1 Introduction

Fractional calculus is becoming a useful and, in some cases, key tool in the analysis of scientific problems in a broad array of fields such as physics, engineering, biology, and economics. In particular, fractional partial differential equations have turned out to be especially relevant. For example, fractional diffusion equations have been successfully used to describe diffusion processes where the diffusion is anomalous [1–8], and fractional diffusion wave equations have been proposed to deal with viscoelastic problems (e.g., in the description of the propagation of stress waves in viscoelastic solids [9–11]). Many other examples can be found in Refs. [8,12–14].

In order for this fractional formalism to be useful in solving practical problems, one should be able to know how to find either exact or at least approximate solutions of these fractional equations. Fortunately, there exist many analytical methods that can provide such solutions [1,8,14–18]. However, as is also the case for the normal fractional equations, numerical methods are the most suitable way, and even the only way, to deal with some kinds of problems. Therefore, the proposal and study of efficient, accurate, and easy to implement numerical methods is quite important. Although in the last few years, many methods for solving fractional partial differential equations have been proposed and analyzed (see Refs. [19–36] and references therein), there is indeed still much work remaining to be done.

Difference methods and, in particular, explicit difference methods, are an important class of numerical methods for solving fractional (and normal) differential equations. The usefulness of the explicit methods and the reason why they are widely employed is based on their particularly attractive features [34,37]: flexibility, simplicity, scanty computational demand, and the possibility of easy generalization to spatial dimensions higher than 1. The method discussed in this paper is an explicit finite difference method designed for solving fractional diffusion and fractional diffusion-wave equations where the fractional derivative is in the Caputo form. As is well known, explicit methods can be unstable in some circumstances. So, it is crucial to determine under which conditions, if any, these methods are stable. This task is carried out in this paper by means of a von Neumann-type stability analysis.

The equation we will use as a testbed is

$$\frac{\partial^\gamma u}{\partial x^\gamma} = K \frac{\partial^2 u}{\partial x^2}$$  \hspace{1cm} (1)

where

$$\frac{\partial^\gamma}{\partial t^\gamma} f(t) = \frac{1}{\Gamma(n-\gamma)} \int_0^t \frac{d^\gamma f(\tau)}{d\tau^n} d\tau$$

$$n-1 < \gamma < n \quad (n \text{ integer})$$ \hspace{1cm} (2)

is the fractional derivative in Caputo’s sense [12,14] and $K$ is a constant (the diffusion constant). For $0 < \gamma < 1$, Eq. (1) is the fractional diffusion equation or subdiffusion equation, whereas for $1 < \gamma < 2$, the equation is the fractional diffusion-wave equation. In order to carry out numerical comparisons, we will consider two problems, both with $K=1$ and defined in the interval $0 \leq x \leq \pi$; the fractional diffusion Eq. (1) with boundary conditions $u(x,0,t) = u(x,\pi,t) = 0$ and initial condition $u(x,0) = f(x) = \sin x$ and the diffusion-wave equation with the same boundary condition $u(x,0,t) = u(x,\pi,t) = 0$ and initial condition $u(x,0) = f(x) = \sin x$ and $\partial u(x,t)/\partial t|_{t=0} = g(x) = 0$. We chose these two problems because their exact solution is known [15] and is easy to compute:

$$u(x,t) = E_\gamma(-t^\gamma) \sin x$$ \hspace{1cm} (3)

where $E_\gamma$ is the Mittag–Leffler function [8,12,14,38].

2 The Finite Difference Schemes

In what follows, we will use the notation $x_j = j \Delta x$, $t_m = m \Delta t$, and $u(x_j,t_m)/u(n) = f^{(n)}$, where $U^{(n)}$ stands for the numerical estimate of the exact solution $u(x,t)$ for $x=x_j$ and $t=t_m$.

