NUMERICAL APPROACH TO SIMULATE DIFFUSION MODEL OF A FLUID-FLOW IN A POROUS MEDIA

by

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Original scientific paper
https://doi.org/10.2298/TSCI21S2255E

When a particle distributes at a rate that deviates from the classical Brownian motion model, fractional space derivatives have been used to simulate anomalous diffusion or dispersion. When a fractional derivative substitutes the second-order derivative in a diffusion or dispersion model, amplified diffusion occurs (named super-diffusion). The proposed approach in this paper allows seeing the physical background of the newly defined Caputo space-time-fractional derivative and indicates that the order of convergence to approximate such equations has increased.

Key words: *diffusion, Caputo derivative, numerical solutions, boundary conditions*

Introduction

The diffusion equation is a PDE based mathematical equation that represents the physical theory of particles moving from a high density to a low density situation randomly and irregularly. It is a term used in physics to explain the macroscopic action of so many micro-particles in Brownian motion, which is caused by the particles' random movements and collisions. In the diffusion procedure, this model defines the variations in place and time of a physical quantity. Various characteristics, including thermal conductivity and electromagnetic wave dispersion, can indeed be represented by using the diffusion model. Moreover, the diffusion process in porous media is a combination of linear and non-linear diffusion equations that offer Darcy-scale estimates of a variety of flow and transport processes in porous media that are associated with diffusion in general [1].

These processes are sometimes not connected to Brownian particle motion in a free fluid, and instead explain pressure diffusion, the diffusive transmission of a phase-field including such fluid saturation, and so on. In fact, the discussed model can be modeled using equations with classical derivatives of space and temporal. But to simulate a particle motion that distributes at varying rates than the classical model, fractional derivatives can be used. The spatial order derivative is frequently among one and two due to physical implementation. In addition, the temporal (time) fractional derivative can be used to represent particle motion in which the period between

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two leaps is longer than usual [2]. The main purpose of the paper is to discuss the numerical method for the 2-D space-time fractional diffusion equation (2-D STFDE):

$$ {}_0^c\mathcal{D}_\tau^\gamma z(x,\tau) = \Delta z(x,\tau) + f(x,\tau), \quad x \in \Omega = (0,1)\times(0,1), \quad 0 < \tau \le T \tag{1}$$

where $\Omega = [0,1]\times[0,1]$, $f(x,\tau)$ is a source term. The operator $\Delta z(x,\tau)$ is:

$$\Delta z(x,\tau) = p(x,\tau){}_0^c\mathcal{D}_x^\alpha z(x,\tau) + q(x,\tau){}_0^c\mathcal{D}_y^\beta z(x,\tau)$$

where the diffusion coefficients are $p(x,\tau), q(x,\tau) \ge 0$ and the fractional orders are $1 < \alpha, \beta \le 2$, and $0 < \gamma \le 1$. The initial $z(x,0) = \psi_0(x)$ and boundary conditions are obtained:

$$\begin{gathered} z(0,y,\tau) = \chi_0(y,\tau), \quad z(1,y,\tau) = \chi_1(y,\tau), \quad z(x,0,\tau) = \psi_0(x,\tau), \\ z(x,1,\tau) = \psi_1(x,\tau), \quad \tau > 0 \end{gathered} \tag{2}$$

where ${}_0^c\mathcal{D}_\tau^\gamma z(x,\tau)$ is the left Caputo fractional derivatives that are defined in [3]. The classical diffusion model is constructed by $\gamma = 1, \alpha = \beta = 2.$

Moreover, we know that the values $1 < \alpha, \beta < 2,$ and $0 < \gamma < 1$ show a super-diffusion and super-slow diffusion model, respectively. For any positive values of γ leads to a super-fast diffusion equation [4]. There are other models such as radiation and absence of fluid motion and transient heat diffusion. Methods for solving these types of models are represented in [5, 6]. Many numerical methods have been used to solve diffusion equation, and several types of numerical methods used in recent years have been described in [7-9].

