

AN EXPLICIT FINITE DIFFERENCE METHOD AND A NEW VON NEUMANN-TYPE STABILITY ANALYSIS FOR FRACTIONAL DIFFUSION EQUATIONS*

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Abstract. A numerical method for solving the fractional diffusion equation, which could also be easily extended to other fractional partial differential equations, is considered. In this paper we combine the forward time centered space (FTCS) method, well known for the numerical integration of ordinary diffusion equations, with the Grünwald–Letnikov discretization of the Riemann–Liouville derivative to obtain an explicit FTCS scheme for solving the fractional diffusion equation. The stability analysis of this scheme is carried out by means of a powerful and simple new procedure close to the well-known von Neumann method for nonfractional partial differential equations. The analytical stability bounds are in excellent agreement with numerical test. A comparison between exact analytical solutions and numerical predictions is made.

Key words. fractional diffusion equation, von Neumann stability analysis, parabolic integro-differential equations, finite difference methods

AMS subject classifications. 26A33, 74S20, 45K05, 60J60

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1. Introduction. The study of fractional differential equations has been a highly specialized and isolated field of mathematics for many years [1]. However, in the last decade there has been increasing interest in the description of physical and chemical processes by means of equations involving fractional derivatives and integrals. This mathematical technique has a broad potential range of application [2]: relaxation in polymer systems, dynamics of protein molecules, and the diffusion of contaminants in complex geological formations are some of the most recently suggested applications [3].

Fractional kinetic equations have proved particularly useful in the context of anomalous slow diffusion (subdiffusion) [4]. Anomalous diffusion is characterized by an asymptotic long-time behavior of the mean square displacement of the form

$$(1.1) \quad \langle x^2(t) \rangle \sim \frac{2K_\gamma}{\Gamma(1+\gamma)} t^\gamma, \quad t \rightarrow \infty,$$

where γ is the anomalous diffusion exponent. The process is usually referred to as subdiffusive when $0 < \gamma < 1$. Ordinary (or Brownian) diffusion corresponds to $\gamma = 1$ with $K_1 = D$ (the diffusion coefficient). From a continuous point of view, the diffusion process is described by the diffusion equation $u_t(x, t) = D u_{xx}(x, t)$, where $u(x, t)$ represents the probability density of finding a “particle” at x at time t , and where $u_{\eta\zeta\dots}$ is the partial derivative with respect to the variables η, ζ, \dots . It turns out that the probability density function $u(x, t)$ that describes anomalous (sub)diffusive particles follows the fractional diffusion equation [4, 5, 6, 7]:

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$$(1.2) \quad \frac{\partial}{\partial t} u(x, t) = K_\gamma {}_0D_t^{1-\gamma} \frac{\partial^2}{\partial x^2} u(x, t), \quad t \geq 0,$$

where ${}_0D_t^{1-\gamma}$ is the fractional derivative defined through the Riemann–Liouville operator (see section 2). Fractional subdiffusion-advection equations, and fractional Fokker–Planck equations, have also been proposed [8, 9, 10, 11], and even subdiffusion-limited reactions have been discussed within this framework [12, 13]. These equations are also referred to as parabolic integrodifferential equations with weakly singular kernels [14].

These current applications of fractional differential equations, and many others that may well be devised in the near future, make it imperative to search for methods of solution. Some exact analytical solutions for a few cases, although important, are already known in terms of special functions such as the Wright function and Fox’s H-function [6, 7, 15, 16]. Some of these results have been obtained by means of the Mellin transform [6, 7] and the method of images [16]. The powerful method of separation of variables can also be applied to fractional equations in the same way as for the usual diffusion equations (an example is given in section 4). Another route to solving fractional equations is through the integration of the product of the solution of the corresponding nonfractional equation (the Brownian counterpart obtained by setting $\gamma \rightarrow 1$) and a one-sided Lévy stable density [4, 17]. However, as also for the Brownian case, the availability of numerical methods for solving (1.2) would be most desirable, especially for those cases where no analytical solution is available. One possibility was discussed recently by Gorenflo and Mainardi [18], Gorenflo, De Fabritiis, and Mainardi [19], and Gorenflo et al. [20], who presented a scheme for building discrete models of random walks suitable for the Monte Carlo simulation of random variables with a probability density governed by fractional diffusion equations. Another, more standard, approach is to build difference schemes of the type used for solving Volterra-type integrodifferential equations [14]. Along this line, some implicit (*backward* Euler and Crank–Nicholson) methods have been proposed [14, 21, 22, 23, 24, 25].

