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Pseudospectral operational matrix for numerical solution of single and multiterm time fractional diffusion equation

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Abstract: This paper presents a new numerical approach to solve single and multiterm time fractional diffusion equations. In this work, the space dimension is discretized to the Gauss – Lobatto points. We use the normalized Grunwald approximation for the time dimension and a pseudospectral successive integration matrix for the space dimension. This approach shows that with fewer numbers of points, we can approximate the solution with more accuracy. Some examples with numerical results in tables and figures displayed.

Key words: Pseudospectral integration matrix, normalized Grunwald approximation, Gauss – Lobatto points, multi-term fractional diffusion equation

1. Introduction

In recent years, due to the accuracy of fractional differential equations in describing a variety of engineering and physics fields, such as kinetics [23, 24, 26, 27, 34, 35, 39], solid mechanics [32], quantum systems [38], magnetic plasma [25], and economics [3], many researchers are interested in fractional calculus. In [39] the concepts of fractional kinetic, such as particle dynamics in different potentials, particle advection in fluids, plasma physics, fusion devices, and quantum optics, were discussed. The fractional kinetics of the diffusion, diffusion-advection, and Fokker – Planck type were presented, which derived from the generalization of the master equations, and the Langevin equations were presented [23].

However, because of the complex structure of the fractional kinetic equations, analytical solutions of these equations are very rare. Hence, the study of the numerical methods to solve these equations is increasing. The time fractional diffusion equation is one of these equations that we will focus on for the new numerical solution for it. In this equation the first-order time derivative is replaced by a fractional derivative of order $0 < \alpha \leq 1$. Some numerical methods for the single-term time fractional diffusion equations are as follows.

Valko and Abate [36] proposed numerical inversion of the 2-D Laplace transform to solve the time fractional diffusion equation on a semiinfinite domain. Li and Xu [15] developed the numerical solution for time fractional diffusion equations based on spectral methods for both time and space dimensions, and they also [17] presented a numerical approach based on FDM in time and the Legendre spectral method in space. Podlubny et al. [31] presented a general method based on the matrix form representation of the discretized fractional operator

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[30]. Murio [24] developed an implicit unconditionally stable numerical approach to solve time fractional diffusion equations on a finite slab. Scherer et al. [33], for numerical solution of time fractional diffusion equations with nonzero initial conditions, presented a modification of the Grunwald − Letnikov approximation for the Caputo time derivative. The authors of [12] proposed a numerical method to solve FPDEs based on the high-order finite element method for space and FDM for time. A numerical method for the solution of time fractional diffusion equations in one- and two-dimensional cases was presented in [5], which applied FDM in time and the Kansa method in the space dimension. Dou and Hon [7] proposed a numerical computation for backward time fractional diffusion equations, and also some examples in one- and two-dimensional cases were considered. Wei and Zhang [37] considered a Cauchy problem of 1-D time fractional diffusion equations. Finally, the Sinc − Harr collocation method [28], a new difference scheme [1] to solve time fractional diffusion equations, was presented.

In this paper, we consider the multiterm time fractional diffusion equation

$$\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}} + \sum_{i=1}^{m} b_i \frac{\partial^{\beta_i} u(x,t)}{\partial t^{\beta_i}} - \frac{\partial^2 u(x,t)}{\partial x^2} = f(x,t), \qquad (x,t) \in [-1,1] \times [0,T] \tag{1}$$

with initial and boundary conditions

$$u(x,0) = v(x), \quad u(-1,t) = g_1(t), \quad u(1,t) = g_2(t), \qquad (x,t) \in [-1,1] \times [0,T]$$

where $0 \leq \beta_i \leq 1$ and $\frac{\partial^{\alpha} u}{\partial t^{\alpha}}$ is the Caputo fractional derivative of order $0 \leq \alpha \leq 1$. Unlike the single-term fractional diffusion equation, mathematical studies on the numerical solution for the multiterm fractional diffusion equation are very rare. Some studies on the multiterm fractional diffusion equation were presented in [13, 16, 19, 21].

Now we present a new numerical approach to solve the time fractional diffusion equation in which the space dimension is discretized to Gauss − Lobatto points, and then a pseudospectral integration matrix is applied. Hence, we review briefly the history of the pseudospectral integration matrix, which is the main method in this paper. El-Gendi [9] presented an operational matrix based on the Clenshaw − Curtis quadrature scheme [6] to solve some linear integral equations of Fredholm and Volterra types, and then he extended this method for the solution of the linear integrodifferential and ODEs. El-Gendi et al. [10] presented a new matrix for successive integration of a function, which was generalization of the El-Gendi operational matrix [9]. Elbarbary [8] used some properties of integrals and derivatives of Chebyshev polynomials and modified the El-Gendi successive integration matrix [10] to derive an operational matrix for n-fold integrations (pseudospectral integration matrix) of a function. This matrix has more accurate results. Gholami [11], for the first time, applied this matrix with the FDM to solve a PDE, and then in [2] with coauthors used this matrix to solve a PDE alone. Now we apply the pseudospectral successive integration matrix for the space dimension and normalized Grunwald approximation for the time dimension to solve single and multiterm time fractional diffusion equations.

2. Preliminaries

2.1. Concepts of fractional derivatives

In this subsection we present the most important definitions for the fractional derivatives.

Definition 2.1.1. The Riemann – Liouville fractional derivative of order $m-1<\alpha<m$ is

$$ {}_aD_x^{\alpha} f(x) = \left[\frac{1}{\Gamma(m-\alpha)} \frac{d^m}{d\xi^m} \int_a^{\xi} (\xi-\eta)^{m-\alpha-1} f(\eta)\, d\eta \right]_{\xi=x}, \tag{2} $$

$$ {}_xD_b^{\alpha} f(x) = \left[\frac{1}{\Gamma(m-\alpha)} \frac{d^m}{d\xi^m} \int_{\xi}^{b} (\eta-\xi)^{m-\alpha-1} f(\eta)\, d\eta \right]_{\xi=x}. \tag{3} $$

Definition 2.1.2. The Caputo fractional derivative of order $m-1<\alpha<m$ is

$$ {}_a^CD_x^{\alpha} f(x) = \frac{1}{\Gamma(m-\alpha)} \int_a^{x} (x-\eta)^{m-\alpha-1} f^{(m)}(\eta)\, d\eta, \tag{4} $$

$$ {}_x^CD_b^{\alpha} f(x) = \frac{1}{\Gamma(m-\alpha)} \int_x^{b} (\eta-x)^{m-\alpha-1} f^{(m)}(\eta)\, d\eta. \tag{5} $$

Definition 2.1.3. [20] The Grunwald – Letnikov fractional derivative of order $m-1<\alpha<m$ is

$$ D_{a^+}^{\alpha} f(x) = \lim_{h\to 0, nh=x-a} h^{-\alpha} \sum_{j=0}^{n} (-1)^j \binom{\alpha}{j} f(x-jh), \tag{6} $$

$$ D_{b^-}^{\alpha} f(x) = \lim_{h\to 0, nh=b-x} h^{-\alpha} \sum_{j=0}^{n} (-1)^j \binom{\alpha}{j} f(x+jh). \tag{7} $$