In our analysis, we will consider separately the subdiffusion equation and the diffusion-wave equation. To obtain the finite difference scheme for solving the subdiffusion equation ($0 < \gamma < 1$), we discretize the Caputo derivative by means of the so-called L1 formula [39].
\[
\frac{\partial^2 f}{\partial t^2} \bigg|_{t_n} = \Delta \gamma f(t_m) + O(\Delta t)
\]  
\[\text{(4)}\]

with

\[
\Delta \gamma f(t_m) = \frac{(\Delta t)^{-\gamma}}{\Gamma(2-\gamma)} \sum_{k=0}^{m-1} b^k \left[ f(t_{m-k}) - f(t_{m-1-k}) \right]
\]  
\[\text{(5)}\]

and

\[
b^k = (k+1)^{1-\gamma} - k^{1-\gamma}
\]  
\[\text{(6)}\]

For the diffusion-wave equation \((1<\gamma\leq2)\), we proceed similarly, but here, using the so-called L2 formula [39]

\[
\frac{\partial^2 f}{\partial t^2} \bigg|_{t_n} = \Delta \gamma f(t_m) + O(\Delta t)^2
\]  
\[\text{(7)}\]

with

\[
\Delta \gamma f(t_m) = \frac{(\Delta t)^{-\gamma}}{\Gamma(3-\gamma)} \sum_{k=0}^{m-1} b^k \left[ f(t_{m-k}) - 2f(t_{m-1-k}) + f(t_{m-2-k}) \right]
\]  
\[\text{(8)}\]

and

\[
b^k = (k+1)^{2-\gamma} - k^{2-\gamma}
\]  
\[\text{(9)}\]

Using Eqs. (4) and (5) in Eq. (1), discretizing the second-order spatial derivative by the usual three-point centered formula

\[
\frac{\partial^2}{\partial x^2} u(x_j,t_m) = \Delta \gamma u(x_j,t_m) + O(\Delta x)^2
\]  
\[\text{(10)}\]

with

\[
\Delta \gamma u(x_j,t_m) = \frac{u(x_{j+1},t_m) - 2u(x_j,t_m) + u(x_{j-1},t_m)}{(\Delta x)^2}
\]  
\[\text{(11)}\]

and neglecting discretization errors of order \(O(\Delta t) + O(\Delta x)^2\) (see Sec. 4), one obtains the following finite difference scheme for solving subdiffusion equations:

\[
U_j^{(m+1)} = U_j^{(m)} + \bar{S}(U_j^{(m)} - 2U_j^{(m)} + U_j^{(m)}) - \sum_{k=1}^{m} b^k \left[U_j^{(m+1-k)} - U_j^{(m-k)} \right]
\]  
\[\text{(12)}\]

with \(\bar{S} = \Gamma(2-\gamma)S\) and

\[
S = \frac{\Gamma(\Delta t)^{-\gamma}}{(\Delta x)^2}
\]  
\[\text{(13)}\]

In the same way, using Eqs. (7) and (8) in Eq. (1), discretizing the second-order spatial derivative by the three-point centered formula and neglecting discretization errors of order \(O(\Delta t) + O(\Delta x)^2\), one obtains a finite difference scheme for solving diffusion-wave equations,

\[
U_j^{(m+1)} = 2U_j^{(m)} - U_j^{(m-1)} + \bar{S}(U_j^{(m)} - 2U_j^{(m)} + U_j^{(m)}) - \sum_{k=1}^{m} b^k \left[U_j^{(m+1-k)} - 2U_j^{(m-k)} + U_j^{(m-k)} \right]
\]  
\[\text{(14)}\]

with \(\bar{S} = \Gamma(3-\gamma)S\).

In Fig. 1, we compare the analytical solution and the numerical solution obtained by using the explicit scheme (12) to solve the fractional subdiffusion problem described at the end of Sec. 1, that is, the fractional diffusion Eq. (1) with \(K=1\) defined in the interval \(0 \leq x \leq \pi\) for the initial condition \(f(x) = \sin x\), boundary conditions \(u(0,t) = u(\pi,t) = 0\), and several values of \(\gamma\). Figure 2 shows the solution for the fractional diffusion-wave equation in the interval \(0 \leq x \leq \pi\) with \(K=1\) and \(f(x) = \sin x\), \(g(x) = 0\), and boundary conditions \(u(0,t) = u(\pi,t) = 0\) for several values of \(\gamma\). We find that the numerical solutions are in excellent agreement with the exact solution in all cases. The quality of these numerical results is similar to those found for other explicit difference methods [34,36,40].

