XLIII CILAMCE
21-25, November, 2022
FOZ DO IGUAÇU - PR - BRAZIL

A Fourier stability study for an explicit numerical scheme applied to the fractional diffusion equation with dimensional correction

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Abstract. This paper presents a study of stability analysis for the generalization of the fractional diffusion equation FDE with constant coefficient, when the dimensional correction parameter τ is inserted in the model. The numerical approach chosen is an explicit finite difference scheme inspired by the classical forward Euler method. The fractional temporal order derivative adopted in the equation is the Riemann-Liouville one, which is approximated by the Grünwald-Letnikov operator. The stability analysis is conducted with the application of the Fourier method, allowing to show that the proposed explicit scheme is conditionally stable. A numerical experiment is also presented with displayed results so as to back up the theoretical conclusions and to point the influence of the dimensional correction parameter.

Keywords: Stability analysis, Fractional diffusion equation, Dimensional correction, Finite differences approximation, Riemann-Liouville fractional derivatives.

1 Introduction

Fractional calculus appeared in 1695, in a letter sent by Leibniz to l'Hôpital, where he questions about the meaning of a derivative of order equal to one half. From that period onwards, the development of fractional calculus took place gradually with contributions of great names, such as Euler, Lagrange, Fourier, Abel, among others. In the last decades, fractional calculus has become an area that has attracted the interest of many research groups due to its success in several applications. These applications are strongly related to systems that present an anomalous superdiffusion or subdiffusion behavior, such as diffusion in plasmas [1], transport of fluids in porous media [2], diffusion in fractals [3], and some others.

Diffusion is a phenomenon which generally occurs when a system is led to the equilibrium process. Brownian motion or usual diffusion is characterized by linear dependence on the time growth of mean square displacement,

$$\langle x^2(t)\rangle \sim K_\alpha t^\alpha$$

with $\alpha = 1$. On the other hand, the anomalous behavior, in general, is characterized by non-linear growth, that is, for $\alpha > 1$, we have a superdiffusive process and for $\alpha < 1$, a subdiffusive process. The fractional diffusion equation that simulates subdiffusive anomalous diffusion is, according to [4],

$$\frac{\partial u(x,t)}{\partial t} = {}_{RL}D^{\alpha}_{0,t}\left(\mathcal{K}\tau^{\alpha}\frac{\partial^2 u(x,t)}{\partial x^2}\right) + f(x,t), \quad 0 < x < L, \;\; 0 < t \le T, \tag{1}$$

where $u(x,t)$ represents the probability density of finding a "particle" in x at time t. The ${}_{RL}D^{\alpha}_{0,t}$ in (1) is the fractional derivative defined through the Riemann-Liouville operator

$${}_{RL}D^{\alpha}_{a,t}f(t) := \frac{1}{\Gamma(m-\alpha)}\frac{d^m}{dt^m}\int_a^t (t-s)^{m-\alpha-1}f(s)ds \,. \tag{2}$$

Here and below, $\alpha > 0$ is the fractional derivative order while m, a positive integer, satisfies $m-1 < \alpha \le m$.

The initial and boundary value problem for the fractional diffusion equation is to determine the temperature distribution, *i.e.*, the function $u(x,t)$ such that

$$\frac{\partial u(x,t)}{\partial t} = {}_{RL}D^{\alpha}_{0,t}\left(\mathcal{K}\tau^{\alpha}\frac{\partial^2 u(x,t)}{\partial x^2}\right) + f(x,t), \quad 0 < x < L, \ 0 < t \leq T, \tag{3a}$$

$$u(x,0) = \phi(x), \quad 0 \leq x \leq L, \tag{3b}$$

$$u(0,t) = l(t), \quad 0 \leq t \leq T, \tag{3c}$$

$$u(L,t) = r(t), \quad 0 \leq t \leq T, \tag{3d}$$

being $\phi(x)$, $l(t)$, $r(t)$ and $f(x,t)$ sufficiently regular functions given herein.