In this paper we shall use the *forward* Euler difference formula for the time derivative $\partial u/\partial t$ in (1.2) to build an *explicit* method that we will call the fractional forward time centered space (FTCS) method. For Brownian ($\gamma = 1$) diffusion equations, this explicit procedure is the simplest numerical methods workhorse [26, 27]. However, for fractional diffusion equations, this explicit method has been overlooked, perhaps because of the difficulty in finding the conditions under which the procedure is stable. This problem is solved here by means of a new stability analysis procedure close to the usual Fourier–von Neumann method for nonfractional partial differential equations.

The plan of the paper is as follows. In section 2 we give a short introduction to some results and definitions in fractional calculus. The numerical procedure for solving the fractional diffusion equation (1.2) by means of the explicit FTCS method is given in section 3. In this section we also discuss the stability and the truncating errors of the FTCS scheme. In section 4 we compare exact analytical solutions with numerical ones and check the reliability of the analytical stability condition. Some concluding remarks are given in section 5.

2. Basic concepts of fractional calculus. The notion of fractional calculus was anticipated by Leibniz, one of the founders of standard calculus, in a letter written in 1695 [1, 4]. But it was in the next two centuries that this subject fully developed into a field of mathematics with the work of Laplace, Cayley, Riemann, Liouville, and many others.

There are two alternative definitions for the fractional derivative ${}_0D_t^{1-\gamma}$ of a function $f(t)$. On the one hand, there is the Riemann–Liouville operator definition

$$(2.1) \quad {}_0D_t^{1-\gamma} f(t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t d\tau \frac{f(\tau)}{(t-\tau)^{1-\gamma}},$$

with $0 < \gamma < 1$. For $\gamma = 1$ one recovers the identity operator and for $\gamma = 0$ the ordinary first-order derivative. On the other hand, the fractional derivative of order $1 - \gamma$ of a function $f(t)$ in the Grünwald–Letnikov form is

$$(2.2) \quad {}_0D_t^{1-\gamma} f(t) = \lim_{h \rightarrow 0} \frac{1}{h^{(1-\gamma)}} \sum_{k=0}^{[t/h]} \omega_k^{(1-\gamma)} f(t - kh), \quad t \geq 0,$$

where $[t/h]$ means the integer part of t/h and $\omega_k^{(1-\gamma)} = (-1)^k \binom{1-\gamma}{k}$. The Grünwald–Letnikov definition is simply a generalization of the ordinary discretization formulas for integer order derivatives [1]. The Riemann–Liouville and the Grünwald–Letnikov approaches coincide under relatively weak conditions: if $f(t)$ is continuous and $f'(t)$ is integrable in the interval $[0, t]$, then for every order $0 < 1 - \gamma < 1$ both the Riemann–Liouville and the Grünwald–Letnikov derivatives exist and coincide for any time inside the interval $[0, t]$ [1, sect. 2.3.7]. This theorem of fractional calculus ensures the consistency of both definitions for most physical applications, where the functions are expected to be sufficiently smooth.

The Grünwald–Letnikov definition is important for our purposes because it allows us to estimate ${}_0D_t^{1-\gamma} f(t)$ numerically in a simple and efficient way:

$$(2.3) \quad {}_0D_t^{1-\gamma} f(t) = \frac{1}{h^{(1-\gamma)}} \sum_{k=0}^{[t/h]} \omega_k^{(1-\gamma)} f(t - kh) + O(h^p).$$

This formula is not unique because there are many different valid choices for $\omega_k^{(\alpha)}$ that lead to approximations of different order p [28]. Let $\omega(z, \alpha)$ be the generating function of the coefficients $\omega_k^{(\alpha)}$, i.e.,

$$(2.4) \quad \omega(z, \alpha) = \sum_{k=0}^{\infty} \omega_k^{(\alpha)} z^k.$$

If the generating function is

$$(2.5) \quad \omega(z, \alpha) = (1 - z)^\alpha,$$

then we get the backward difference formula of order $p = 1$ (BDF1) [1, 28]. This is also called the backward Euler formula of order 1 or, simply, the Grünwald–Letnikov formula. These coefficients are $\omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ and can be evaluated recursively:

$$(2.6) \quad \omega_0^{(\alpha)} = 1, \quad \omega_k^{(\alpha)} = \left(1 - \frac{\alpha + 1}{k}\right) \omega_{k-1}^{(\alpha)}.$$