3 Stability of the Fractional Difference Schemes

The two explicit difference schemes considered in Sec. 2 are not always stable. For any \(\gamma\), there are always choices of \(\Delta x\) and \(\Delta t\) (or, equivalently, choices of \(S\)) for which the numerical schemes become unstable. In these cases, the numerical solution eventually becomes useless and even absurd (two examples of this are shown in Figs. 3 and 5). Therefore, it is important to determine the conditions, if any, under which these two explicit methods are stable. For this purpose, we will use here a kind of fractional von Neumann stability analysis already employed in Refs. [34–36].

In order to analyze the stability of the numerical scheme (12) that solves subdiffusion equations, we start by analyzing the stability of a generic subdiffusive mode \(U_j^{(m)} = e^{iqx}e^{\Delta x}\), where \(q\) is any of the real spatial wave-numbers supported by the lattice. Inserting this expression into Eq. (12), one gets

\[
\dot{v}_{m+1} = v_m - \sum_{k=1}^{m} b^k (v_{m+1-k} - v_{m-k}) + \bar{S}(e^{iq\Delta x} - 2 + e^{-iq\Delta x}) v_m
\]  
\[\text{(15)}\]

The stability of the mode and, consequently, the stability of the numerical scheme will be determined by the behavior of \(\dot{v}_m\). If we write

![Fig. 1 Numerical solutions (symbols) and exact solutions \(u(\pi/2,t) = E_j(-t^\gamma)\) (lines) at the midpoint \(x = \pi/2\) of the fractional diffusion problem described in the main text for \(\gamma = 1\) (squares), \(\gamma = 0.75\) (triangles), and \(\gamma = 0.5\) (circles). We have used \(\Delta x = \pi/20\) in all cases and \(\bar{S} = 0.5\) for \(\gamma = 1\), \(\bar{S} = 0.44\) for \(\gamma = 3/4\), and \(\bar{S} = 0.38\) for \(\gamma = 1/2\).](image1)

![Fig. 2 Numerical solutions (symbols) and exact solutions \(u(\pi/2,t) = E_j(-t^\gamma)\) (lines) at the midpoint \(x = \pi/2\) of the fractional diffusion problem described in the main text for \(\gamma = 1.25\) (triangles), \(\gamma = 1.5\) (circles), \(\gamma = 1.75\) (squares), and \(\gamma = 2\) (stars) with \(\Delta t = 0.01\) and \(\Delta x = \pi/20\).](image2)
and assume that $\xi = \xi(q)$ is independent of time, then we obtain the following expression for the amplification factor $\xi$ of the subdiffusive mode:

$$\xi = 1 - \sum_{k=1}^{m} b_k(\xi^{-k} - \xi^{-k}) + \tilde{S}e^{iq\Delta t} - 2 + e^{-iq\Delta t}\xi$$ (17)

If $|\xi| > 1$ for some $q$, the temporal factor of the solution grows to infinity according to Eq. (16) and the mode is unstable. Considering the extreme value $\xi = -1$, we obtain from Eq. (17) the following stability bound on $\tilde{S}$:

$$\tilde{S} \sin^2\left(\frac{q\Delta t}{2}\right) \leq \tilde{S}_x^{\infty} = \frac{1}{2} + \frac{1}{2} \sum_{k=1}^{m} (-1)^{k(1-\gamma) - k^{1-\gamma}}$$ (18)

For $m$ to be large enough, we can estimate $\tilde{S}_x^{\infty}$ by $\tilde{S}_x = \lim_{m \to \infty} \tilde{S}_x^{\infty}$ and we get

$$\tilde{S} \sin^2\left(\frac{q\Delta t}{2}\right) \leq \tilde{S}_x$$ (19)

where $\tilde{S}_x$ can be written as $-\sum_{k=1}^{m} (-1)^{k(1-\gamma)}$ or, in terms of the Riemann zeta function,

$$\tilde{S}_x = (1 - 2^{1-\gamma})\zeta(\gamma - 1)$$ (20)