The constant $\mathcal{K}$ in (3a) is called thermal diffusivity, and this parameter depends on the thermal conductivity κ, the density ρ and the material specific heat C_p, that is, $\mathcal{K} = \kappa/\rho C_p$. In the international system (SI) its unit equals to $[K] = [m^2/s]$. The adequacy of the diffusion equation of integer order to the one of arbitrary order generates an imbalance of dimensions and units, that is, $\left[\frac{d^{\alpha}}{dt^{\alpha}}\right] = s^{-\alpha}$. Thus, based on [5, 6] a new parameter τ is applied together with the fractional derivative as seen in (3a), τ being a parameter whose unit is time, so that the fractional equation (3a) preserves the dimension consistency. From now on we call $\mathcal{K}\tau^{\alpha}$ the fractional diffusion coefficient.

2 An explicit numerical approximation scheme for FDE

We have chosen the finite difference method to perform some numerical tests on (3), having applied a scheme based on forward Euler [7]. The computational mesh in the domain for (3) was defined by

$$x_i := i\Delta x, \ \ i = 0,1,2,\ldots,M, \ \ L = M\Delta x \ ,$$

$$t_n := n\Delta t, \ \ n = 0,1,2,\ldots,N, \ \ T = N\Delta t \ .$$

Grünwald-Letnikov fractional derivative for a sufficiently regular function $u(t)$ is equivalent to its fractional derivative in Riemann-Liouville sense [8]. This fact makes it possible to get approximations for the Riemann-Liouville fractional derivative if we employ Grünwald-Letnikov's, by what we mean

$${}_{RL}D^{\alpha}_{0,t}u(t)\big|_{t=t_n} \approx \frac{1}{\Delta t^{\alpha}}\sum_{k=0}^{n}(-1)^k\binom{\alpha}{k}u(t_{n-k}). \tag{4}$$

Expression (4) is a linear (order 1) approximation for any $\alpha > 0$. Applying forward and centered differences to integer derivatives and (4) to (3a), we get

$$\frac{U_i^n - U_i^{n-1}}{\Delta t} = \frac{\mathcal{K}\tau^{\alpha}}{\Delta t^{\alpha}}\sum_{k=0}^{n}\omega(k)\left(\frac{U_{i-1}^{n-k} - 2U_i^{n-k} + U_{i+1}^{n-k}}{\Delta x^2}\right) + f_i^n, \tag{5a}$$

$$U_i^0 = \phi(x_i) \ \ (i = 0,1,\ldots,M), \tag{5b}$$

$$U_0^n = l(t_n) \ \ (n = 0,1,\ldots,N), \tag{5c}$$

$$U_M^n = r(t_n) \ \ (n = 0,1,\ldots,N), \tag{5d}$$

where U_i^n is the approximation of $u(x_i,t_n)$ by the scheme (5a), $\omega(k) = (-1)^k\binom{\alpha}{k}$ and $f_i^n = f(x_i,t_n)$. From (5a), we get

$$U_i^{n+1} = U_i^n + r\sum_{k=0}^{n}\omega(k)(U_{i-1}^{n-k} - 2U_i^{n-k} + U_{i+1}^{n-k}) + \Delta t f_i^n, \tag{6}$$