The generating function for the backward difference formula of order $p = 2$ (BDF2) is [1, 28]

$$(2.7) \quad \omega(z, \alpha) = \left(\frac{3}{2} - 2z + \frac{1}{2}z^2\right)^\alpha.$$

These coefficients can be easily calculated using fast Fourier transforms [1]. However, for the fractional FTCS method discussed in this paper, we will show in the next section that nothing is gained by using second-order approximations for the fractional derivative. Additionally, the stability bound is smaller if one uses the BDF2 formula. Finally, it is important to note that the error estimates given in (2.3) are valid only if either $t/h \gg 1$ [1] or $u(x, t)$ is sufficiently smooth at the time origin $t = 0$ [29].

3. Fractional FTCS method. We will use the customary notation $x_j = j\Delta x$, $t_m = m\Delta t$, and $u(x_j, t_m) \equiv u_j^{(m)} \simeq U_j^{(m)}$, where $U_j^{(m)}$ stands for the numerical estimate of the exact value of $u(x, t)$ at the point (x_j, t_m) . In the usual FTCS method, the diffusion equation is replaced with a difference recurrence system for the quantities $u_j^{(m)}$:

$$(3.1) \quad \frac{u_j^{(m+1)} - u_j^{(m)}}{\Delta t} = D \frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{(\Delta x)^2} + T(x, t),$$

with $T(x, t)$ being the truncation term [26]. In the same way, the fractional equation is replaced with

$$(3.2) \quad \frac{u_j^{(m+1)} - u_j^{(m)}}{\Delta t} = K_\gamma {}_0D_t^{1-\gamma} \frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{(\Delta x)^2} + T(x, t).$$

The estimate of the truncation term will be given in section 3.2. Inserting the Grünwald–Letnikov definition of the fractional derivative given in (2.3) into (3.2), neglecting the truncation term, and rearranging the terms, we finally get the explicit FTCS difference scheme

$$(3.3) \quad U_j^{(m+1)} = U_j^{(m)} + S_\gamma \sum_{k=0}^m \omega_k^{(1-\gamma)} \left[U_{j-1}^{(m-k)} - 2U_j^{(m-k)} + U_{j+1}^{(m-k)} \right],$$

where $S_\gamma = K_\gamma \Delta t / [h^{1-\gamma} (\Delta x)^2]$. In this scheme, $U_j^{(m+1)}$, for every position j , is given *explicitly* in terms of all the previous states $U_j^{(n)}$, $n = 0, 1, \dots, m$. Because the estimates $U_j^{(m)}$ of $u(x_j, t_m)$ are made at the times $m\Delta t$, $m = 1, 2, \dots$, and because the evaluation of ${}_0D_t^{1-\gamma} u(x_j, t)$ by means of (2.3) requires knowing $u(x_j, t)$ at the times nh , $n = 0, 1, 2, \dots$, it is natural to choose $h = \Delta t$. In this case,

$$(3.4) \quad S_\gamma = K_\gamma \frac{\Delta t^\gamma}{(\Delta x)^2}.$$

We assume that the system is prepared in an initial state $u_j^{(0)} = U_j^{(0)}$ with $u_j^{(n)} = 0$ if $n \leq -1$. The iteration process described by (3.3) is easily implementable as a computer algorithm, but the resulting program is far more memory hungry than the elementary Markov diffusive analogue because, in evaluating $U_j^{(m+1)}$, one has to save all the previous estimates $U_{j-1}^{(n)}$, $U_j^{(n)}$, and $U_{j+1}^{(n)}$ for $n = 0, 1, \dots, m$. However, the use of the short-memory principle [1] or the nested mesh procedure [30] could alleviate this burden. Regardless, before tackling (3.3) seriously we must first discuss two fundamental questions concerning any integration algorithm: its stability and the magnitude of the errors committed by the replacement of the continuous equation with the discrete algorithm.

3.1. Stability of the fractional FTCS method. Here we will show that the stability of the fractional numerical schemes can be analyzed very easily and efficiently with a method close to the well-known Von Neumann (or Fourier) method of nonfractional partial differential equations. In this section, we will apply it to the fractional FTCS difference scheme (3.3).