Because the sine function is bounded by 1, one finds that, a fortiori, the algorithm is stable if $\tilde{S} \leq \tilde{S}_x$, that is, if

$$S \leq S_x = \frac{(1 - 2^{1-\gamma})\zeta(\gamma - 1)}{\Gamma(2 - \gamma)}$$ (21)

In the same way, one can find the stability bound for the diffusion-wave equation ($1 < \gamma \leq 2$). Here, the equation for the amplification factor is

$$\xi = 2 + \xi^{-1} + \sum_{k=1}^{m} b_k(\xi^{1-k} - 2 \xi^{-k} + \xi^{-1-k}) = \tilde{S}e^{iq\Delta t} - 2 + e^{-iq\Delta t}\xi$$ (22)

Inserting the extreme value $\xi = -1$ into this equation, we obtain the following stability bound on $S$:

$$\tilde{S} \sin^2\left(\frac{q\Delta t}{2}\right) \leq \tilde{S}_x = 1 + \sum_{k=1}^{m} (-1)^{k(1-\gamma) - k^{1-\gamma}}$$ (23)

Proceeding as before for the subdiffusion, we get again Eq. (19) from this equation but now with

$$\tilde{S}_x = \sum_{k=1}^{m} (-1)^{k(1-\gamma) - k^{1-\gamma}}$$ (24)

or, in terms of the Riemann zeta function,

$$\tilde{S}_x = 2(1 - 2^{1-\gamma})\zeta(\gamma - 2)$$ (25)

This means that, a fortiori, the method is stable when

$$S \leq S_x = \frac{2^{1-\gamma}(\gamma - 2)\zeta(\gamma - 2)}{\Gamma(3 - \gamma)}$$ (26)

Figures 3 and 4 show the numerical solution $u(x,t)$ for the problem considered in Fig. 1 but for two values of $S$, respectively, larger and smaller than the stability bound provided by Eq. (21). Figures 5 and 6 show the numerical solution $u(x,t)$ for the problem considered in Fig. 2 for three values of $S$: one larger and two smaller than the stability bound provided by Eq. (26). One sees that the value of $S$ is crucial: When this parameter is inside the stability region, the solid line is to guide the eye.
stable region, one gets a sensible numerical solution; otherwise, one gets an evidently wrong solution with wild oscillations, which are the signature of an unstable scheme.

Finally, it should be noted that when one uses either of the two numerical schemes with a given mesh \( \Delta x \), the corresponding time step \( \Delta t \) for a given value of \( S \) (of course, smaller than \( S_\text{cr} \)) cannot be larger than a quantity of the order \( (\Delta x)^2 \gamma \). Therefore, for fractional subdiffusion equations where \( 0 < \gamma \leq 1 \), \( \Delta t \) could become extremely small even for not too small values of \( \Delta x \), especially if \( \gamma \) is close to zero. In this case, the number of steps needed to find the solution for moderate or even small times could become very large, making the numerical procedure inefficient. On the other hand, for diffusion-wave equations, because here \( \gamma \) is larger than 1, one realizes that the explicit numerical scheme could be stable even for large values of \( \Delta t \). Note, however, that in this case, the numerical solution would be inaccurate because, as we will show in Sec. 4, one expects the numerical error to be of order \( \Delta t \).

4 Truncation Error

In Sec. 2, we found the present finite difference method essentially by replacing the integro-differential Eq. (1) evaluated at the point \((x_j, t_m)\)

\[
\left[ \frac{\partial^2 u}{\partial t^2} - \frac{1}{K} \frac{\partial^2 u}{\partial x^2} \right]_{(x_j, t_m)} = 0
\]

by the difference equation

\[
\Delta u_j^{(m+1)} - K \Delta^2 u_j^{(m)} = T(x_j, t_m)
\]

(28)

Note that the temporal derivative and the spatial derivative are evaluated at different times, \( t_{m+1} \) and \( t_m \), respectively. Neglecting the truncation (error) term \( T(x_j, t) \), we got in Sec. 2 the explicit difference schemes (12) and (14). Of course, the smaller the term \( T(x_j, t) \), the better the approximate solution \( U \) obtained from these numerical schemes. So, it is important to estimate the size of \( T(x_j, t) \).