From [29] we can write

$$ D_{a^+}^{\alpha} f(x) = \sum_{j=0}^{m-1} \frac{f^{(j)}(a)(x-a)^{j-\alpha}}{\Gamma(j-\alpha+1)} + \frac{1}{\Gamma(m-\alpha)} \int_a^{x} (x-\eta)^{m-\alpha-1} f^{(m)}(\eta)\, d\eta, \tag{8} $$

$$ D_{b^-}^{\alpha} f(x) = \sum_{j=0}^{m-1} \frac{(-1)^j f^{(j)}(b)(b-x)^{j-\alpha}}{\Gamma(j-\alpha+1)} + \frac{(-1)^m}{\Gamma(m-\alpha)} \int_x^{b} (\eta-x)^{m-\alpha-1} f^{(m)}(\eta)\, d\eta, \tag{9} $$

for $m-1<\alpha<m$. Using repeated integration by parts and then differentiation of the Riemann – Liouville fractional derivative we have

$$ \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{d\xi^m} \int_a^{\xi} (\xi-\eta)^{m-\alpha-1} f(\eta)\, d\eta = \sum_{j=0}^{m-1} \frac{f^{(j)}(a)(\xi-a)^{j-\alpha}}{\Gamma(j-\alpha+1)} $$

$$ + \frac{1}{\Gamma(m-\alpha)} \int_a^{\xi} (\xi-\eta)^{m-\alpha-1} f^{(m)}(\eta)\, d\eta. \tag{10} $$

Similarly,

$$ \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{d\xi^m} \int_{\xi}^{b} (\eta-\xi)^{m-\alpha-1} f(\eta)\, d\eta = \sum_{j=0}^{m-1} \frac{(-1)^j f^{(j)}(b)(b-\xi)^{j-\alpha}}{\Gamma(j-\alpha+1)} $$

$$+\frac{(-1)^m}{\Gamma(m-\alpha)}\int_\xi^b (\eta-\xi)^{m-\alpha-1} f^{(m)}(\eta)\, d\eta. \tag{11}$$

These equations show that

$${}_aD_x^\alpha f(x) = D_{a^+}^\alpha f(x), \qquad {}_bD_x^\alpha f(x) = D_{b^-}^\alpha f(x). \tag{12}$$

Indeed, the Grunwald − Letnikov derivative and the Riemann − Liouville derivative are equivalent if the function $f(x)$ has $m-1$ continuous derivatives and $f^{(m)}(x)$ is integrable on closed interval $[a,b]$. Using this fact [18], by the relationship between the Riemann − Liouville fractional derivative and the Grunwald − Letnikov fractional derivative we will derive a numerical solution such that we use the Riemann − Liouville definition during problem formulation and then the Grunwald − Letnikov definition for achieving the numerical solution. From the standard Grunwald definition we have:

Definition 2.1.4. [40] The standard Grunwald formula for $u(x,t)$ for which $a \le x \le b$ is

$$D_{a^+}^\alpha u(x,t) = \lim_{M_1\to\infty} h_1^{-\alpha}\sum_{j=0}^{M_1}(-1)^j\binom{\alpha}{j}u(x-jh_1,t), \tag{13}$$

$$D_{b^-}^\alpha u(x,t) = \lim_{M_2\to\infty} h_2^{-\alpha}\sum_{j=0}^{M_2}(-1)^j\binom{\alpha}{j}u(x+jh_2,t), \tag{14}$$

where $M_1, M_2 \in N, h_1 = \frac{x-a}{M_1}, h_2 = \frac{b-x}{M_2}$ and $g_\alpha^{(j)}$ are the normalized Grunwald weights functions defined as

$$g_\alpha^{(j)} = -\frac{\alpha-j+1}{j}\, g_\alpha^{(j-1)}, \qquad j = 1,2,3,... \tag{15}$$

with $g_\alpha^{(0)} = 1$.

Let $\Omega = [a,b]\times[0,T], (x,t)\in\Omega, t_k = k\tau, k = 0(1)n, x_i = a+ih, i = 0(1)m$, with $\tau = \frac{T}{n}$ and $h = \frac{b-a}{m}$ being time and space steps, respectively. From [22], for $u(x,t)\in L^1(\Omega), D_{a^+}^\alpha u(x,t)\in \ell(\Omega)$ and $D_{b^-}^\alpha u(x,t)\in\ell(\Omega)$, we obtain

$$D_{a^+}^\alpha u(x_i,t_k) = h^{-\alpha}\sum_{j=0}^{i}(-1)^j\binom{\alpha}{j}u(x_{i-j},t_k) + O(h), \tag{16}$$

$$D_{b^-}^\alpha u(x_i,t_k) = h^{-\alpha}\sum_{j=0}^{m-i}(-1)^j\binom{\alpha}{j}u(x_{i+j},t_k) + O(h). \tag{17}$$

2.2. Pseudospectral integration matrix

We assume that $(P_N f)(x)$ is the Nth order Chebyshev interpolating polynomial of the function $f(x)$ at the points $(x_k, f(x_k))$ where

$$(P_N f)(x) = \sum_{j=0}^{N} f_j\,\varphi_j(x), \tag{18}$$

with

$$\varphi_j(x) = \frac{2\alpha_j}{N} \sum_{r=0}^{N} \alpha_r \, T_r(x) \, T_r(x_j), \tag{19}$$

where $\varphi_j(x_k) = \delta_{j,k}$ ($\delta_{j,k}$ is the Kronecker delta) and $\alpha_0 = \alpha_N = 1/2$, $\alpha_j = 1$ for $j = 1(1)N-1$. Since $(P_N f)(x)$ is a unique interpolating polynomial of order N, it can be expressed in terms of a series expansion of the classical Chebyshev polynomials, and hence we have

$$(P_N f)(x) = \sum_{r=0}^{N} a_r \, T_r(x), \tag{20}$$

where

$$a_r = \frac{2\alpha_r}{N} \sum_{j=0}^{N} \alpha_j \, f(x_j) \, T_r(x_j). \tag{21}$$

The successive integration of $f(x)$ in the interval $[-1, x_k]$ can be estimated by successive integration of $(P_N f)(x)$. Thus, we have

$$I_n(f) \simeq \sum_{r=0}^{N} a_r \int_{-1}^{x} \int_{-1}^{t_{n-1}} \int_{-1}^{t_{n-2}} \dots \int_{-1}^{t_2} \int_{-1}^{t_1} T_r(t_0) \, dt_0 \, dt_1 \dots dt_{n-2} \, dt_{n-1}. \tag{22}$$

