SOLVING THE TIME-FRACTIONAL DIFFUSION EQUATION USING A LIE GROUP INTEGRATOR

by

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In this paper, we propose a numerical method to approximate the solutions of time fractional diffusion equation which is in the class of Lie group integrators. Our utilized method, namely fictitious time integration method transforms the unknown dependent variable to a new variable with one dimension more. Then the group preserving scheme is used to integrate the new fractional partial differential equations in the augmented space R^{3+1}*. Effectiveness and validity of method demonstrated using two examples.*

Key words: *time fractional diffusion equation, fictitious time integration method, Caputo fractional derivative, group-preserving scheme*

Introduction

Partial differential equations of parabolic type have a significant role in the many branches of science and engineering. Diffusion equation as an example of this class describes the transport of a substance due to the molecular motion of the surrounding medium. The applications of anomalous diffusion equation can be found in electron transportation, heat conduction, compared with normal diffusion phenomena, dissipation, magnetic plasma, seepage, and turbulence, anomalous diffusion.

On the other hand, the fractional calculus started recently to become very significant in several branches of science and engineering [1-5]. Many important phenomena, *e. g.* electro-chemistry, electro-magnetics, control processing, acoustics, anomalous diffusion and visco-elasticity are well described by fractional differential equations. It is well known that new fractional order models are more satisfactory than integer ones and this is our motivation to consider the time fractional diffusion equation (TFDE) as [6, 7]:

$$D_t^\alpha u + u = \kappa \nabla^2 u + \mathrm{C}(x,t), \quad x \in \Omega \subset \mathrm{R}^2, \quad 0 < \alpha < 1 \tag{1}$$

with initial condition:

$$u(x,0) = w(x), \quad t = 0 \tag{2}$$

and boundary condition:

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$$u(x,t) = h(x,t), \quad x \in \partial\Omega, \quad t > 0 \tag{3}$$

where $D_t^\alpha u$ is the Caputo fractional derivative, $u(x,t)$ – the solute concentration, $C(x, t)$ – the source term, $w(x,t)$ – the initial solute concentration, $h(x,t)$ – the boundary solute concentration, α – the fractional derivative order, and κ – the diffusion coefficient.

Fu *et al.* [8] have applied the Laplace transformed boundary particle method which is an approach in the class of meshless methods, for solving the eq. (1) in two and three dimensions. Based on the meshless collocation formulation and moving least squares, an implicit meshless method is introduced by Gu *et al.* [9] to approximate the solution of TFDE. Pirkhedri and Javadi [10] considered the eq. (1) with the Sinc-Haar collocation method with exponential convergence rate. Moreover, some alternatives of finite difference schemes have been applied to the TFDE in [11-13].

In this paper, we construct a simple and accurate numerical method of FTIM to solve the TFDE. This method firstly proposed by Liu [14] to solve an inverse Sturm-Liouville problem. In the sense of stability and accuracy of FTIM, it would be very remarkable that it is much satisfactory than other conventional numerical approaches.

The Fictitious time integration method

Several mathematical definitions about the fractional derivative have been proposed until now [1-5]. Here we adopt the one usually used definition: the Caputo fractional differential operator:

$$D_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u_s(x,s)}{(t-s)^\alpha} \mathrm{d}s, \qquad 0 < \alpha < 1 \tag{4}$$

By using the above fractional derivatives we can write eq. (1) as:

$$\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u_s(x,s)}{(t-s)^\alpha} \mathrm{d}s + u = \kappa\nabla^2 u + C(x,t) \tag{5}$$

Now, we introduce a fictitious damping coefficient $\nu_0 > 0$ into eq. (5) to increase the stability of numerical integration:

$$\frac{\nu_0}{\Gamma(1-\alpha)} \int_0^t \frac{u_s(x,s)}{(t-s)^\alpha} \mathrm{d}s + \nu_0 u - \nu_0 \kappa\nabla^2 u - \nu_0 C(x,t) = 0 \tag{6}$$

Then, we are ready to introduce the pivotal transformation:

$$v(x,t,\tau) = (1+\tau)^\gamma u(x,t), \qquad 0 < \gamma \le 1 \tag{7}$$

Thus eq. (5) transforms to the following form:

$$\frac{\nu_0}{(1+\tau)^\gamma} \left[\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{v_s(x,s,\tau)}{(t-s)^\alpha} \mathrm{d}s + v - \kappa\nabla^2 v - C(x,t) \right] = 0 \tag{8}$$

