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Comparison of different numerical methods for the solution of the time-fractional reaction-diffusion equation with variable diffusion coefficient

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Abstract

In this work we perform a comparison of two different numerical schemes for the solution of the time-fractional diffusion equation with variable diffusion coefficient and a nonlinear source term. The two methods are the implicit numerical scheme presented in [M.L. Morgado, M. Rebelo, Numerical approximation of distributed order reaction-diffusion equations, Journal of Computational and Applied Mathematics 275 (2015) 216-227] that is adapted to our type of equation, and a colocation method where Chebyshev polynomials are used to reduce the fractional differential equation to a system of ordinary differential equations.

Key words: Time-fractional diffusion equation, Caputo derivative, Chebyshev polynomials

1 Introduction

It is well known that several diffusion processes that occur in nature, present super-diffusive or a sub-diffusive behavior. Therefore, for the correct modeling of these physical phenomena, fractional differential models were proposed in the literature, allowing this way to overcome the difficulty in predicting reliable results by using classical models for the modeling of such extreme diffusion processes. Most of these models are complex, and, analytical solutions are only possible for a small number of particular cases. Therefore, the numerical solution of these fractional models is a demand.

In this work we are interested on the numerical solution of the time-fractional diffusion equation with a variable diffusion coefficient and a non-linear source term [1, 2], given by

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} - \frac{\partial}{\partial x}\left(k\left(x\right)\frac{\partial u(x,t)}{\partial x}\right) = f\left(x,\, t, u(x,t)\right), \quad 0 \le x \le L,\, t > 0 \tag{1}$$

with boundary conditions:

$$u(0,\, t) = \phi_0\left(t\right),\, u(L,\, t) = \phi_L\left(t\right) \tag{2}$$

and an initial condition,

$$u(x,0) = g\left(x\right), \tag{3}$$

where $\frac{\partial^\alpha}{\partial t^\alpha}$ is the fractional Caputo derivative given by [3],

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma\left(1-\alpha\right)}\int_0^t \left(t-s\right)^{-\alpha}\frac{\partial u(x,s)}{\partial s}ds \tag{4}$$

with $0 < \alpha < 1$. Note that $k\left(x\right)$ is a function of x, meaning that we can deal with possible anisotropy.

2 Numerical solution

Method 1

For the numerical solution of Eq. 1, we will use a similar method to the one proposed in [4] for the numerical solution of distributed order reaction-diffusion equations.

The method is now briefly explained. The diffusive term (second term on the left-hand-side of Eq. 1) is approximated using a second order finite difference formula,

$$\frac{\partial}{\partial x}\left(k\left(x\right)\frac{\partial u(x,t)}{\partial x}\right) \approx \frac{k\left(x_i+\frac{\Delta x}{2}\right)u(x_{i+1},t) - \left(k\left(x_i+\frac{\Delta x}{2}\right)+k\left(x_i-\frac{\Delta x}{2}\right)\right)u(x_i,t) + k\left(x_i-\frac{\Delta x}{2}\right)u(x_{i-1},t)}{(\Delta x)^2} \tag{5}$$

and for the fractional derivative we use the backward finite difference formula provided by Diethelm [3] ($\mathcal{O}\left((\triangle t)^{2-\alpha}\right)$),

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} \approx \frac{(\triangle t)^{-\alpha}}{\Gamma\left(2-\alpha\right)}\sum_{m=0}^{l} a_{m,l}^{(\alpha)}\left(u\left(x_i, t_{l-m}\right) - u\left(x_i, 0\right)\right) + c_\alpha\left(\triangle t\right)^{2-\alpha}\frac{\partial^2 u}{\partial t^2}(x_i,\eta_l),\, \eta_l \in (0,\, t_l) \tag{6}$$

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$$a_{m,l}^{(\alpha)} = \begin{cases} 1, & m=0 \\ (m+1)^{1-\alpha} - 2m^{1-\alpha} + (m-1)^{1-\alpha} & 0<m<l \\ (1-\alpha)\, l^{-\alpha} - l^{1-\alpha} + (l-1)^{1-\alpha} & m=l \end{cases}$$

The source term, $f\left(x,t,u(x,t)\right)$, is simply given by

$$f\left(x_i,t_l,u(x_i,t_l)\right) = f\left(x_i,t_{l-1},u(x_i,t_{l-1})\right) + \mathcal{O}\left(\triangle t\right). \tag{7}$$

We assume uniform meshes for both spatial ($\Delta x = L/K$) and time discretizations ($\Delta t = T/R$), with K and R the number of divisions of each grid.