Theorem 1. *[14] The exact relation between Chebyshev functions and their derivatives is expressed as*

$$T_r(x) = \sum_{m=0}^{n} \frac{(-1)^m \binom{n}{m}}{2^n \chi_m} T^{(n)}_{r+n-2m}, \qquad r > n,$$

where

$$\chi_m = \prod_{\substack{j=0 \\ j \neq n-m}}^{n} (r + n - m - j).$$

Theorem 2. *[8] The successive integration of Chebyshev polynomials is expressed in terms of Chebyshev polynomials as*

$$\int_{-1}^{x} \int_{-1}^{t_{n-1}} \int_{-1}^{t_{n-2}} \dots \int_{-1}^{t_2} \int_{-1}^{t_1} T_r(t_0) \, dt_0 \, dt_1 \dots dt_{n-2} \, dt_{n-1} = \sum_{m=0}^{n-\gamma_r} \beta_r \, \frac{(-1)^m \binom{n}{m}}{2^n \chi_m} \, \xi_{n,m,r}(x),$$

where

$$\xi_{n,m,r}(x) = T_{r+n-2m}(x) - \sum_{i=0}^{n-1} \eta_i \, T^{(i)}_{r+n-2m}(-1),$$

$$\eta_i = \sum_{j=0}^{i} \frac{x^j}{(i-j)! j!}, \qquad \chi_m = \prod_{\substack{j=0 \\ j \neq n-m}}^{n} (r + n - m - j),$$

$$\beta_i = \begin{cases} 2 & i = 0, \\ 1 & i > 0, \end{cases} \qquad \gamma_i = \begin{cases} n & i = 0, \\ n - i + 1 & 1 \leq i \leq n, \\ 0 & i > n. \end{cases}$$

Thus, from Theorem 2 and relations (21) and (22), we have

$$I_n(f) \simeq \sum_{j=0}^{N} \left(\frac{2\alpha_j}{N} \sum_{r=0}^{N} \alpha_r \, T_r(x_j) \sum_{m=0}^{n-\gamma_r} \beta_r \, \frac{(-1)^m \binom{n}{m}}{2^n \chi_m} \, \xi_{n,m,r}(x) \right) f(x_j).$$

The matrix form of the successive integration of the function $f(x)$ at the Gauss–Lobatto points x_k is

$$[I_n(f)] = \left[\sum_{j=0}^{N} \left(\frac{2\alpha_j}{N} \sum_{r=0}^{N} \alpha_r \, T_r(x_j) \sum_{m=0}^{n-\gamma_r} \beta_r \, \frac{(-1)^m \binom{n}{m}}{2^n \chi_m} \, \xi_{n,m,r}(x) \right) f(x_j) \right] = \Theta^{(n)}[f]. \tag{23}$$

The elements of the matrix $\Theta^{(n)}$ are

$$\vartheta_{k,j}^{(n)} = \frac{2\alpha_j}{N} \sum_{r=0}^{N} \alpha_r \, T_r(x_j) \sum_{m=0}^{n-\gamma_r} \beta_r \, \frac{(-1)^m \binom{n}{m}}{2^n \chi_m} \, \xi_{n,m,r}(x_k). \tag{24}$$

The matrix $\Theta^{(n)}$ in (23), presented in [8], is called the pseudospectral integration matrix.

3. Single and multiterm fractional diffusion equations

3.1. Time fractional diffusion equation

We consider the time fractional diffusion equation

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = k(t) \frac{\partial^2 u(x,t)}{\partial x^2} + q(t)\, u(x,t) + f(x,t), \qquad (x,t) \in [-1,1] \times [0,T], \tag{25}$$

with initial condition

$$u(x,0) = v(x), \qquad -1 \le x \le 1,$$

and boundary conditions

$$u(-1,t) = g_1(t), \quad u(1,t) = g_2(t), \qquad 0 \le t \le T,$$

where $\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}$ is the Caputo fractional derivative of order $0 \le \alpha \le 1$ and $v(x)$, g_1 and g_2 are known functions. In equation (12) it is illustrated that the Grunwald − Letnikov derivative and Riemann − Liouville derivative are equivalent under the discussed conditions. Hence, we use this fact to derive a numerical approach [18] for the solution of fractional differential equations such that in these equations we use the Riemann − Liouville definition during problem formulation and then the Grunwald − Letnikov definition for deriving the numerical solution. The relationship between Caputo derivative $\frac{\partial^\alpha}{\partial t^\alpha}$ and Riemann − Liouville derivative ${}_0D_t^\alpha$ is [4]

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = {}_0D_t^\alpha u(x,t) - \frac{u(x,0)}{t^\alpha \Gamma(1-\alpha)}, \qquad 0 \le \alpha \le 1.$$

Hence, we can write equation (25) for $0 \le \alpha \le 1$ as

$${}_0D_t^\alpha u(x,t) - \frac{v(x)}{t^\alpha \Gamma(1-\alpha)} = k(t) \frac{\partial^2 u(x,t)}{\partial x^2} + q(t)\, u(x,t) + f(x,t), \qquad (x,t) \in [-1,1] \times (0,T]. \tag{26}$$

Now we apply the pseudospectral integration matrix for discretization of the space dimension to the Gauss − Lobatto points $x_i = -\cos\frac{i\pi}{N}$ for $N \in \mathbb{N}$. Assume that

$$\frac{\partial^2 u(x,t)}{\partial x^2}\bigg|_{x_i} = \varphi(x_i,t), \tag{27}$$

$$\frac{\partial u(x,t)}{\partial x}\bigg|_{x_i} = \sum_{j=0}^{N} \vartheta_{i,j}^{(1)}\,\varphi(x_j,t) + c_1, \tag{28}$$

$$u(x_i,t) = \sum_{j=0}^{N} \vartheta_{i,j}^{(2)}\,\varphi(x_j,t) + c_1(x_i+1) + c_2, \tag{29}$$

for $i = 0(1)N$. We can find the constants c_1 and c_2 to satisfy the boundary conditions. From these conditions we obtain

$$c_1 = -\frac{1}{2}\bigg(\sum_{j=0}^{N} \vartheta_{N,j}^{(2)}\,\varphi(x_j,t) + g_1(t) - g_2(t)\bigg), \qquad c_2 = g_1(t).$$

By substituting c_1 and c_2 into (29), we have

$$u(x_i,t) = \sum_{j=0}^{N} \vartheta_{i,j}^{(2)}\,\varphi(x_j,t)\; - \frac{1}{2}(x_i+1)\sum_{j=0}^{N} \vartheta_{N,j}^{(2)}\,\varphi(x_j,t)\; + p_i(t), \tag{30}$$

in which

$$P_i(t) = -\frac{1}{2}(x_i+1)\big(g_1(t) - g_2(t)\big) + g_1(t). \tag{31}$$

Now, we substitute (27) and (30) into main equation (26) to obtain

$$\sum_{j=0}^{N} \vartheta_{i,j}^{(2)}\,{}_0D_t^{\alpha}\varphi(x_j,t)\; - \frac{1}{2}(x_i+1)\sum_{j=0}^{N} \vartheta_{N,j}^{(2)}\,{}_0D_t^{\alpha}\varphi(x_j,t)$$

$$= q(t)\bigg(\sum_{j=0}^{N} \vartheta_{i,j}^{(2)}\,\varphi(x_j,t)\; - \frac{1}{2}(x_i+1)\sum_{j=0}^{N} \vartheta_{N,j}^{(2)}\,\varphi(x_j,t)\; + p_i(t)\bigg)$$

$$+k(t)\varphi(x_i,t) - {}_0D_t^{\alpha}p_i(t) + \frac{v(x_i)}{t^{\alpha}\Gamma(1-\alpha)} + f(x_i,t), \qquad i = 0(1)N. \tag{32}$$