Implementation of numerical method for 2-D STFDE

To obtain the full discretization of eq. (1), two subsections are required. Since the convergence order of the linear approximation for the left Caputo time fractional derivative in the infinite interval is $\mathcal{O}(\delta\tau^{2-\gamma})$ in [10], we use the quadratic interpolation of [11, 12] and make some remarks on the relationship between cofficients them in the first subsection. The technique for the 2-D issue of eq. (1) is shown in the second subsection with using the second shifted Chebyshev basis and the full discrete scheme of 2-D STFDE is obtained.

Discretizations for the right Caputo fractional derivative

Let $\tau_j = j\delta\tau, j = 0,1,\ldots,J$ be the node points of the temporal sense in each interval [0, *T*] that $\delta\tau = T/J$ is the temporal step size. The quadratic approach is applied to discrete the Caputo derivative for $0 < \alpha \le 1$ is [11]:

$$ {}_0^c\mathcal{D}_\tau^\gamma z(x,\tau) = \frac{\delta\tau^{-\gamma}}{\Gamma(2-\gamma)}\sum_{k=0}^{j} S_{j,k} z(x,\tau_k) + \mathcal{O}(\delta\tau^{3-\gamma}) \tag{3}$$

where $S_{j,k}$ is the unknown coefficients that can be described for the variant values *j* in the following form:

$$S_{1,k} = \begin{cases} -\mathcal{A}_1, & k = 0, \\ \mathcal{A}_1, & k = 1, \end{cases} \quad S_{2,k} = \begin{cases} -\mathcal{A}_2 + \mathcal{B}_{2,2}, & k = 0, \\ \mathcal{A}_2 + \mathcal{C}_{2,2}, & k = 1, \\ \mathcal{D}_{2,2}, & k = 2, \end{cases} \quad S_{j,k} = \begin{cases} -\mathcal{A}_j + \mathcal{B}_{j,k+2}, & k = 0, \\ \mathcal{A}_j + \mathcal{B}_{j,k+2} + \mathcal{C}_{j,k+1}, & k = 1, \\ \mathcal{B}_{j,k+2} + \mathcal{C}_{j,k+1} + \mathcal{D}_{j,k}, & 2 \le k \le j-2 \\ \mathcal{C}_{j,k+1} + \mathcal{D}_{j,k}, & k = j-1, \\ \mathcal{D}_{j,k}, & k = j, \end{cases}$$

Now, by substituting eq. (3) in eq. (1) and after simplifying the following relation is obtained:

$$S_{J,J}z^j-\overline{\Delta}z^j=\sum_{k=0}^{j-1}\overline{S}_{j,k}z^k+\overline{f}^j+R^j,\quad j=1,2,\ldots,J$$

where $z^j=z(x,y,t_j),$, $\overline{\Delta}z^j=\delta\tau^{\gamma}\Gamma(2-\gamma)\Delta z(x,y,t_j)$ and $\overline{f}^j=\delta\tau^{\gamma}\Gamma(2-\gamma)f(x,\tau)$. Furthermore, the truncation error fulfills $R^j\leq\mathcal{O}(\delta\tau^3)$. Deleting R^j, we obtain the semi-discrete scheme of the eq. (1):

$$S_{J,J}Z^j-\overline{\Delta}Z^j=\sum_{k=0}^{j-1}\overline{S}_{j,k}Z^k+\overline{f}^j,\quad j=1,2,\ldots,J \tag{4}$$

where Z^j is the approximate solution in the time *j*.