We start by assuming a solution (a subdiffusion mode or eigenfunction) with the form $u_j^{(m)} = \zeta_m e^{iqj\Delta x}$, where q is a real spatial wave number. Inserting this expression into (3.3) one gets

$$(3.5) \quad \zeta_{m+1} = \zeta_m - 4S \sin^2 \left(\frac{q\Delta x}{2} \right) \sum_{k=0}^m \omega_k^{(1-\gamma)} \zeta_{m-k}.$$

It is interesting to note that this equation is the discretized version of

$$(3.6) \quad \frac{d\psi(t)}{dt} = -4C \sin^2 \left(\frac{q\Delta x}{2} \right) {}_0D_t^{1-\gamma} \psi(t)$$

(with $C = S(\Delta t)^\gamma$) whose solution can be expressed in terms of the Mittag-Leffler function $E_\gamma(-\lambda t^\gamma)$ [2, 4]. This result is not unexpected because the subdiffusion modes of (1.2) decay as Mittag-Leffler functions [4] (e.g., see (4.4)).

The stability of the solution is determined by the behavior of ζ_m . Unfortunately, solving (3.5) is much more difficult than solving the corresponding equation for the diffusive case. However, let us write

$$(3.7) \quad \zeta_{m+1} = \xi \zeta_m,$$

and let us *assume* for the moment that $\xi \equiv \xi(q)$ is independent of time. Then (3.5) implies a closed equation for the amplification factor ξ of the subdiffusion mode:

$$(3.8) \quad \xi = 1 - 4S_\gamma \sin^2 \left(\frac{q\Delta x}{2} \right) \sum_{k=0}^m \omega_k^{(1-\gamma)} \xi^{-k}.$$

If $|\xi| > 1$ for some q , the temporal factor of the solution grows to infinity according to (3.7) and the mode is unstable. Considering the extreme value $\xi = -1$, we obtain from (3.8) the following stability bound on S_γ :

$$(3.9) \quad S_\gamma \sin^2 \left(\frac{q\Delta x}{2} \right) \leq \frac{1/2}{\sum_{k=0}^m (-1)^k \omega_k^{(1-\gamma)}} \equiv S_{\gamma,m}^\times.$$

The bound expressed in (3.9) depends on the number of iterations m . Nevertheless, this dependence is weak: $S_{\gamma,m}^\times$ approaches $S_\gamma^\times \equiv \lim_{m \rightarrow \infty} S_{\gamma,m}^\times$ in the form of oscillations with small decaying amplitudes (see Figure 3.1). The value of S_γ^\times can be deduced from (3.9) by taking into account that $\sum_{k=0}^\infty (-1)^k \omega_k^{(1-\gamma)} \equiv \omega(-1, 1-\gamma)$ (see (2.4)). Therefore, we find that the FTCS method is stable as long as

$$(3.10) \quad S_\gamma \sin^2 \left(\frac{q\Delta x}{2} \right) \leq S_\gamma^\times$$