Let

$$t_k = k\tau, \qquad k = 0(1)m, \qquad \tau = \frac{T}{m},$$

and use the Grunwald − Letnikov approximation instance with the Riemann − Liouville derivative in the time dimension to obtain the numerical formula as

$${}_0D_{t_k}^{\alpha}\varphi(x_j,t) = \tau^{-\alpha}\sum_{r=0}^{k} g_{\alpha}^{(r)}\varphi(x_j,t_{k-r}), \qquad k = 0(1)m, \tag{33}$$

where $g_\alpha^{(r)}$ are normalized Grunwald weights functions. Hence, we insert (33) into (32) to obtain

$$\tau^{-\alpha}\sum_{r=0}^{k} g_\alpha^{(r)}\Big(\sum_{j=0}^{N}\vartheta_{i,j}^{(2)}\,\varphi(x_j,t_{k-r})\,-\frac{1}{2}(x_i+1)\sum_{j=0}^{N}\vartheta_{N,j}^{(2)}\,\varphi(x_j,t_{k-r})\Big)$$

$$=q(t_k)\Big(\sum_{j=0}^{N}\vartheta_{i,j}^{(2)}\,\varphi(x_j,t_k)\,-\frac{1}{2}(x_i+1)\sum_{j=0}^{N}\vartheta_{N,j}^{(2)}\,\varphi(x_j,t_k)\,+p_i(t_k)\Big)+k(t_k)\varphi(x_i,t_k)$$

$$+\frac{v(x_i)}{t_k^\alpha\Gamma(1-\alpha)}-{}_0D_{t_k}^\alpha p_i(t_k)+f(x_i,t_k),\qquad i=0(1)N,k=1(1)m. \tag{34}$$

We recall from [2] to summarize

$$\mathbf{A_i}=\big[\vartheta_{i,0}^{(2)},\vartheta_{i,1}^{(2)},...,\vartheta_{i,N}^{(2)}\big]-\frac{1}{2}(X_i+1)\big[\vartheta_{N,0}^{(2)},\vartheta_{N,1}^{(2)},...,\vartheta_{N,N}^{(2)}\big], \tag{35}$$

$$\Phi^k=\big[\varphi_{0,k},\varphi_{1,k},...,\varphi_{N,k}\big]^t, \tag{36}$$

and then apply $g_\alpha^{(0)}=1$ to obtain

$$\Big[\big(\tau^{-\alpha}-q(t_k)\big)\mathbf{A_i}\Big]\Phi^k-k(t_k)\varphi(x_i,t_k)=\frac{v(x_i)}{t_k^\alpha\Gamma(1-\alpha)}-{}_0D_{t_k}^\alpha p_i(t_k)$$

$$+p_i(t_k)q(t_k)+f(x_i,t_k)-\tau^{-\alpha}\sum_{r=1}^{k}g_\alpha^{(r)}\mathbf{A_i}\Phi^{k-r} \tag{37}$$

for $i=0(1)N$ and $k=1(1)m$. Indeed, (37) is the following system:

$$\mathbb{A}^k\Phi^k=\mathbb{B}^k \tag{38}$$

for $i=0(1)N$ and $k=1(1)m$ since $\Phi^0=\varphi(x_i,0)=V''(x_i)$ from the initial condition. With all unknowns $\varphi(x_i,t_k)$ obtained by solving this system, finally we can approximate the solutions from equation (30).

3.2. The multiterm time fractional diffusion equation

We consider the multiterm time fractional diffusion equation (1) for $m=1$ and $b_1=1$ as

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}+\frac{\partial^\beta u(x,t)}{\partial t^\beta}=\frac{\partial^2 u(x,t)}{\partial x^2}+f(x,t),\qquad (x,t)\in[-1,1]\times[0,T], \tag{39}$$

with initial condition

$$u(x,0)=v(x),\qquad -1\le x\le 1,$$

and boundary conditions

$$u(-1,t)=g_1(t),\quad u(1,t)=g_2(t),\qquad 0\le t\le T,$$

with $0 \leq \alpha, \beta \leq 1$. Similar to the previous subsection, we apply a pseudospectral integration matrix for $x_i = -cos(\frac{i\pi}{N})$ and we have the same procedure as in (27)–(31) exactly. Now, from the relationship between Caputo and Riemann–Liouville fractional derivatives, we can write equation (39) as

$$ {}_0D_t^{\alpha} u(x,t) + {}_0D_t^{\beta} u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + \mathbf{F}(x,t), \qquad (x,t) \in [-1,1] \times [0,T], \tag{40}$$

in which

$$\mathbf{F}(x,t) = f(x,t) + v(x)\left(\frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{t^{-\beta}}{\Gamma(1-\beta)}\right).$$

Substituting (27) and (30) into main equation (40) gives us

$$\sum_{j=0}^{N} \vartheta_{i,j}^{(2)} \, {}_0D_t^{\alpha} \varphi(x_j,t) - \frac{1}{2}(x_i+1) \sum_{j=0}^{N} \vartheta_{N,j}^{(2)} \, {}_0D_t^{\alpha} \varphi(x_j,t)$$

$$+ \sum_{j=0}^{N} \vartheta_{i,j}^{(2)} \, {}_0D_t^{\beta} \varphi(x_j,t) - \frac{1}{2}(x_i+1) \sum_{j=0}^{N} \vartheta_{N,j}^{(2)} \, {}_0D_t^{\beta} \varphi(x_j,t)$$

$$= \varphi(x_i,t) + \mathbf{H}_{\alpha,\beta}(x_i,t), \qquad i = 0(1)N, \tag{41}$$

in which

$$\mathbf{H}_{\alpha,\beta}(x_i,t) = \mathbf{F}(x_i,t) - {}_0D_t^{\alpha} P_i(t) - {}_0D_t^{\beta} P_i(t).$$

Let

$$t_k = k\tau, \qquad k = 0(1)m, \qquad \tau = \frac{T}{m},$$

and use the normalized Grunwald–Letnikov approximation instance of the Riemann–Liouville derivative as

$$ {}_0D_{t_k}^{\alpha} \varphi(x_j,t) = \tau^{-\alpha} \sum_{r=0}^{k} g_{\alpha}^{(r)} \varphi(x_j, t_{k-r}), \qquad k = 0(1)m, \tag{42}$$

$$ {}_0D_{t_k}^{\beta} \varphi(x_j,t) = \tau^{-\beta} \sum_{r=0}^{k} g_{\alpha}^{(r)} \varphi(x_j, t_{k-r}), \qquad k = 0(1)m. \tag{43}$$

By using the notations in [2] and equations (42) and (43) we can write equation (41) as

$$\left(\tau^{-\alpha} \sum_{r=0}^{k} g_{\alpha}^{(r)} + \tau^{-\beta} \sum_{r=0}^{k} g_{\beta}^{(r)}\right) \mathbf{A_i} \, \Phi^{k-r} - \varphi(x_i,t_k) = \mathbf{H}_{\alpha,\beta}(x_i,t_k), \tag{44}$$

for $i = 0(1)N$ and $k = 1(1)m$. Finally, because $g_{\alpha}^{(0)} = 1$ for any α, we have

$$\left(\tau^{-\alpha} + \tau^{-\beta}\right) \mathbf{A_i} \, \Phi^{k} - \varphi(x_i,t_k) = \mathbf{H}_{\alpha,\beta}(x_i,t_k) - \mathbf{A_i} \sum_{r=1}^{k} \left[\tau^{-\alpha} g_{\alpha}^{(r)} + \tau^{-\beta} g_{\beta}^{(r)}\right] \Phi^{k-r}, \tag{45}$$

for $i = 0(1)N$ and $k = 1(1)m$. Indeed, (45) is the following system:

$$\mathrm{A}\,\Phi^k = \mathrm{B}^k, \qquad i = 0(1)N, \qquad k = 1(1)N. \tag{46}$$

For $k = 0$ from the initial condition we have $\Phi^0 = \varphi(x_i, 0) = V''(x_i)$. All unknowns $\varphi(x_i, t_k)$ are obtained by solving this system and finally we can approximate the solutions from equation (30).