Full scheme for 2-D fractional diffusion model

Now we'll examine the full discretization scheme for 2-D STFDE. In the time direction, we apply the quadratic approach to get the semi-discrete scheme (4). But to get the full discrete, we need to do spatial discretization. To do this, we use the collocation method based on the shifted Chebyshev polynomials of the second kind. The extension of function $z(x,\tau_j)$ can be written to a finite number of sentences, $(N+1)\times(M+1)$, using this type of polynomial:

$$z(x,\tau_j)=\sum_{n=0}^{N}\sum_{m=0}^{M}\mathrm{u}_{nm}^j u_{nm}(x) \tag{5}$$

where $u_{nm}(x)$ and u_{nm}^j are SCP and the unknown coefficients, respectively. The unknown coefficients are determined:

$$\mathrm{u}_{nm}^j=\frac{\langle u_n(x),\langle z(x,t_j),u_m(y)\rangle\rangle}{\langle u_n(x),u_n(x)\rangle\langle u_m(y),u_m(y)\rangle}=\frac{64}{\pi^2}\int_0^1\int_0^1\frac{(x-x^2)^{1/2}}{(y-y^2)^{-1/2}}z(x,t_j)u_{nm}(x)\mathrm{d}x\mathrm{d}y \tag{6}$$

where $\langle.\rangle$ denotes the inner product in the space $L^2[(0,1)\times(0,1)]$. To continue the discretization of eq. (4), we need to have the closed form of the fractional derivative of the $\alpha,\beta-$order for basis polynomials. This form is obtained in the paper [13]:

$$\begin{aligned}{}_0^c\mathcal{D}_x^{\alpha}u_n(x) &= \sum_{\kappa=0}^{n-\lceil\alpha\rceil}\mathbf{N}_{n,\kappa}^{\alpha}\times x^{n-\kappa-\alpha},\quad x\in(0,1),\quad n=0,1,\ldots,N\\ {}_0^c\mathcal{D}_y^{\alpha}u_m(y) &= \sum_{\kappa=0}^{m-\lceil\beta\rceil}\mathbf{N}_{m,\kappa}^{\beta}\times y^{m-\kappa-\beta},\quad y\in(0,1),\quad m=0,1,\ldots,M\end{aligned} \tag{7}$$

where $\lceil\alpha\rceil$ and $\lceil\beta\rceil$ are the ceiling of α and β, respectively. The known cofficient $\mathbf{N}_{n,k}^{\alpha}$ is defined:

$$\mathbf{N}_{n,\kappa}^{\alpha}=\frac{(-1)^{\kappa}4^{n-\kappa}\Gamma(2n-\kappa+2)\Gamma(n-\kappa+1)}{\Gamma(\kappa+1)\Gamma(2n-2\kappa+2)\Gamma(n-\kappa+1-\alpha)}$$

For $\mathbf{N}_{m,\kappa}^{\beta}$, a relation like the previous one is defined. Substituting eqs. (5) and (7) in eq. (4), we have:

$$\sum_{n=0}^{N}\sum_{m=0}^{M}\mathrm{u}_{nm}^{j}u_{nm}(x)-p(x,\tau)\sum_{n=\lceil\alpha\rceil}^{N}\sum_{m=0}^{M}\sum_{\kappa=0}^{n-\lceil\alpha\rceil}\mathrm{u}_{nm}^{j}u_{m}(y)\mathbf{N}_{n,\kappa}^{\alpha}\times x^{n-\kappa-\alpha}-$$
$$-q(x,\tau)\sum_{n=0}^{N}\sum_{m=\lceil\beta\rceil}^{M}\sum_{\kappa=0}^{m-\lceil\beta\rceil}\mathrm{u}_{nm}^{j}u_{n}(x)\mathbf{N}_{m,\kappa}^{\beta}\times y^{m-\kappa-\beta}= \tag{8}$$
$$=\sum_{k=0}^{j-1}\sum_{n=0}^{N}\sum_{m=0}^{M}\overline{S}_{j,k}\mathrm{u}_{nm}^{k}u_{nm}(x)+\overline{f}^{\,j},\quad j=1,2,\ldots,J$$