Denoting the approximate value of $u\left(x_i,t_l\right)$ by u_i^l, and $k\left(x_i \pm \frac{\Delta x}{2}\right)$ by $k_{i\pm\frac{1}{2}}$ the finite difference scheme is then given by,

$$\frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{m=0}^{l} a_{m,l}^{(\alpha)} \left(u_i^{l-m} - u_i^0\right) = \frac{k_{i+\frac{1}{2}} u_{i+1}^l - \left(k_{i+\frac{1}{2}} + k_{i-\frac{1}{2}}\right) u_i^l + k_{i-\frac{1}{2}} u_{i-1}^l}{(\Delta x)^2} + f\left(x_i,t_{l-1},u_i^{l-1}\right)$$
$$i = 1,....,N-1,\ \ l = 1,....,R \tag{8}$$

together with the initial and boundary conditions:

$$u_i^0 = g\left(x_i\right),\ \ i = 1,...,N-1 \tag{9}$$

$$u_0^l = \varphi_0\left(t_l\right),\ \ u_k^l = \varphi_L\left(t_l\right),\ \ l = 1,2,...R \tag{10}$$

Method 2

A second numerical method is now proposed, based on the assumption that the solution can be written in terms of a Chebyshev series expansion.

Chebyshev polynomials are defined in the interval $[-1,1]$ and can be obtained through the following recurrence formula:

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

Alternatively, they can also be obtained from:

$$T_n(z) = n\sum_{i=0}^{[n/2]} (-1)^i 2^{n-2i-1} \frac{(n-i-1)!}{i!(n-2i)!} z^{n-2i},\quad n = 0,1,\ldots,$$

($[n/2]$ represents the integer part of $n/2$) and satisfy the following orthogonality conditions:

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

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In order to use these polynomials in the interval $[0, T]$, we introduce the change of variable $z = (2t/T - 1)$ and obtain the so-called shifted Chebyshev polynomials:

$$T_{T,n}(t) = T_n\left(2t/T - 1\right).$$

These shifted Chebyshev polynomials can also be obtained from the following expression (see [5]):

$$T_{T,n}(t) = n \sum_{k=0}^{n} (-1)^{n-k} \frac{2^{2k}(n+k-1)!}{(2k)!(n-k)!T^k} t^k, \quad n = 1, 2, \ldots,$$

where

$$T_{T,i}(0) = (-1)^i \ \text{ and } \ T_{T,i}(T) = 1, \tag{11}$$

and satisfy the following orthogonality relation:

$$\int_0^T T_{T,j}(t) T_{T,k}(t) \omega_T(t) dt = \delta_{kj} h_k,$$

where $\omega_T(t) = \dfrac{1}{\sqrt{Tt - t^2}}$ and $h_0 = \pi$, $h_k = \frac{\pi}{2}$, $k = 1, 2, \ldots$.

A function $y(t)$ belonging to the space of square integrable functions on $[0, T]$, may be expressed as

$$y(t) = \sum_{i=0}^{\infty} c_i T_{T,i}(t), \tag{12}$$

where the coefficients c_i are given by:

$$c_i = \frac{1}{h_i} \int_0^T y(t) T_{T,i}(t) \omega_T(t)\, dt, \quad i = 0, 1, 2, \ldots \ .$$

For computational purposes, only the first $(m + 1)$ terms in (12) are considered, and then the following result holds:

Theorem 1. *([5])*
Let $y(t)$ be a square integrable function on $[0, T]$ approximated as

$$y(t) = \sum_{i=0}^{m} c_i T_{T,i}(t). \tag{13}$$

Then, for $\alpha > 0$ we have:

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

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where

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

and the error $|E(m)| = |D^\alpha y(t) - D^\alpha y_m(t)|$ *is bounded by*

$$|E(m)| \leq \sum_{i=m+1}^{\infty} c_i \left(\sum_{k=\lceil\alpha\rceil}^{i} \sum_{j=0}^{k-\lceil\alpha\rceil} \theta_{i,j,k} \right),$$

where

$$\theta_{i,j,k} = \frac{(-1)^{i-k} 2i(i+k-1)!\Gamma\left(k-\alpha+\frac{1}{2}\right)}{h_j \Gamma\left(k+\frac{1}{2}\right)(i-k)!\Gamma(k-\alpha-j+1)\Gamma(k+j-\alpha+1)T^\alpha},$$

$h_0 = 2,\ h_j = 1,\ j = 1, 2, \ldots$.

For the numerical solution of (1) let

$$u(t,x) \approx u_m(t,x) = \sum_{i=0}^{m} v_i(x) T_{T,i}(t),$$

Using the results given before, and taking into account that $0 < \alpha < 1$, we can discretize the time fractional diffusion equation as:

$$\sum_{i=1}^{m} \sum_{k=0}^{i-1} v_i(x) w_{i,k}^{\alpha} t^{i-k-\alpha} = k'(x) \sum_{i=0}^{m} v'(x) T_{T,i}(t) + k(x) \sum_{i=0}^{m} v''(x) T_{T,i}(t) + f\left(t, x, \sum_{i=0}^{m} v_i(x) T_{T,i}(t)\right). \tag{14}$$

We now collocate this equation at the m zeros of the shifted Chebyshev polynomial $T_{T,m}(t)$, T_p, $p = 0, 1, \ldots, m-1$, obtaining the following m second order ordinary differential equations on the $(m+1)$ unknowns $v_i(x)$, $i = 0, 1, ..., m$:

$$\sum_{i=1}^{m} \sum_{k=0}^{i-1} v_i(x) w_{i,k}^{\alpha} t_p^{i-k-\alpha} = k'(x) \sum_{i=0}^{m} v'(x) T_{T,i}(t_p) + k(x) \sum_{i=0}^{m} v''(x) T_{T,i}(t_p) + f\left(t_p, x, \sum_{i=0}^{m} v_i(x) T_{T,i}(t_p)\right). \tag{15}$$

The extra equation is achieved considering the initial condition,

$$\sum_{i=0}^{m} (-1)^i v_i(x) = g(x),$$

obtaining in this way, a system of $(m+1)$ differential equations.

Taking into account the boundary conditions (2), we obtain the following $2m$ conditions:

$$\sum_{i=0}^{m} v_i(0) T_{T,i}(t_p) = \phi_0(t_p),\ p = 0, \ldots, m-1, \tag{16}$$

$$\sum_{i=0}^{m} v_i(L) T_{T,i}(t_p) = \phi_L(t_p),\ p = 0, \ldots, m-1. \tag{17}$$

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From the initial condition when $x = 0$, we obtain also that

$$\sum_{i=0}^{m} (-1)^i v_i(0) = g(0), \quad (18)$$

$$\sum_{i=0}^{m} (-1)^i v_i(L) = g(L). \quad (19)$$

The approximate solution of the time-fractional diffusion equation, may then be reduced to a system of second order ordinary boundary value problems, which is linear if f is linear with respect to the third argument, and nonlinear otherwise.

3 Results and Discussion

In order to illustrate the feasibility of the methods, an example for which the analytical solution is known is now presented. The numerical error is measured by determining the maximum error at the mesh points (x_i, t_l):

$$\varepsilon_{\Delta x, \Delta t} = \max_{i=1,\dots,N,\, l=0,\dots,R} \left| u(x_i, t_j) - u_i^l \right|, \quad (20)$$

where u_i^l is the numerical solution at (x_i, t_l).