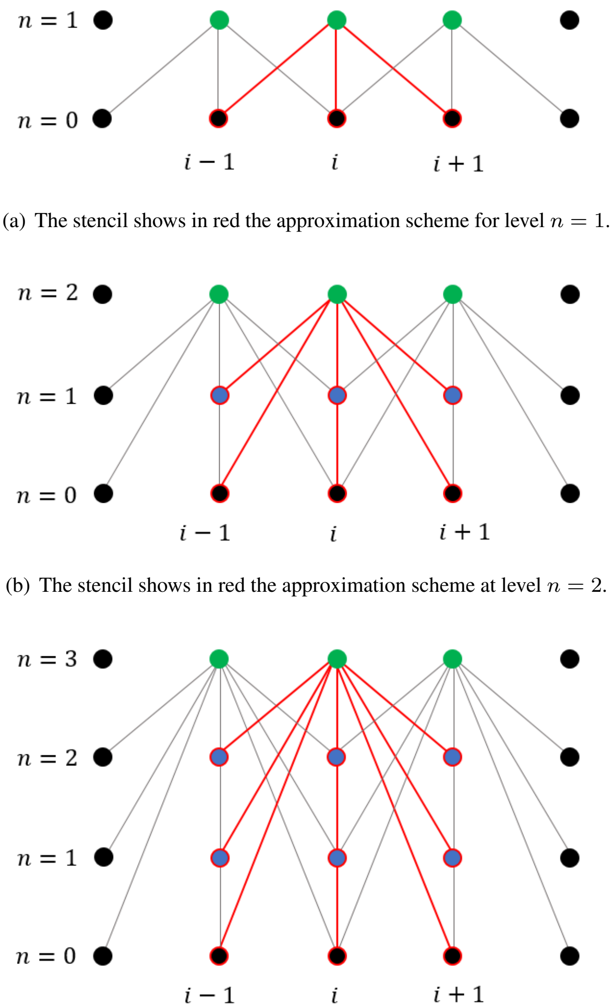
with $r := \mathcal{K}\frac{\Delta t}{\Delta x^2}\left(\frac{\tau}{\Delta t}\right)^{\alpha}$. For $1 \leq i \leq M-1$, the matrix form for (6) is

$$\boldsymbol{U^{n+1}} = \boldsymbol{U^n} + \sum_{k=0}^{n}\omega(k)\left(A\boldsymbol{U^{n-k}} + \boldsymbol{C^{n-k}}\right) + \Delta t\boldsymbol{f^n}, \tag{7}$$

where $\boldsymbol{f^n} = \left(f_1^n, f_2^n, \ldots, f_{N-1}^n\right)^t$, $\boldsymbol{U^n} := \left(U_1^n, U_2^n, \ldots, U_{N-1}^n\right)^t$, $\boldsymbol{C^{n-k}} := \left(rU_0^{n-k}, 0, \ldots, 0, rU_N^{n-k}\right)^t$ and

$$A := \begin{pmatrix} -2r & r & 0 & \ldots & 0 \\ r & -2r & r & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & r & -2r & r \\ 0 & \ldots & 0 & r & -2r \end{pmatrix}.$$

More details about its matrix form and computational implementation can be found in [9]. Figures 1 (a) – (c) show the dependence of the calculated values with respect to the nodes in the first three levels. The stencil formed by the red edges shows the values required for the calculation of node i in step n.



(a) The stencil shows in red the approximation scheme for level $n = 1$.

(b) The stencil shows in red the approximation scheme at level $n = 2$.

(c) The stencil shows in red the approximation scheme at level $n = 3$.

Figure 1. Stencil showing in red the calculating scheme for the explicit Euler type method in the first three levels.

3 Stability of the forward Euler Type Method

The study of stability will be done by the Von Neumann or Fourier method. We are assuming a solution in the form $U_i^n = d_n \, \mathrm{e}^{j\sigma i \Delta x}$, where $j^2 = -1$ and $\sigma = 2\pi m/L$. Inserting this expression into (6) one gets

$$d_{n+1} = d_n - 4r \,\mathrm{sen}^2\left(\frac{\sigma \Delta x}{2}\right) \sum_{k=0}^{n} \omega(k) d_{n-k} \; . \tag{8}$$

Lemma 3.1. *The sum* $\sum_{k=0}^{n} (-1)^{-k} \omega(k) = 2^{\alpha}$ *holds.*

Proof. See [10]. □

Teorema 3.1. *The explicit Euler type methods* (5) *is stable for* $\mathcal{K}\frac{\Delta t}{\Delta x^2}\left(\frac{\tau}{\Delta t}\right)^{\alpha} \leq \frac{1}{2^{1+\alpha}}$.