In eq (8), there are $(N+1)(M+1)$ unknowns that must be specified. By placing $(N-1)(M-1)$ roots of SCP, $(N-1)(M-1)$ equations are created, which, considering the following boundary conditions the above relation, becomes a linear system in each time step:

$$\begin{gathered}\sum_{n=0}^{N}\sum_{m=0}^{M}(-1)^{n+2}(n+1)\mathrm{u}_{nm}^{j}u_{m}(y)=\chi_0(y,\tau_j),\ \sum_{n=0}^{N}\sum_{m=0}^{M}(n+1)\mathrm{u}_{nm}^{j}u_{m}(y)=\chi_1(y,\tau_j)\\ \sum_{n=0}^{N}\sum_{m=0}^{M}(-1)^{m+2}(m+1)\mathrm{u}_{nm}^{j}u_{n}(x)=\psi_0(x,\tau_j),\ \sum_{n=0}^{N}\sum_{m=0}^{M}(m+1)\mathrm{u}_{nm}^{j}u_{n}(x)=\psi_1(x,\tau_j)\end{gathered} \tag{9}$$

Furthermore, we apply $z(x,0)=\psi_0(x)$ in eq. (5) combining with eq. (6) to achieve the initial solution u_{nm}^{0}.

Numerical results

This part demonstrates the performance of the suggested method on two test issues in order to illustrate its efficacy for the various values of *J*, *M*, and *N*. The considerable matter of the provided results is to illustrate that the numerical results approve the related proved theorems about the temporal-discrete schemes convergence order. We calculate the convergence order and rate in temporal

$$CO=\log_2\left(\frac{\|L_\infty(2\delta\tau)\|}{\|L_\infty(\delta\tau)\|}\right),\quad CR=2^{CO}$$

to showcase the new method validity. We took the following examples from papers [8-10] and compared the numerical results with these results. In these papers, the order of convergence is equal to $TCO=\mathcal{O}(\delta\tau^{2-\gamma})$, while the new method has the convergence order of $TCO=\mathcal{O}(\delta\tau^{3-\gamma})$.

Example 1 Investigate the following 2-D STFDE with the exact solution $z(x,\tau)=(\tau^2+1)x^3y^3,\ x\in\Omega$.

$${}_0^c\mathcal{D}_\tau^{0.5}z(x,\tau)=\frac{\Gamma(2.8)}{6}x^{1.2}{}_0^c\mathcal{D}_x^{1.2}z(x,\tau)+\frac{\Gamma(2.2)}{6}y^{1.8}{}_0^c\mathcal{D}_y^{1.8}z(x,\tau)+x^3y^3\left[\frac{8}{3\Gamma(0.5)}\tau^{1.5}-2\tau^2-2\right]$$
$$z(0,y,\tau)=z(x,0,\tau)=0,\quad z(1,y,\tau)=(\tau^2+1)y^3,\quad z(x,1,\tau)=(\tau^2+1)x^3,\quad 0<\tau\le T$$

The exact solution is used to determine the initial condition. Table 1 makes a comparable evaluation of the error L_∞ between the methods of [8-10] and the proposed method. It is clear that the proposed method can better approximate the exact solution $v(x,\tau)$. The order of convergence of the approximating solution in L_∞ and L_2-norms is close to $\mathcal{O}(\delta\tau^{3-\gamma})$, as shown by the convergence results shown in tab. 2.

Table 1. Comparing the absolute error L_∞ using the suggested technique and the methods [8-10] at T = 1 for *Example 1*

$\Delta\tau$	$M = N$	[8]	[9]	N, M	[10]	Current method
1/10	10	9.93756×10^{-2}	8.43962×10^{-3}	3, 5	1.56003×10^{-3}	2.57562×10^{-5}
1/20	20	7.14376×10^{-2}	8.34223×10^{-3}	5, 7	4.30068×10^{-4}	4.30422×10^{-6}
1/40	40	4.23914×10^{-2}	7.23612×10^{-3}	7, 9	1.46784×10^{-4}	7.29734×10^{-7}
1/100	100	1.87382×10^{-2}	5.40802×10^{-3}	9, 11	3.70882×10^{-5}	7.20669×10^{-8}

Table 2. The convergence order, CO, and convergance rate, CR, of the current method with $N = M = 5$ at T = 1 for *Example 1*