4. Numerical results

Example 1. *Consider the time fractional diffusion equation in [1] by translating $0 \le x \le 1$ to $-1 \le X \le 1$ as*

$$\frac{\partial^\alpha w(X,t)}{\partial t^\alpha} = 4k(t)\frac{\partial^2 w(X,t)}{\partial X^2} - q(t)w(X,t) + f(X,t), \tag{47}$$

where $0 \le t \le 1$ and $0 \le \alpha \le 1$ with initial condition

$$w(x,0) = 0, \qquad -1 \le X \le 1,$$

and boundary conditions

$$w(-1,t) = w(1,t) = 0, \qquad 0 \le t \le 1,$$

in which $k(t) = e^t$, $q(t) = 1 - \sin(2t)$ and

$$f(X,t) = \left[\pi^2\, t^2\, e^t + t^2(1 - \sin(2t)) + \frac{2t^{2-\alpha}}{\Gamma(3-\alpha)}\right] \sin\Big(\frac{\pi(X+1)}{2}\Big).$$

The exact solution of this equation is $w(X,t) = t^2 \sin\big(\frac{\pi(X+1)}{2}\big)$. The numerical results of this problem are presented in the Tables 1–3 and Figures 1–4.

Table 1. Max errors for example 1 when $N = 4$ and $m = 4$.

t	$\alpha = 0.1$	$\alpha = 0.75$	$\alpha = 0.85$	$\alpha = 0.95$
0.25	4.98E –4	8.47E –3	1.07E –2	1.32E –2
0.5	8.64E –4	9.74E –3	1.18E –2	1.40E –2
0.75	1.13E –3	9.12E –3	1.06E –2	1.20E –2
1	1.35E –3	8.02E –3	8.95E –3	9.77E –3

Example 2. *We consider the one-dimensional multiterm time fractional diffusion equation in [13] by translating $0 \le x \le 1$ to $-1 \le X \le 1$ as*

$$\frac{\partial^\alpha w(X,t)}{\partial t^\alpha} + \frac{\partial^\beta w(X,t)}{\partial t^\beta} - 4\frac{\partial^2 w(X,t)}{\partial X^2} = f(X,t), \quad (X,t) \in [-1,1]\times[0,1], \quad 0 \le \alpha,\beta \le 1, \tag{48}$$

with initial and boundary conditions

$$w(X,0) = \frac{1-X^2}{4}, \qquad w(-1,t) = w(1,t) = 0,$$

and

$$f(X,t) = \left(\frac{t^{2-\alpha}}{\Gamma(3-\alpha)} + \frac{t^{2-\beta}}{\Gamma(3-\beta)}\right)\Big(\frac{1-X^2}{2}\Big) + 2(1+t^2).$$

Table 2. Max errors for example 1 when $N = 4$ and $m = 10$.

t	$\alpha = 0.1$	$\alpha = 0.75$	$\alpha = 0.85$	$\alpha = 0.95$
0.1	$9.56E$ –5	$2.49E$ –3	$3.26E$ –3	$4.14E$ –3
0.2	$1.84E$ –4	$3.50E$ –3	$4.54E$ –3	$5.77E$ –3
0.3	$2.65E$ –4	$3.94E$ –3	$5.00E$ –3	$6.25E$ –3
0.4	$3.43E$ –4	$4.11E$ –3	$5.08E$ –3	$6.20E$ –3
0.5	$4.18E$ –4	$4.13E$ –3	$4.98E$ –3	$5.93E$ –3
0.6	$4.92E$ –4	$4.06E$ –3	$4.79E$ –3	$5.57E$ –3
0.7	$5.67E$ –4	$3.94E$ –3	$4.57E$ –3	$5.19E$ –3
0.8	$6.44E$ –4	$3.80E$ –3	$4.32E$ –3	$4.82E$ –3
0.9	$7.24E$ –4	$3.65E$ –3	$4.09E$ –3	$4.48E$ –3
1	$8.07E$ –4	$3.51E$ –3	$3.87E$ –3	$4.18E$ –3

Table 3. Max errors for example 1 when $N = 4, 8$ and $m = 20$.

t	$\alpha = 0.1$	$\alpha = 0.75$	$\alpha = 0.85$	$\alpha = 0.95$
0.05	$2.62E$ –5	$8.73E$ –4	$1.15E$ –3	$1.45E$ –3
0.1	$5.18E$ –5	$1.35E$ –3	$1.80E$ –3	$2.31E$ –3
0.15	$7.69E$ –5	$1.65E$ –3	$2.18E$ –3	$2.81E$ –3
0.2	$1.02E$ –4	$1.84E$ –3	$2.40E$ –3	$3.09E$ –3
0.25	$1.27E$ –4	$1.96E$ -3	$2.53E$ –3	$3.22E$ –3
0.3	$1.53E$ –4	$2.04E$ -3	$2.59E$ –3	$3.26E$ –3
0.35	$1.79E$ –4	$2.09E$ –3	$2.62E$ –3	$3.24E$ –3
0.4	$2.06E$ -4	$2.12E$ –3	$2.62E$ –3	$3.19E$ –3
0.45	$2.34E$ –4	$2.13E$ –3	$2.60E$ –3	$3.12E$ –3
0.5	$2.63E$ –4	$2.14E$ –3	$2.57E$ –3	$3.04E$ –3
0.55	$2.93E$ –4	$2.13E$ –3	$2.53E$ –3	$2.96E$ –3
0.6	$3.25E$ –4	$2.12E$ –3	$2.49E$ –3	$2.87E$ –3
0.65	$3.57E$ –4	$2.10E$ –3	$2.44E$ –3	$2.78E$ –3
0.7	$3.91E$ –4	$2.08E$ –3	$2.39E$ –3	$2.70E$ –3
0.75	$4.26E$ –4	$2.06E$ –3	$2.35E$ –3	$2.62E$ –3
0.8	$4.62E$ –4	$2.04E$ –3	$2.30E$ –3	$2.54E$ –3
0.85	$5.00E$ –4	$2.02E$ –3	$2.26E$ –3	$2.48E$ –3
0.9	$5.40E$ –4	$2.01E$ –3	$2.22E$ –3	$2.41E$ –3
0.95	$5.80E$ –4	$1.99E$ –3	$2.19E$ –3	$2.35E$ –3
1	$6.23E$ –4	$1.97E$ –3	$2.15E$ –3	$2.30E$ –3

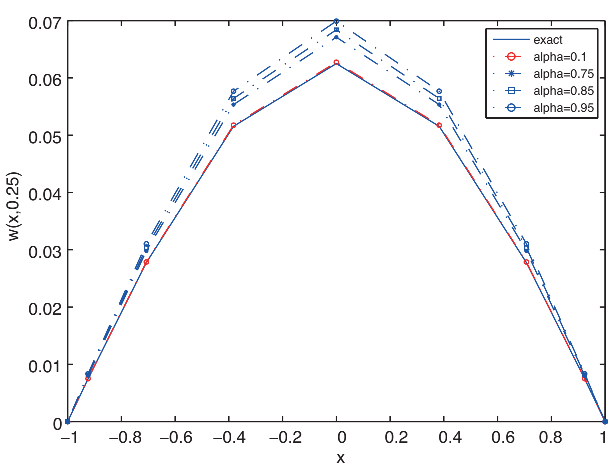

Figure 1. Comparison of numerical solutions of example 1 at $t = 0.25$.