Proof. Let us write by Von Neumann $d_{n+1} = \xi(\sigma) d_n$ and assume for the moment that $\xi := \xi(\sigma)$ is independent of time. Then (8) implies a closed equation for the amplification factor ξ of the subdiffusion mode:

$$\xi = 1 - 4r \sin^2\left(\frac{\sigma \Delta x}{2}\right) \sum_{k=0}^{n} \omega(k) \xi^{-k} \; . \tag{9}$$

If $|\xi| > 1$ for some σ, the factor of the solution d_n grows to infinity according to (9) and the method is unstable. Considering the extreme value $\xi = -1$, we obtain from (9) the following stability bound on r:

$$r \sin^2\left(\frac{\sigma \Delta x}{2}\right) \leq \frac{1/2}{\sum_{k=0}^{n} (-1)^{-k} \omega(k)} \; . \tag{10}$$

Applying Lemma 3.1 in (10), we obtain

$$r \leq \frac{1}{(2^{1+\alpha}) \sin^2(\sigma \Delta x / 2)} \; . \tag{11}$$

As the maximum squared value of the sine function is bounded by one, we can give a more conservative and also easier to apply bound estimate for the stability of the forward Euler-type method, that is,

$$\mathcal{K}\frac{\Delta t}{\Delta x^2}\left(\frac{\tau}{\Delta t}\right)^{\alpha} \leq \frac{1}{2^{1+\alpha}} \; . \tag{12}$$

□

4 Numerical experiments

We considered a problem with absorbing boundaries, $l(t) = t^{1+\alpha} \exp(\pi\alpha)$, $r(t) = t^{1+\alpha} \exp(\pi(\alpha - 1))$, initial condition $\phi(x) = 0$ and source term $f(x,t) = \left[(1+\alpha)t^{\alpha} - \pi^2 \Gamma(\alpha+2) t\right] \exp(\pi(\alpha - x))$. The exact solution of (3a) is then $u(x,t) = t^{1+\alpha} \exp\left(\pi(\alpha - x)\right)$, on the domain $D := \{(x,t) |\; 0 < x < 1,\; 0 < t < 1\}$.

The values shown in Table 1 confirm the ones that theoretical numerical analysis has previewed. Furthermore, it exhibits an influence of the order α on the stability condition. We consider $\mathcal{K} = 1$ and set the parameter $\tau = 1$.

Table 1. Error in norm L^2 of forward Euler method with $\Delta t = 1/40000$.

M	$\alpha = 0,1$	$\frac{\Delta t^{0.9}}{\Delta x^2} \leq \frac{1}{2^{1.1}}$	$\alpha = 0,3$	$\frac{\Delta t^{0.7}}{\Delta x^2} \leq \frac{1}{2^{1.3}}$	$\alpha = 0,5$	$\frac{\Delta t^{0.5}}{\Delta x^2} \leq \frac{1}{2^{1.5}}$
10	2.3886×10^{-3}	0.0072	4.4266×10^{-3}	0.0601	NaN	0.5000
20	5.9948×10^{-4}	0.0289	1.1092×10^{-3}	0.2402	NaN	2.0000
30	2.6635×10^{-4}	0.0649 0.4665	NaN	0.5405 0.4061	NaN	4.5000 0.3536
40	1.4962×10^{-4}	0.1154	NaN	0.9609	NaN	8.0000
50	9.5564×10^{-5}	0.1803	NaN	1.5014	NaN	12.500

The displayed results on table 1 confirm the stability condition (12) of the proposed method. However, they motivate the search for another scheme in approaching the problem (5) since, even taking $\Delta t = 1/40000$ no convergence was obtained "NaN (Not a Number)" for values of α greater than or equal to 0.5, which could preclude more elaborate adjustments in the model. A mesh refinement in the temporal variable can lead to reach new values for α. However, the memory effect of the fractional derivatives advises us against making this option since the fractional derivative performance in the temporal variable generates a sum dependent on the number of steps in this variable. The consequent increase in the code processing time as well as in the demand for required memory may then turn its employment unfeasible.

Figures 2 show the effect caused by changes in the order α, having the parameter τ value being fixed as one. Taking $\Delta x = 1/20$ and $\Delta t = 1/20000$.