Example

$$\begin{cases} \frac{\partial^\alpha u(x,t)}{\partial t^\alpha} &= \frac{\partial}{\partial x}\left((x+1)\frac{\partial u(x,t)}{\partial x}\right) - t^2\left(2-2x-9x^2\right)x + t^2\left(1-x\right)x^2 \\ & -u(x,t) - \frac{2t^{2-\alpha}x^2(x-1)}{(2-3\alpha+\alpha^2)\Gamma(1-\alpha)} \\ u(x,0) &= 0, \;\; x \in (0,1) \\ u(x,t)|_{x=0,1} &= 0, \;\; t \in (0,1) \end{cases} \quad (21)$$

whose analytical solution is $T(x,t) = t^2 x^2 (1-x)$.

Tables 1 and 2 show the convergence order obtained for method 1. We obtained convergence orders of approximately 2 and 1 for the space and time. Note that the convergence order in time is reduced due to the assumption that the reaction term comes from the previous iteration. For this particular case, there is no need for this approximation, since we are dealing with a linear source term, but, we want to test the basic behavior of the method.

In Table 3 we compare the different methods by numerically solving the equation given in the example.

It can be seen that for Method 2, the absolute errors are much lower when compared to Method 1. For Method 1 we have used $\Delta t = 0.025$ and $\Delta x = 0.1$, but, even refining the mesh to $\Delta t = 0.005$ and $\Delta x = 0.005$, the small error obtained with Method 2 could not be achieved.

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Step sizes		$\alpha = 0.5$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	q
0.002	1/6	0.001958	–
0.002	1/12	0.000475	2.04
0.002	1/24	0.000097	2.29

Table 1: Numerical results obtained for the problem given in Eq. 21 (Method 1), for $\alpha = 0.5$: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence q, for the variable x ($\Delta t = 0.002$).

Step sizes		$\alpha = 0.5$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p
1/10	0.01	0.001544	–
1/20	0.01	0.000770	1.00
1/40	0.01	0.000380	1.02

Table 2: Numerical results obtained for the problem given in Eq. 21 (Method 1), for $\alpha = 0.5$: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p, for the variable t ($\Delta x = 0.01$).

		Method 1	Method 2		
x	u_{exact}	$\lvert u_{ex.} - u_{app.}\rvert$	$\lvert u_{ex.} - u_{app.}\rvert$ $m=1$	$\lvert u_{ex.} - u_{app.}\rvert$ $m=2$	$\lvert u_{ex.} - u_{app.}\rvert$ $m=3$
0.1	0.009	2.08590E-04	3.92491E-03	2.92558E-08	3.51328E-08
0.2	0.032	3.20917E-04	1.49104E-02	3.53476E-08	4.17026E-08
0.3	0.063	3.64312E-04	2.99838E-02	4.16731E-08	4.85743E-08
0.4	0.096	3.61761E-04	4.61841E-02	4.83157E-08	5.58276E-08
0.5	0.125	3.31354E-04	6.05480E-02	5.53470E-08	6.35323E-08
0.6	0.144	2.85839E-04	7.01013E-02	6.28303E-08	7.17508E-08
0.7	0.147	2.32238E-04	7.18517E-02	7.08234E-08	8.05412E-08
0.8	0.128	1.71492E-04	6.27843E-02	7.93813E-08	8.99593E-08
0.9	0.081	9.81395E-05	3.98576E-02	8.85571E-08	1.00060E-07

Table 3: Absolute error obtained for the two different methods ($\alpha = 0.5$ and $t = 1$). For Method 1 we have used $\Delta t = 0.025$ and $\Delta x = 0.1$.

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It should be noted that these results were obtained for the particular function shown in example 1, and, more studies should be performed in order to formulate accurate conclusions.

4 Conclusions

We derived two different numerical methods for the solution of the time-fractional diffusion equation with variable a diffusion coefficient and a nonlinear source term, together with Dirichlet boundary conditions. One of the methods is based on a straightforward finite difference method, while the second method assumes that the solution can be written in terms of Chebyshev polynomials. From simple simulations, we concluded that the second method provides smaller absolute errors, but, more studies need to be performed.

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