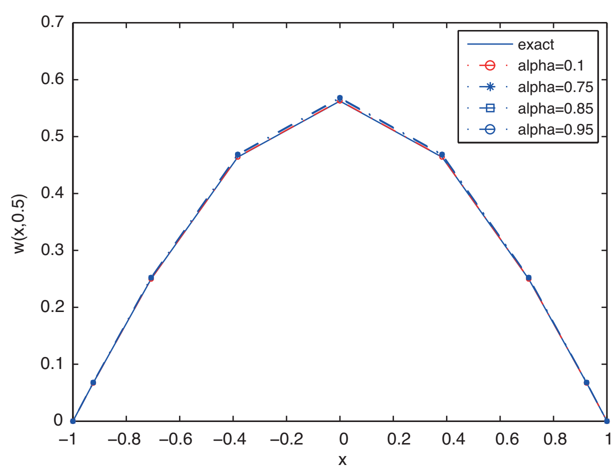

Figure 2. Comparison of numerical solutions of example 1 at $t = 0.75$.

The exact solution of (48) *is*

$$w(X,t) = (1+t^2)\left(\frac{1-X^2}{4}\right).$$

The numerical results of this problem are presented in the Tables 4 and 5 and Figures 5–7.

Example 3. *Considering the time fractional diffusion equation in [28] by translating* $0 \le x \le 1$ *to* $-1 \le X \le 1$

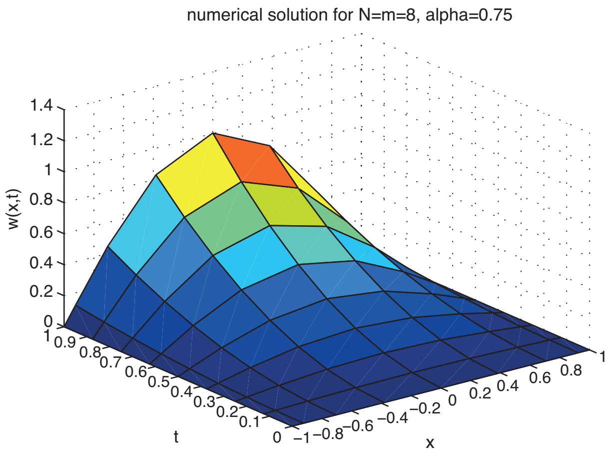

Figure 3. The approximation solution of example 1 when $\alpha = 0.75$.

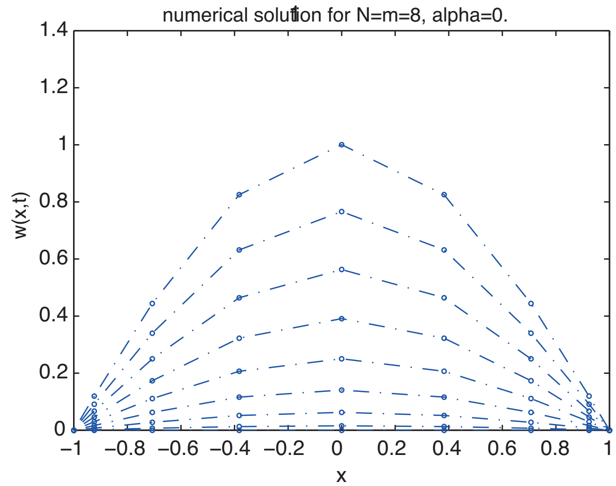

Figure 4. The approximation solution of example 1 when $\alpha = 0.1$.

Table 4. Max errors for example 2 when $N = m = 4$ and $\beta = 0.2$.

t	$\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 0.95$
0.25	$4.25E-3$	$5.55E-3$	$5.54E-3$
0.5	$3.19E-3$	$4.59E-3$	$6.59E-3$
0.75	$3.16E-3$	$4.65E-3$	$6.99E-3$
1	$3.39E-3$	$5.00E-3$	$7.28E-3$

Table 5. Max errors for example 2 when $N = 5, m = 10$ and $\beta = 0.2$.

t	$\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 0.95$
0.1	$3.76E-3$	$4.92E-3$	$2.17E-3$
0.2	$2.12E-3$	$2.97E-3$	$2.52E-3$
0.3	$1.57E-3$	$2.23E-3$	$2.56E-3$
0.4	$1.33E-3$	$1.92E-3$	$2.55E-3$
0.5	$1.22E-3$	$1.79E-3$	$2.53E-3$
0.6	$1.18E-3$	$1.74E-3$	$2.53E-3$
0.7	$1.17E-3$	$1.73E-3$	$2.54E-3$
0.8	$1.18E-3$	$1.75E-3$	$2.57E-3$
0.9	$1.21E-3$	$1.79E-3$	$2.59E-3$
1	$1.24E-3$	$1.84E-3$	$2.61E-3$

as

$$\frac{\partial^\alpha w(X,t)}{\partial t^\alpha} - 4\frac{\partial^2 w(X,t)}{\partial X^2} = f(X,t), \qquad (X,t) \in [-1,1]\times[0,1], \qquad 0 \le \alpha \le 1, \tag{49}$$

with initial and boundary conditions

$$w(X,0) = 0, \qquad w(-1,t) = w(1,t) = 0,$$

and

$$f(X,t) = \left(\frac{\Gamma(3)}{\Gamma(3-\alpha)}\, t^{2-\alpha} + 4\pi^2\, t^2\right)\sin\big(\pi(X+1)\big),$$

the exact solution of (49) *is*

$$w(X,t) = t^2 \sin\big(\pi(X+1)\big).$$

The numerical results of this problem are presented in the Tables 6–8 and Figures 8–10.

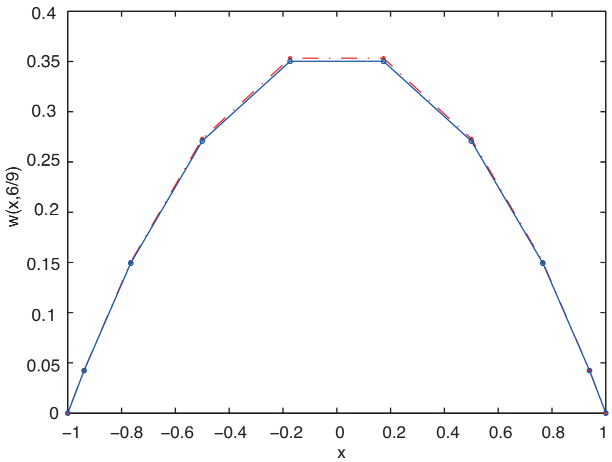

Figure 5. Comparison of numerical and exact solutions of example 2 for $\alpha = 0.95, \beta = 0.2$ at $t = \frac{6}{9}$.