Differentiation of eq. (8) regards to the fictitious time τ, concludes:

$$\frac{\partial v(x,t,\tau)}{\partial \tau} = \gamma(1+\tau)^{\gamma-1} u(x,t) \tag{9}$$

Hence, we can obtain:

$$\frac{\partial v}{\partial \tau}=\frac{\nu_0}{(1+\tau)^\gamma}\left[\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{v_s(x,s,\tau)}{(t-s)^\alpha}\mathrm{d}s+v-\kappa\nabla^2 v-\mathrm{C}(x,t)\right]+\gamma(1+\tau)^{\gamma-1}u \tag{10}$$

Then upon using $u=v/(1+\tau)^\gamma$, eq. (10) can be converted into a new type of functional PDE for v:

$$\frac{\partial v}{\partial \tau}=\frac{\nu_0}{(1+\tau)^\gamma}\left[\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{v_s(x,s,\tau)}{(t-s)^\alpha}\,\mathrm{d}s+v-\kappa\nabla^2 v-\mathrm{C}(x,t)\right]+\frac{\gamma v}{1+\tau} \tag{11}$$

From

$$\frac{\partial}{\partial \tau}\left[\frac{v}{(1+\tau)^\gamma}\right]=\frac{v_\tau}{(1+\tau)^\gamma}-\frac{\gamma v}{(1+\tau)^{1+\gamma}} \tag{12}$$

and after multiplying the integrating factor $1/(1+\tau)^\gamma$ on both sides of eq. (11), one can obtain:

$$\frac{\partial}{\partial \tau}\left[\frac{v}{(1+\tau)^\gamma}\right]=\frac{\nu_0}{(1+\tau)^{2\gamma}}\left[\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{v_s(x,s,\tau)}{(t-s)^\alpha}\,\mathrm{d}s+v-\kappa\nabla^2 v-\mathrm{C}(x,t)\right] \tag{13}$$

Now, by using $u=v/(1+\tau)^\gamma$ again, we can obtain a new type of functional PDE for u:

$$u_\tau=\frac{\nu_0}{(1+\tau)^\gamma}\left[\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{u_s(x,s,\tau)}{(t-s)^\alpha}\,\mathrm{d}s+u-\kappa\nabla^2 u-\mathrm{C}(x,t)\right] \tag{14}$$

Here, we must stress that above τ, is a fictitious time, and is used to embed eq. (5) into a new functional PDE in the space of R^{3+1}. As well as, u is an unknown function with $u=u(x,t,\tau)$ subjecting to the constraints in eq. (1), for all $\tau\geq 0$, and $u(x,t,\tau)|_{\tau=0}$ is given initially by a guess.

Let $u_i^j(\tau):=u(x_i,t_j,\tau)$ be a numerical value of u at a grid point (x_i, t_j), and at a fictitious time τ. Note that in one dimensional case we have $x_i = x_i$ and in two dimensional case $x_i=(x_{i_1},y_{i_2})$. Applying a semi-discretization to the eq. (14) we get:

$$\frac{\mathrm{d}}{\mathrm{d}\tau}u_i^j(\tau)=\frac{\nu_0}{(1+\tau)^\gamma}\left[\frac{1}{\Gamma(1-\alpha)}\int_0^{t_j}\frac{u_s(x_i,s,\tau)}{(t_j-s)^\alpha}\,\mathrm{d}s+\right.$$
$$\left.+u_i^j-\kappa\left(\frac{\breve{u}_{i+1}^j-2\breve{u}_i^j+\breve{u}_{i-1}^j}{\Delta x^2}+\frac{\breve{u}_i^{j+1}-2\breve{u}_i^j+\breve{u}_i^{j-1}}{\Delta t^2}\right)-\mathrm{C}(x_i,t_j)\right] \tag{15}$$

where in two dimensional case we have:

$$\frac{\breve{u}_{i+1}^j-2\breve{u}_i^j+\breve{u}_{i-1}^j}{\Delta x^2}=\frac{u_{i_1+1,i_2}^j-2u_{i_1,i_2}^j+u_{i_1-1,i_2}^j}{\Delta x^2}+\frac{u_{i_1,i_2+1}^j-2u_{i_1,i_2}^j+u_{i_1,i_2-1}^j}{\Delta y^2}$$

and

$$\frac{\breve{u}_i^{j+1}-2\breve{u}_i^j+\breve{u}_i^{j-1}}{\Delta t^2}=\frac{u_{i_1,i_2}^{j+1}-2u_{i_1,i_2}^j+u_{i_1,i_2}^{j-1}}{\Delta t^2}$$

