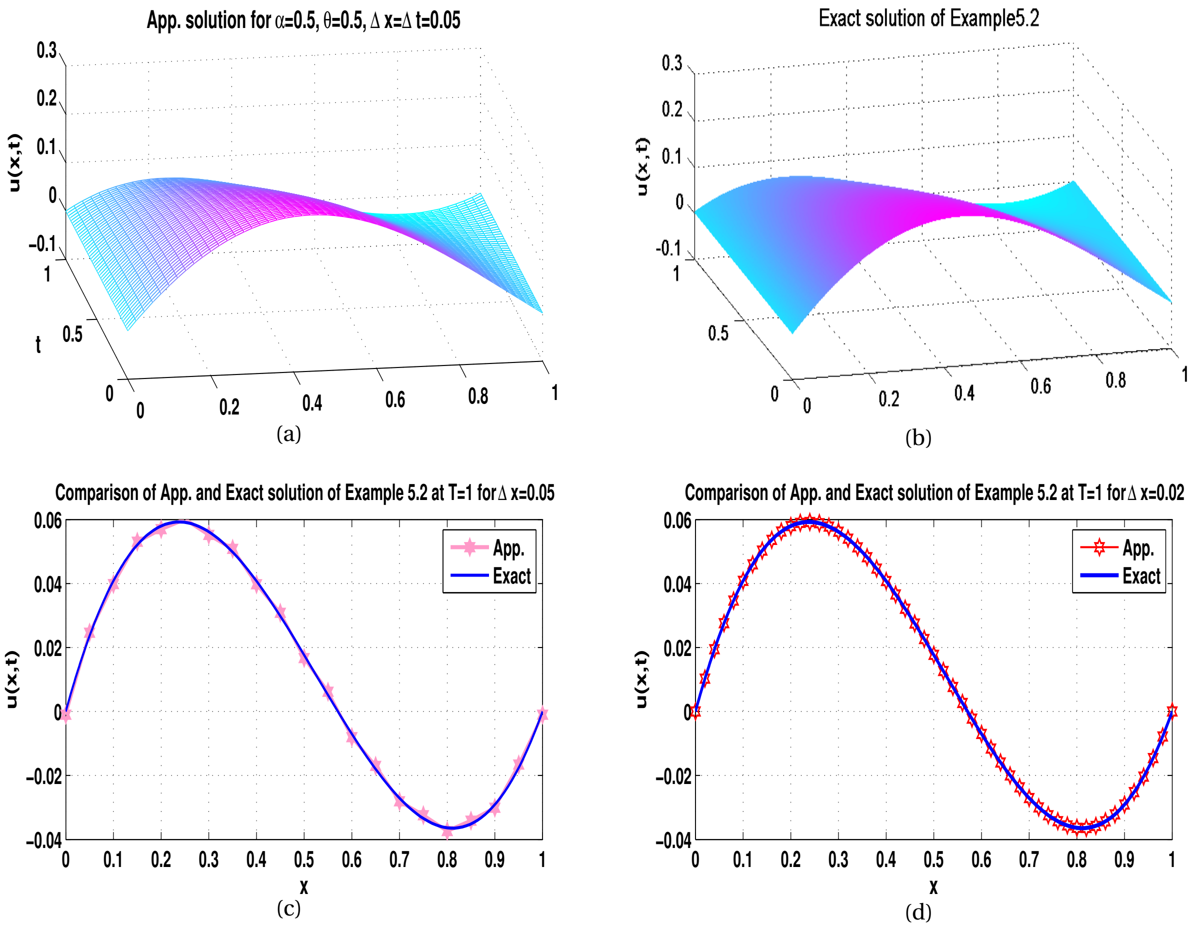

Fig. 2. The behavior of numerical solutions for the Example 5.2 for different $\Delta x, \Delta t$ and $\alpha = 0.5, \theta = 0.5$,

6. Conclusion

In this paper we presented a numerical scheme for solving one-dimensional time-fractional diffusion equation defined by Caputo fractional derivative. The method employed to find the numerical solutions of these equations is based on the approximation for Caputo fractional derivative. The computational results are found to be in good agreement with the exact solutions.

Acknowledgements

The authors would like to thank the referees and reviewers for their valuable comments and suggestions to improve the quality of the paper.

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