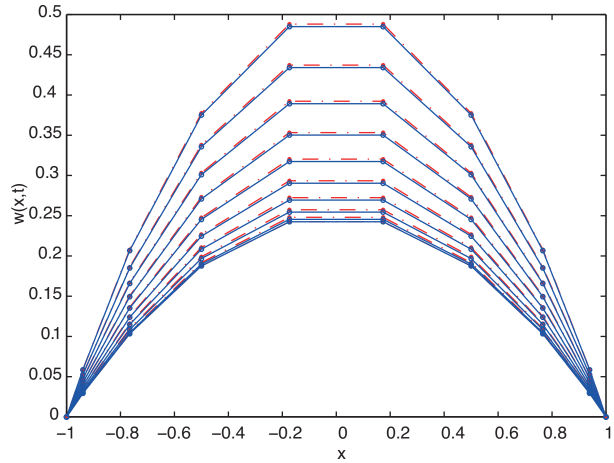

Figure 6. Comparison of numerical and exact solutions of example 2 for $\alpha = 0.95, \beta = 0.2$.

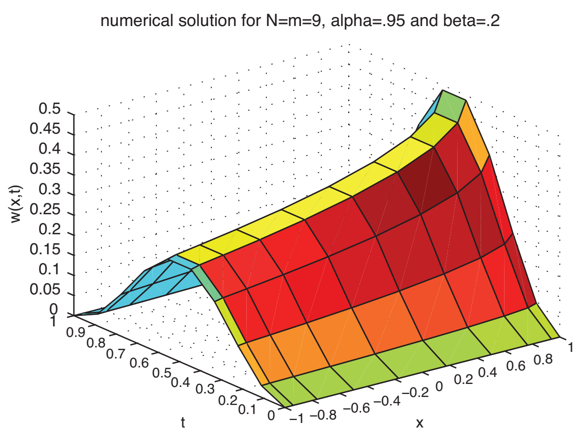

Figure 7. The approximation solution of example 2 when $\alpha = 0.95$ and $\beta = 0.2$.

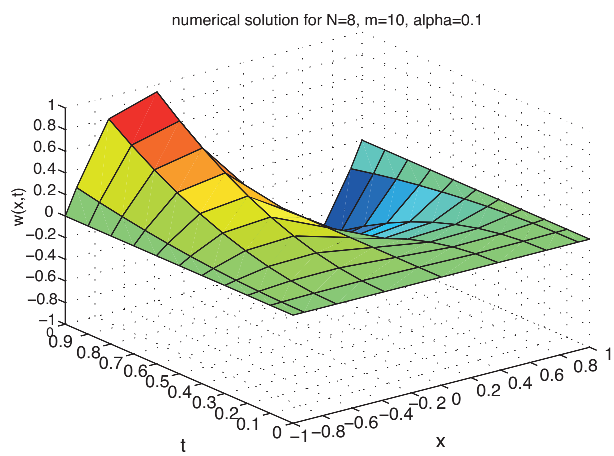

Figure 8. The approximation solution of example 3 for $N = m = 8$ when $\alpha = 0.1$.

Table 6. Max errors for example 3 when $N = 4$ and $m = 4$.

t	$\alpha = 0.1$	$\alpha = 0.5$	$\alpha = 0.99$
0.25	$4.50E -3$	$3.43E -3$	$2.58E -4$
0.5	$1.82E -2$	$1.66E -2$	$1.33E -2$
0.75	$4.13E -2$	$3.91E -2$	$3.61E -2$
1	$7.36E -2$	$7.11E -2$	$6.83E -2$

Table 7. Max errors for example 3 when $N = 8$ and $m = 4$.

t	$\alpha = 0.1$	$\alpha = 0.5$	$\alpha = 0.99$
0.25	$1.55E -4$	$1.42E -3$	$5.25E -3$
0.5	$3.00E -4$	$2.15E -3$	$5.77E -3$
0.75	$4.36E -4$	$2.70E -3$	$5.84E -3$
1	$5.64E -4$	$3.15E -3$	$5.85E -3$

5. Conclusion

In this paper, a new numerical approach for solutions of single and multiterm time fractional diffusion equations is presented, in which the pseudospectral operational matrix has a critical role. For the first attempt, two numerical methods, the pseudospectral integration matrix and normalized Grunwald approximation, are applied

Table 8. Max errors for example 3 when $N = 8$ and $m = 10$.

t	$\alpha = 0.1$	$\alpha = 0.5$	$\alpha = 0.99$
0.1	$2.70E-5$	$3.49E-4$	$1.84E-3$
0.2	$5.25E-5$	$5.35E-4$	$2.21E-3$
0.3	$7.64E-5$	$6.73E-4$	$2.30E-3$
0.4	$9.90E-5$	$7.88E-4$	$2.32E-3$
0.5	$1.21E-4$	$8.89E-4$	$2.32E-3$
0.6	$1.41E-4$	$9.78E-4$	$2.32E-3$
0.7	$1.61E-4$	$1.06E-3$	$2.31E-3$
0.8	$1.81E-4$	$1.13E-3$	$2.30E-3$
0.9	$2.00E-4$	$1.20E-3$	$2.27E-3$
1	$2.17E-4$	$1.27E-3$	$2.09E-3$

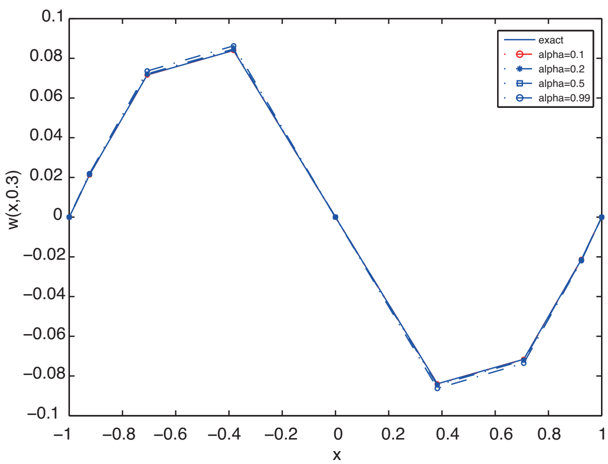

Figure 9. Comparison of numerical solutions of example 3 at $t = 0.3$.