Moreover:

$$\int_0^{t_j} \frac{u_s(x_i, s, \tau)}{(x_i - s)^\alpha} \mathrm{d}s = \sum_{l=1}^{j-1} \frac{u(x_i, t_{l+1}, \tau) - u(x_i, t_1, \tau)}{(t_j - t_l)^\alpha} \tag{16}$$

and in the two dimensional case we have:

$$\int_0^{t_j} \frac{u_s(x_i, s, \tau)}{(x_i - s)^\alpha} \mathrm{d}s = \sum_{l=1}^{j-1} \frac{u(x_{i_1}, y_{i_2}, t_{l+1}, \tau) - u(x_{i_1}, y_{i_2}, t_1, \tau)}{(t_j - t_l)^\alpha}$$

where $\Delta x = (\Delta x, \Delta y) = [a/(n_1 - 1), b/(n_2 - 1)],$, $x_i = (i-1)\Delta x$, and $t_j = (j-1)\Delta t.$

The GPS for differential equations system

Upon letting $u = (u_1^1, u_1^2, ..., u_N^{n_3})^T = (u_{1,1}^1, u_{1,1}^2, ..., u_{n_1,n_2}^{n_3})^T$ eq. (15) converts to a system of ODE:

$$u' = \Upsilon(u, \tau), \quad u \in \mathrm{R}^M, \quad \tau \in \mathrm{R} \tag{17}$$

where Υ denotes a vector with $i_1 i_2 j$ - component being the right-hand side of eq. (15), and $M = n_1 \times n_2 \times n_3$ is the number of total grid point inside the domain $\Omega = (0, a) \times (0, b) \times (0, T].$

Now, we can develop a GPS, introduced by Liu [15], to solve eq. (17):

$$X_{l+1} = \mathrm{G}(l) X_l \tag{18}$$

where X_l denotes the discrete value of X at τ_l, and $\mathrm{G}(l) \in SO_0(M,1)$ is the group value of G at τ_l. Note that, $X := (u^T, \|u\|)^T$ is a vector in the Minkowskian space which transforms eq. (16) into $\mathrm{d}X/\mathrm{d}\tau = \mathrm{A}X$ where:

$$\mathrm{A} = \begin{pmatrix} 0_{M\times M} & \dfrac{\Upsilon(u,\tau)}{\|u\|} \\ \dfrac{\Upsilon^T(u,\tau)}{\|u\|} & 0 \end{pmatrix} \in so(M,1)$$

is a Lie algebra of the proper orthochronous Lorentz group $SO_0(M,1).$

An closed-form representation of exponential mapping of $\mathrm{G}(l)$ can be written:

$$\mathrm{G}_l = \exp[\Delta\tau \mathrm{A}(l)] = \begin{bmatrix} I_M + \dfrac{\alpha_l - 1}{\|\Upsilon_l\|^2} \Upsilon_l \Upsilon_l^T & \dfrac{\beta_l \Upsilon_l}{\|\Upsilon_l\|} \\ \dfrac{\beta_l \Upsilon_l^T}{\|\Upsilon_l\|} & \alpha_l \end{bmatrix} \tag{19}$$

where

$$\alpha_l = \cosh \frac{\Delta\tau \|\Upsilon_l\|}{\|u_l\|}, \quad \beta_l = \sinh \frac{\Delta\tau \|\Upsilon_l\|}{\|u_l\|} \tag{20}$$

Substituting eq. (19) for G_l into eq. (18), concludes:

$$u_{l+1} = u_l + \frac{(\alpha_l - 1)\Upsilon_l . u_l + \beta_l \|u_l\| \|\Upsilon_l\|}{\|\Upsilon_l\|^2} \Upsilon_l = u_l + \eta_l \Upsilon_l \tag{21}$$

This scheme (GPS) keeps group properties for every $\Delta\tau > 0$. More details of this method can be found in [16-18].