From Eqs. (1) and (28), we get

\[
\left[ \frac{\partial^2 u}{\partial t^2} \right]_{(x_j, t_m)} = \Delta u_j^{(m+1)} - K \Delta^2 u_j^{(m)} = T(x_j, t_m)
\]

(29)

But from Eq. (4), we see that

\[
\Delta u_j^{(m+1)} = \frac{\partial u}{\partial t}\bigg|_{(x_j, t_{m+1})} + O(\Delta t)
\]

(30)

But

\[
\frac{\partial u}{\partial t}\bigg|_{(x_j, t_{m+1})} = \frac{\partial u}{\partial t}\bigg|_{(x_j, t_m)} + \Delta t \frac{d}{dt} \frac{\partial u}{\partial t}\bigg|_{(x_j, t_m)} + O(\Delta t^2)
\]

(31)

so that

\[
\Delta u_j^{(m+1)} = \Delta u_j^{(m)} + O(\Delta t)
\]

(32)

From this result and from taking into account Eq. (10), we find

\[
T(x, t) = O(\Delta t) + O(\Delta t)^2
\]

(33)

Note that the stability condition (21) imposes that the largest value of \( \Delta t \) that one can choose should be of order \( (\Delta x)^2 \gamma \), so that for a given value of \( \Delta x \), the truncation error is of order \( (\Delta t)^2 \) for fractional subdiffusion equations, as \( 2/\gamma > 2 \) for these equations.

For the diffusion-wave equation \((1 < \gamma \leq 2)\), we proceed in the same form. The only difference is that now (see Eq. (7))

\[
\Delta u_j^{(m+1)} = \frac{\partial u}{\partial t}\bigg|_{(x_j, t_{m+1})} + O(\Delta t^2)
\]

(34)

But due to Eq. (31), we find that

\[
\Delta u_j^{(m+1)} = \Delta u_j^{(m)} + O(\Delta t) + O(\Delta t)^2
\]

so that finally, we obtain Eq. (33) in this case also. Finally, note that the stability condition (26) imposes that the largest value of \( \Delta t \) that one can choose is of order \( (\Delta x)^2 \gamma \), so that for a given value of \( \Delta x \), the truncation error would be of order \( (\Delta t)^2 \) for fractional diffusion-wave equations, as \( 2/\gamma < 2 \) for this kind of equations.

5 Numerical Check of the Stability Analysis

In this section, we check the stability bounds of the explicit schemes (4) and (5) given by Eqs. (20) and (21), respectively.

The stability bound (20), i.e., the largest value of \( \tilde{S} \) for which the numerical method (4) for solving fractional diffusion equations is stable, is checked in the following way: For a given value of \( \gamma \) chosen from the interval [0,1] and for \( \tilde{S} = 0.245(1+\gamma) + 0.001n \), with \( n = 0, 1, 2, \ldots \), we integrate the fractional diffusion problem described preceding Eq. (3) by means of the numerical scheme (4) until step \( M \). The simple linear function we have chosen for the initial value of \( \tilde{S} \) (the one corresponding to \( n=0 \)) is well below the theoretical stability bound predicted by Eq. (20). We consider that the numerical algorithm for some given values of \( \gamma \) and \( \tilde{S} \) is unstable when the absolute difference between two values corresponding to two consecutive steps is larger than a given value \( \Xi \), that is,

\[
|U_j^{(m+1)} - U_j^{(m)}| > \Xi
\]

(35)