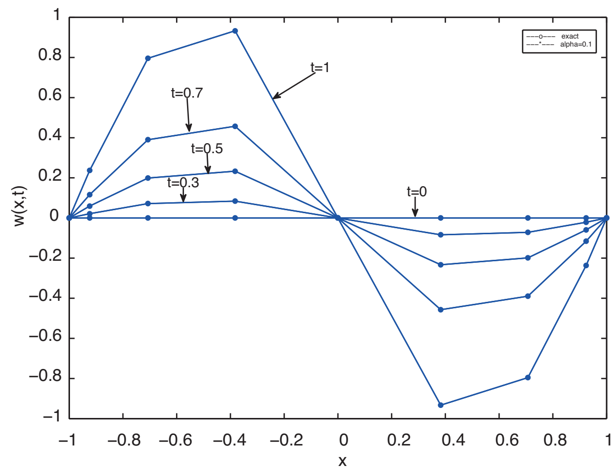

Figure 10. Comparison of numerical solutions of example 3 at some values of t.

simultaneously. The significance of this work is the presentation of a new discretization of the space dimension based on the Gauss−Lobatto points. This method shows that with fewer number of points we can approximate the solutions with enough accuracy. Finally, we hope to use the pseudospectral operational matrix for the solution of fractional partial differential equations alone.

References

[1] Alikhanov AA. A new difference scheme for the time fractional diffusion equation. J Comput Phys 2015; 280: 424-438.

[2] Babolian E, Gholami S, Javidi M. A numerical solution for one-dimensional parabolic equation based on pseudo-spectral integration matrix. Appl Comput Math 2014; 13: 306-315.

[3] Baillie RT. Long memory processes and fractional integration in econometrics. J Econom 1996; 73: 5-59.

[4] Chen S, Liu F, Zhuang P, Anh V. Finite difference approximations for the fractional Fokker-Planck equation. Appl Math Model 2009; 33: 256-273.

[5] Chen W, Ye L, Sun H. Fractional diffusion equations by the Kansa method. Comp Math Appl 2010; 59: 1614-1620.

[6] Clenshaw CW. The numerical solution of linear differential equations in Chebushev series. P Camb Philos Soc 1957; 53: 134-149.

[7] Dou FF, Hon YC. Numerical computation for backward time-fractional diffusion equation. Eng Anal Bound Elem 2014; 40: 138-146.

[8] Elbarbary EME. Pseudo-spectral integration matrix and boundary value problems. Int J Comp Math 2007; 84: 1851-1861.

[9] El-Gendi SE. Chebyshev solution of differential, integral, and integro-differential equations. Comp J 1969; 12: 282-287.

[10] El-Gendi SE, Nasr H, El-Hawary HM. Numerical solution of Poisson's equation by expansion in Chebyshev polynomials. Bull Calcutta Math Soc 1992; 84: 443-449.

[11] Gholami S. A numerical solution for one-dimensional parabolic equation using pseudo-spectral integration matrix and FDM. R J Appl Sci Eng Tech 2014; 7: 801-806.

[12] Jiang Y, Ma J. High-order finite element methods for time-fractional partial differential equations. J Comput Appl Math 2011; 235: 3285-3290.

[13] Jin B, Lazarov R, Liu Y, Zhou Z. The Galerkin finite element method for a multi-term time-fractional diffusion equation. J Comput Phys 2015; 281: 825-843.

[14] Khalifa AK, Elbarbary EME, Abd-Elrazek MA. Chebyshev expansion method for solving second and fourth order elliptic equations. Appl Math Comput 2003; 135: 307-318.

[15] Li X, Xu C. A space-time spectral method for the time fractional diffusion equation. SIAM J Numer Anal 2009; 47: 21082131.

[16] Li Z, Liu Y, Yamamoto M. Initial-boundary value problems for multi-term time-fractional diffusion equations with positive constant coefficients. Appl Math Comput 2013; 257: 381-397.

[17] Lin Y, Xu C. Finite difference/spectral approximations for the time fractional diffusion equation. J Comput Phys 2007; 225: 1533-1552.

[18] Liu F, Anh V, Turner I. Numerical solution of the space fractional Fokker-Planck equation. J Comput Appl Math 2004; 166: 209-219.

[19] Liu F, Meerschaert MM, McGough RJ, Zhuang P, Liu X. Numerical methods for solving the multi-term time-fractional wave-diffusion equation. Frac Cal Appl Anal 2013; 16: 9-25.

[20] Lorenzo CF, Hartley TT. Initialization, Conceptualization, and Application in the Generalized Fractional Calculus. Cleveland, OH, USA: Lewis Research Center, 1998.

[21] Luchko Y. Initial-boundary-value problems for the generalized multi-term time-fractional diffusion equations. J Math Anal Appl 2011; 374: 538-548.

[22] Meerschaert MM, Tadjeran C. Finite difference approximations for fractional advection-dispersion equations. J Comput Appl Math 2004; 172: 65-77.

[23] Metzler R, Klafter J. The random walk's guide to anomalous diffusion: a fractional dynamics approach. Phys Reports 2000; 339: 1-77.

[24] Murio AD. Implicit finite difference approximation for time fractional diffusion equations. Comp Math Appl 2008; 56: 1138-1145.

[25] Negrete DDC, Carreras BA, Lynch VE. Front dynamics in reaction-diffusion systems with Levy flights: a fractional diffusion approach. Phys Rev Lett 2003; 91: 018301-018304.

[26] Pagnini G. Short note on the emergence of fractional kinetics. Physica A 2014; 409: 29-34.

[27] Philippa B, Robson RE, White RD. Generalized phase-space kinetic and diffusion equations for classical and dispersive trasnport. New J Phys 2014; 16: 073040.

[28] Pirkhedri A, Javadi HHS. Solving the time fractional diffusion equation via Sinc-Haar collocation method. Appl Math Comput 2015; 257: 317-326.

[29] Podlubny I. Fractional Differential Equations. San Diego, CA, USA: Academic Press, 1999.

[30] Podlubny I. Matrix approach to discrete fractional calculus. Fractional Calculus and Applied Analysis 2000; 3: 359-386.

[31] Podlubny I, Chechkin A, Skovranek T, Chen Y, Jara VB. Matrix approach to discrete fractional calculus II: partial fractional differential equations. J Comput Phys 2009; 228: 3137-3153.

[32] Rossikhin YA, Shitikova MV. Applications of fractional calculus to dynamic problems of linear and nonlinear hereditary mechanics of solids. Appl Mech Rev 1997; 50: 15-67.

[33] Scherer R, Kalla SL, Boyadjiev L, Al-Saqabi B. Numerical treatment of fractional heat equations. Appl Numer Math 2008; 58: 1212-1223.

[34] Sibatov RT, Uchaikin VV. Fractional differential kinetics of charge transport in unordered semiconductors. Semiconductors 2007; 41: 335-340.

[35] Sokolov IM, Klafter J, Blumen A. Fractional kinetics. Phys Today 2002; 55: 48-54.

[36] Valko PP, Abate J. Numerical inversion of 2-d Laplace transforms applied to fractional diffusion equation. Appl Numer Math 2005; 53: 73-88.

[37] Wei T, Zhang ZQ. Stable numerical solution to a Cauchy problem for a time fractional diffusion equation. Eng Anal Bound Elem 2014; 40: 128-137.

[38] Wu JN, Huang HC, Cheng SC, Hsieh WF. Fractional Langevin equation in quantum systems with memory effect. Appl Math 2014; 5: 1741-1749.

[39] Zaslavsky G. Chaos, fractional kinetics and anomalous transport. Phys Rep 2002; 371: 461-580.

[40] Zhuang P, Liu F, Anh V, Turner I. Numerical methods for the variable-order fractional advection-diffusion equation with a nonlinear source term. SIAM J Numer Anal 2009; 47: 1760-1781.