Now we can utilize the GPS, by supposing the initial value of $u_i^j(0) = u_{i_1,i_2}^j(0)$, to integrate eq. (17) from the initial fictitious time $\tau = 0$ to a selected final fictitious time τ_f. Stopping criterion for this numerical integration is:

$$\sqrt{\sum_{i=1}^{N}\sum_{j=1}^{n_3}\left[u_i^j(l+1) - u_i^j(l)\right]^2} = \sqrt{\sum_{i_1=1}^{n_1}\sum_{i_2=1}^{n_2}\sum_{j=1}^{n_3}\left[u_{i_1,i_2}^j(l+1) - u_{i_1,i_2}^j(l)\right]^2} \le \varepsilon \tag{22}$$

where ε is a selected convergence criterion. The solution of u is obtainable from:

$$u_i^j = \frac{v_i^j(\tau_0)}{(1+\tau_0)^\gamma} \tag{23}$$

where $\tau_0(\le \tau_f)$ satisfies at the above criterion. The parameters v_0 and γ can strengthen the stability of and enhancing the convergence speed of numerical integration, respectively.

Numerical examples

In this section, we examine the performance of our FTIM to solve the TFDE.

Example 1

Consider the one-dimensional TFDE [6]:

$$D_t^\alpha u(x,t) + u(x,t) = u_{xx}(x,t) + \mathrm{C}(x,t), \qquad \alpha \in (0,1), \qquad x \in [0,2], \qquad t \ge 0$$

$$u(x,0) = 0, \quad x \in [0,2] \quad u(0,t) = u(2,t) = 0, \quad t \ge 0$$

where $\mathrm{C}(x,t) = [2/\Gamma(3-\alpha)]x(2-x)t^{2-\alpha} + t^2 x(2-x) + 2t^2$ and exact solution of this problem is given by $u(x,t) = t^2 x(2-x)$. From one-dimensionless of space direction, we have $n_2 = 0$ and other applied parameters in FTIM are $n_1 = 19$, $n_3 = 19$, $v_0 = 0.4$, $\gamma = 1\mathrm{e}-4$, $\Delta\tau = 1\mathrm{e}-5$, and $u_j^i(0) = 1\mathrm{e}-3$. Here, we suppose the final time $T = 10$ and fractional order $\alpha = 0.5$. In fig. 1 we plot the approximate solution and absolute error plot of this example. High accurate solutions of applied method for this equation can be seen from these figures.

Example 2

Let us consider the two-dimensional TFDE [6]:

$$D_t^\alpha u(x,z,t) + u(x,z,t) = u_{xx}(x,z,t) + u_{zz}(x,z,t) + \mathrm{C}(x,z,t), \qquad x, z \in [0,2], \qquad t > 0$$

$$u(x,z,0) = 0, \quad x, z \in [0,2] \quad u(0,z,t) = u(2,z,t) = t^2 z(2-z)$$

$$u(x,0,t) = u(x,2,t) = t^2 x(2-x)$$

where $\mathrm{C}(x,z,t) = [2/\Gamma(3-\alpha)]t^{2-\alpha}[x(2-x) + z(2-x)] + t^2[x(2-x) + z(2-z)] + 4z^2$ and analytical solution is given by $u(x,z,t) = t^2[x(2-x) + z(2-z)]$. In this example we use the values $v0 = 0.401$, $n_1 = n_2 = n_3 = 19$, $\gamma = 1\mathrm{e}-4$, $\Delta\tau = 1\mathrm{e}-5$, and $u_j^i(0) = 1\mathrm{e}-3$. Also, the fractional order is supposed $\alpha = 0.7$ in figs. 2 and 3 where $T = 10$ is the final time in both of them. Approximate solutions and related error contour plots are demonstrated in fig. 2 and fig. 3 with $z = 2.5$ and $z = 1.5$ respectively. Efficiency and power of FTIM can be seen from these figures.

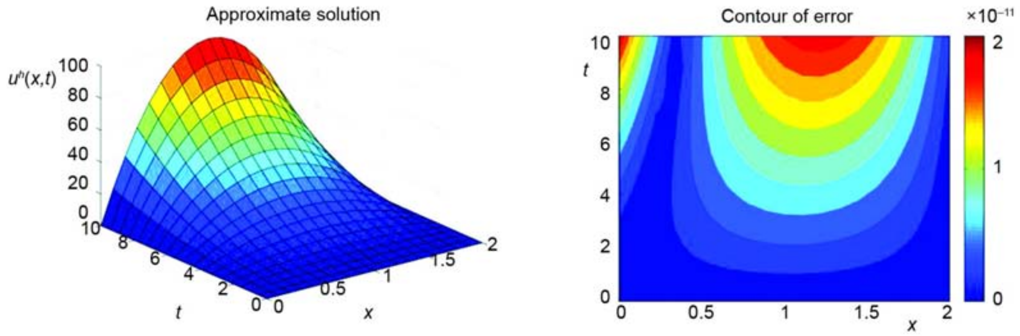

Figure 1. Plotting the numerical solution and contour plot error of Example 1 for a TFDE *(for color image see journal web-site)*