$\delta\tau$	L_∞	CO	CR	L_2	*CO*	CR
1/10	2.56872×10^{-5}			5.17407×10^{-5}		
1/20	4.29776×10^{-6}	2.59059	6.02343	8.58292×10^{-6}	2.59176	6.02833
1/40	7.32854×10^{-7}	2.55199	5.86441	8.58292×10^{-6}	2.55278	5.8674
1/80	1.26830×10^{-7}	2.53063	5.77824	2.53034×10^{-7}	2.53129	5.78087
1/160	2.2335×10^{-8}	2.51859	5.73023	4.41423×10^{-8}	2.51910	5.73223

Example 2 Investigate the following 2-D STFDE with the exact solution $u(x,\tau) = [\exp(\tau) - 1]x^3 y^{3.6}$.

$$ {}_0^c\mathcal{D}_\tau^{0.5} z(x,\tau) = a(x,\tau) {}_0^c\mathcal{D}_x^{1.8} z(x,\tau) + b(x,\tau) {}_0^c\mathcal{D}_y^{1.6} z(x\tau) + f(x,\tau), \quad x \in \Omega, \quad 0 < \tau \le T $$

$$ a(x,\tau) = \frac{\Gamma(2.2)}{6} x^{2.8} y, \; b(x,\tau) = \frac{2}{\Gamma(4.6)} y^{2.6} x $$

$$ f(x,\tau) = -2[\exp(\tau) - 1] y^{4.6} x^4 + \frac{2}{\Gamma(0.5)} \exp(\tau) \tau^{0.5} {}_1F_1(0.5, 1.5, -\tau) $$

where ${}_1F_1(0.5,1.5,-\tau)$ is the Kummer confluent hypergeometric operator. The exact solution is used to determine the initial and boundary conditions. Table 3 shows a comparable evaluation of the error L_∞ between the methods of [9, 10] and the proposed method. It is clear that the proposed method can better approximate the exact solution $v(x,\tau)$. The order and rate of convergence of the approximating solution in L_∞ and L_2-norms is close to $\mathcal{O}(\delta\tau^{3-\gamma})$, as shown by the convergence results shown in tab. 4.

Table 3. Comparing the absolute error L_∞ using the suggested technique and the methods [9, 10] at T = 1 for *Example 2*

$\delta\tau$	$M = N$	L_∞ [9]	$M = N$	L_∞ [10]	L_∞ of current method
1/10	10	1.54478×10^{-2}	4	1.78543×10^{-3}	4.63807×10^{-4}
1/20	20	1.46362×10^{-2}	6	4.67992×10^{-4}	1.96365×10^{-5}
1/40	40	1.20455×10^{-2}	8	1.72900×10^{-4}	2.25629×10^{-6}
1/80	80	9.43800×10^{-3}	10	6.21019×10^{-5}	2.25629×10^{-6}
1/100	100	8.66339×10^{-3}	12	4.46008×10^{-5}	1.89227×10^{-7}

Table 4. The convergence order, CO, and convergence rate, CR, of the current method with $N = M = 7$ at T = 1 for *Example 2*

$\delta\tau$	L_∞	CO	CR	L_2	*CO*	CR
1/5	4.39825×10^{-4}			7.24368×10^{-4}		
1/10	8.11468×10^{-5}	2.43833	5.42012	1.32653×10^{-4}	2.44907	5.46063
1/20	1.27847×10^{-5}	2.66611	6.34718	2.14175×10^{-5}	2.63007	6.19367

Conclusion

Using the spectral method based on SCP, this paper suggested a numerical method for solving the 2-D STFDE. This approach is divided into two parts: the first part in which the time-fractional derivative is approximated using the quadratic interpolation of the order $\mathcal{O}(\delta\tau^{2-\gamma})$, and the second part in which the spectral method is used for spatial approximation. The numerical results are showed that the technique is unconditionally stable and convergent. It confirmed the theoretical results and comparing to exact solutions and existing schemes in the literature demonstrates the new method accuracy and efficiency.

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Paper submitted: April 13, 2021
Paper revised: April 25, 2021
Paper accepted: May 17, 2021