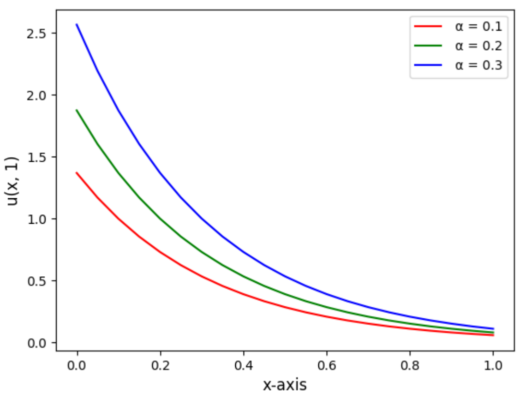
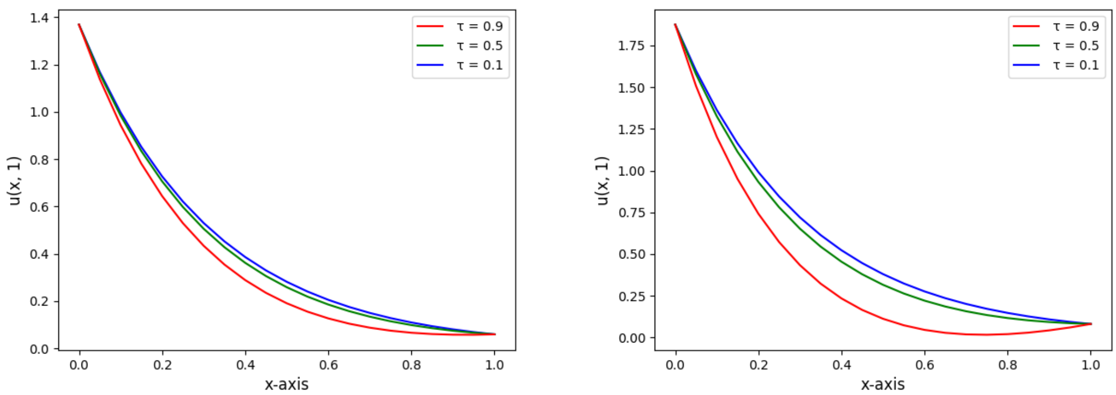


Figure 2. Numerical solutions at $T = 1$ with $\tau = 1$.

Figures 3(a) and (b) exhibit numerical results for different values of the dimensional correction parameter τ and the fracional derivative order α.



(a) Order $\alpha = 0.1$.

(b) Order $\alpha = 0.2$.

Figure 3. Numerical solutions at $T = 1$, taking $\Delta x = 1/20$ and $\Delta t = 1/10000$.

The numerical results shown in Figure 2 of the proposed example suggest that the order α of the fractional derivative has a considerable influence on the modeling. From another perspective, for a fixed value of α, the dimensional correction parameter τ also plays a role in adjusting the mathematical model to the problem, as seen in Figures 3(a)–(b).

Analysis of the stability condition (12) through table 1 confirms requirements on the stride length Δt to catch up information related to corresponding order values for α. In fact, it is possible to assign values to the parameter τ so that the method stability is obtained with a lower dependence on the step related to the temporal variable.

5 Conclusions

This work proposes an explicit finite difference approximation scheme – here called progressive Euler-type method – applied to a temporal fractional diffusion equation in the Riemann-Liouville sense, a dimensional correction parameter τ being considered. The stability condition for the numerical scheme is established by use of the Von Neumann method.

The performed computational tests have confirmed the theoretical results as regards to the numerical method stability. From the first look, the explicit scheme is particularly interesting due to its simplicity and easy implementation. On the other hand, the required stability condition can make it inadvisable when considering processing time and memory requiments. Inserting the dimension correction parameter τ in the modeling generates new alternatives, even for the adjustments of the method stability condition. On other hand, it imposes dealing with a new challenge, namely, the choice of the best value for τ.

Continuing this work, implicit schemes will be studied aiming at unconditionally stable methods and with more precise approximations. It is also planned to analyze the influence of the dimensional correction parameter with respect to different fractional derivative operators.

Acknowledgements. This work has been performed under financial support of CAPES – Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brazil, Financial Code 001

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