at any position \( j \) within the first \( M \) integration steps. Here, we use \( \Xi = 1 \), but the results do not change substantially for any other reasonable choice. Let \( \tilde{S}_{\text{crit}} \) be the smallest value of \( \tilde{S} = 0.245(1+\gamma) + 0.001n \) that satisfies the criterion (35). For a lattice with \( 2N+1 \) points (including the absorbing boundaries), the maximum value of \( \sin(\pi/2) / (2N+1) \) in Eq. (19) occurs for \( \pi/2 = (2N+1) \pi/2(2N+1) \), so that the stability criterion (19) becomes \( \tilde{S}_{\text{crit}} \sin^2[(2N+1) \pi/(4N+2)] \approx \tilde{S}_{\text{cr}} \), or, in terms of \( \tilde{S} \), \( S_{\text{crit}} \equiv \tilde{S}_{\text{crit}} \), where \( \tilde{S}_{\text{crit}} = \tilde{S}_{\text{cr}} \sin^2[(2N+1) \pi/(4N+2)] / (G-\gamma) \). In Fig. 7, we check this stability bound by comparing \( S_{\text{crit}} \) evaluated numerically for \( M \)
The result of this analysis in terms of the quantity $S$ proves when bound corresponding to two other explicit difference methods, integration time step and $\frac{x}{H^2}$. The stability of the method was investigated by means of a fractional derivative that appears in the fractional diffusion-wave equations where the fractional Caputo form. It is remarkable that the stability region for the method is stable as long as the parameter $S$ of the von Neumann analysis and the symbols belong to the numerical results with the criterion in Eq. (31).

We proceed in a similar way to check the stability bound corresponding to the explicit methods of $\frac{x}{H^2}$ and $\frac{M}{H^2}$. The solid line is the size of the spatial discretization.

We thus determined that the method is stable as long as the parameter $S$ defined by $S=\frac{x}{H^2}$ satisfies the criterion (31) and $\frac{x}{H^2}$ is shown in Fig. 7. We again find that the agreement between numerical estimates and the prediction of the von Neumann stability analysis improves when $M$ increases. In this figure, we also show the stability bound corresponding to two other explicit difference methods, namely, the method of Yuste and Acedo [34] designed for fractional equations in the Riemann–Liouville form and the method by Gorenflo et al. [40] designed for fractional equations in the Caputo form. It is remarkable that the stability region for the present method is the largest.

6 Conclusions

An explicit difference method has been considered for solving fractional diffusion and diffusion-wave equations where the fractional derivative is in the Caputo form. The fractional derivative appearing in the fractional diffusion equation is approximated by means of the so-called L1 formula, the L2 formula employed for the fractional derivative that appears in the fractional diffusion-wave equation, and the spatial Laplacian approximated by the standard three-point centered formula for both equations. The truncation error is of order $O(\Delta t)+O(\Delta x^2)$, where $\Delta t$ is the integration time step and $\Delta x$ is the size of the spatial discretization. The stability of the method was investigated by means of a fractional version of the von Neumann (or Fourier) stability analysis. We thus determined that the method is stable as long as the parameter $S=K(\Delta t)^{\alpha}/(\Delta x^2)$ is below a given value (the stability bound) that can be easily expressed in terms of the Riemann zeta function (see Eqs. (21) and (26)). This region of stability is larger than the stability region of two other similar explicit difference methods, namely, the methods of Gorenflo et al. [40] and of Yuste and Acedo [34]. The predicted stability bound was checked numerically over the whole interval $0<\gamma \leq 2$, that is, for the two types of fractional equations (diffusion and diffusion-wave equations) considered in this paper.

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**References**


=200 and $M=1000$ with the theoretically predicted bound $S$. The convergence of the numerical values toward $S$ when $M$ increases is clear.

Proceed in a similar way to check the stability bound (21) of the algorithm (5) that integrates diffusion-wave equations. Here, we use the numerical scheme (5) to solve the diffusion-wave problem described preceding Eq. (3) with $S=\frac{x}{H^2}$. Again, we will denote the smallest value of $S=\frac{x}{H^2}$ that satisfies the criterion (31) by $S_{\text{crit}}$. The result of this analysis in terms of the quantity $S_{\text{crit}}$ defined by $S_{\text{crit}} = \frac{x}{H^2} \frac{\sin((2N-1)\pi/(4M))/\sin(3-\gamma)}{\gamma}$ is shown in Fig. 7. We also show the stability bound corresponding to two other explicit difference methods, namely, the method of Yuste and Acedo [34] designed for fractional equations in the Riemann–Liouville form and the method by Gorenflo et al. [40] designed for fractional equations in the Caputo form. It is remarkable that the stability region for the present method is the largest.

> **Fig. 7** Numerical values of $S_{\text{crit}}$ corresponding to the onset of instability versus the subdiffusion exponent $\gamma$. The solid line is the stability bound corresponding to the explicit methods of Refs. [34,36,40].