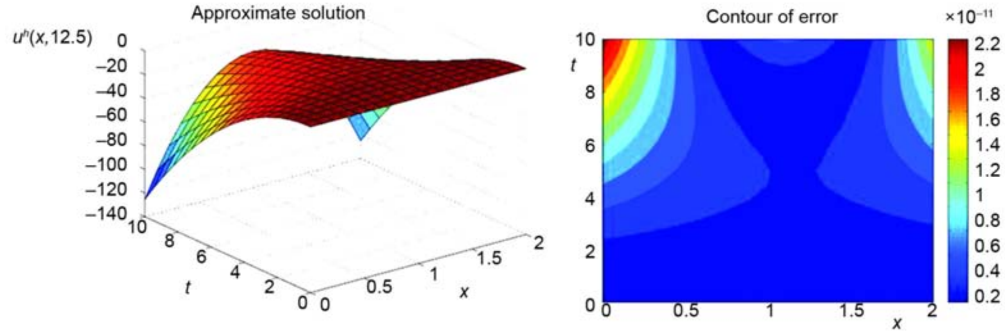

Figure 2. Plotting the numerical solution and contour plot error of Example 2 with *z* = 2.5 for a TFDE *(for color image see journal web-site)*

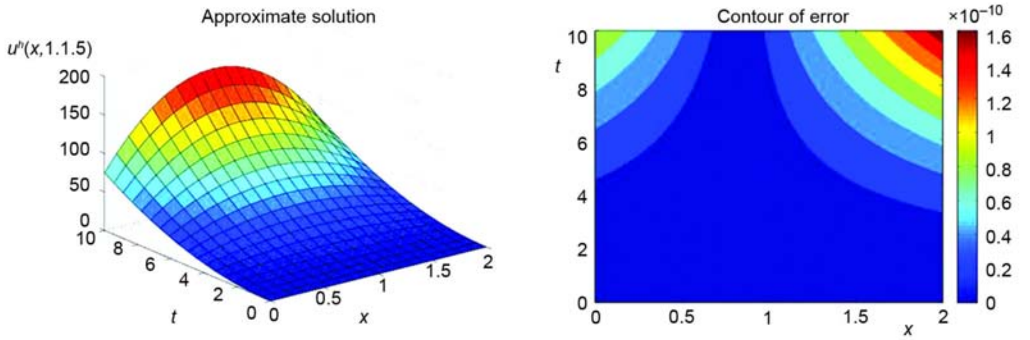

Figure 3. Plotting the numerical solution and contour plot error of Example 2 with *z* = 1.5 for a TFDE *(for color image see journal web-site)*

Conclusions

Using the novel FTIM and introducing a fictitious variable, we have transformed TFDE into another type of fractional differential equation in a one-dimension higher space. By employing the GPS we numerically integrated the discretized equations that the coefficient ν_0 is utilized to enhance the stability of current method. After suitably choose of the constant γ, to fast the convergence of numerical solutions, two numerical examples were devised, which demonstrate that FTIM is applicable to the numerical solutions of TFDE.

Nomenclature

A	– augmented matrix
C(x, t)	– source term
G	– an element of Lorentz group
$h(x, t)$	– boundary solute concentration
I_M	– M-dimensional unit matrix
M	– number of discretized points
$SO_0(M, 1)$	–M-dimensional Lorentz group
$so(M, 1)$	– the Lie algebra of $SO_0(M,1)$
t	– time
Δt	– time stepsize
u	– solute concentration
$w(x, t)$	– initial solute concentration
x	– space dimension

Greek symbols

α	– fractional derivative order
γ	– convergence rate parameter
κ	– diffusion coefficient
τ	– fictitious time
ν_0	– fictitious damping coefficient
Υ	– M-dimensional vector field in eq. (17)
$\|\cdot\|$	– Euclidean norm

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