with

$$(3.11) \quad S_\gamma^\times = \frac{1}{2\omega(-1, 1-\gamma)}.$$

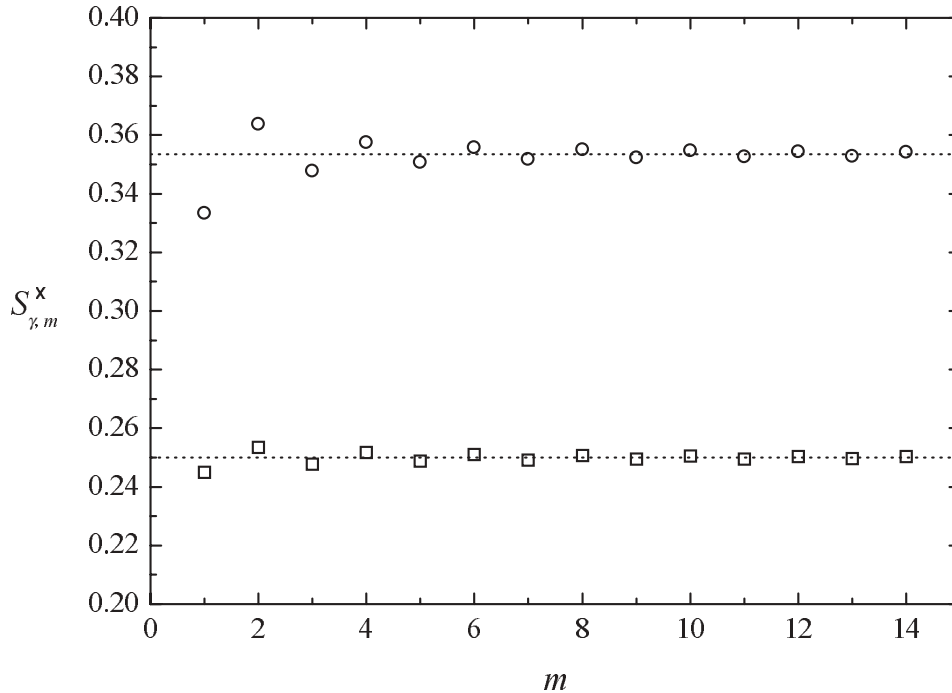


FIG. 3.1. First values of $S_{\gamma,m}$ versus m for $\gamma = 1/2$ when the first-order coefficients (circles) and second-order coefficients (squares) are used. The lines mark the corresponding limit values S_{γ}^x given by (3.12) and (3.13).

In particular, when the BDF1 coefficients given by (2.5) are used, one gets

$$(3.12) \quad S_{\gamma}^x = \frac{1}{2(1 - \xi)^{1-\gamma} \Big|_{\xi \rightarrow -1}} = \frac{1}{2^{2-\gamma}}.$$

Similarly, when the BDF2 coefficients given by (2.7) are used, one gets

$$(3.13) \quad S_{\gamma}^x = \frac{1}{2 \left(\frac{3}{2} - 2\xi + \frac{1}{2}\xi^2 \right)^{1-\gamma} \Big|_{\xi \rightarrow -1}} = \frac{1}{4^{3/2-\gamma}}.$$

We will verify numerically in section 4 that the explicit integration method as given by (3.3) is stable when

$$(3.14) \quad S_{\gamma} \leq \frac{S_{\gamma}^x}{\sin^2 \left(\frac{q\Delta x}{2} \right)}$$

and unstable otherwise. As the maximum value of the square of the sine function is bounded by 1, we can give a more conservative but simpler bound: the fractional FTCS method will be stable when

$$(3.15) \quad S_{\gamma} = K_{\gamma} \frac{\Delta t^{\gamma}}{(\Delta x)^2} \leq S_{\gamma}^x.$$

The physical interpretation of this restriction is the same as for the diffusive case, namely, (3.15) means that the maximum allowed time step Δt is, up to a numerical factor, the (sub)diffusion time across a distance of length Δx (cf. (1.1)).

Notice that the value of $S_\gamma^\times = 1/4^{3/2-\gamma}$ given by (3.13) is smaller than $1/2^{2-\gamma}$ for any $\gamma < 1$ (if $\gamma = 1$, we recover the bound $S^\times = 1/2$ of the usual explicit FTCS method for the ordinary diffusion equation [26, 27]). Consequently, the fractional FTCS method that uses a second-order approximation in the fractional derivative is “less robust” than the fractional FTCS method that uses the first-order coefficients $\omega_k^{(1-\gamma)}$. Taking into account that the two methods (BDF1 and BDF2) have the same precision (see section 3.2) we note that nothing is gained by using the fractional derivative with higher precision. Therefore, in practical applications, here we will use only the first-order coefficients (2.6).

3.2. Truncating error of the fractional FTCS method. The truncating error $T(x, t)$ of the fractional FTCS difference scheme is (see (3.2))

$$(3.16) \quad T(x, t) = \frac{u_j^{(m+1)} - u_j^{(m)}}{\Delta t} - K_\gamma D_t^{1-\gamma} \left[\frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{(\Delta x)^2} \right].$$

But

$$(3.17) \quad \frac{u_j^{(m+1)} - u_j^{(m)}}{\Delta t} = u_t + \frac{1}{2}u_{tt}\Delta t + O(\Delta t)^2$$

and

$$(3.18) \quad {}_0D_t^{1-\gamma} \left[u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)} \right] = \frac{1}{h^{1-\gamma}} \sum_{k=0}^m \omega_k^{1-\gamma} \left[u_{xx} + \frac{1}{12}u_{xxxx}(\Delta x)^2 + \dots \right] + O(h^p)$$

so that, taking into account that $u(x, t)$ is the exact solution of (1.2), we finally get from (3.16), (3.17), and (3.18) the following result:

$$(3.19) \quad T(x, t) = O(h^p) + \frac{1}{2}u_{tt}\Delta t - \frac{K_\gamma(\Delta x)^2}{12} {}_0D_t^{1-\gamma}u_{xxxx} + \dots$$

$$(3.20) \quad = O(h^p) + O(\Delta t) + O(\Delta x)^2.$$

Therefore, (i) assuming that the initial boundary data for u are consistent (as assumed for the usual FTCS method [26]) and (ii) assuming that u is sufficiently smooth at the origin $t = 0$ (see the remark below (2.7)), we conclude that the method discussed in this paper is unconditionally consistent for any order p because $T(x, t) \rightarrow 0$ as $h, \Delta t, \Delta x \rightarrow 0$. As remarked above, in practical calculations it is convenient to use $h = \Delta t$ so that, due to the term $O(\Delta t)$ in (3.20), no improvements are achieved by considering higher orders than $p = 1$ in the fractional derivative. It is interesting to note that for the diffusion equation ($\gamma = 1$) it is possible to cancel out the last two terms in (3.19) with the choice $\Delta t = (\Delta x)^2/(6K_\gamma)$, thereby obtaining a scheme that is “second-order accurate” [26]. This is not possible for the fractional case because of the fractional operator.

4. Numerical solutions and the stability bound on S_γ . The objective of this section is twofold: first, we want to test the reliability of the numerical algorithm defined in (3.3) by applying it to two fractional problems with known exact solutions and, second, we want to check the stability bounds obtained in section 3.1.

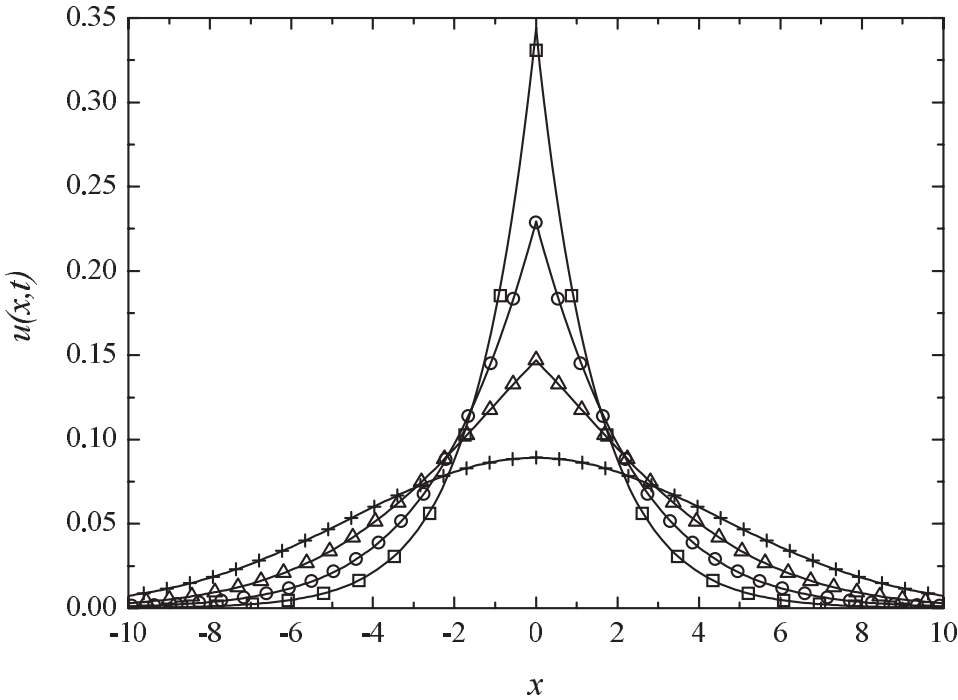


FIG. 4.1. Numerical solution of the subdiffusion equation for the problem defined in the unbounded space, $-\infty < x < \infty$ with initial condition $u(x, t = 0) = \delta(x)$ for $\gamma = 1/4$ (squares), $\gamma = 1/2$ (circles), $\gamma = 3/4$ (triangles), and $\gamma = 1$ (crosses), and $t = 10$. The lines correspond to the exact analytical solution.

4.1. Numerical solution versus exact solution: Two examples. The fundamental solution of the subdiffusion equation in (1.2) corresponds to the problem defined in the unbounded space, $-\infty < x < \infty$, where the initial condition is $u(x, t = 0) = \delta(x)$. This solution is called the propagator, or Green’s function, and can be expressed in terms of Fox’s H-function [4]:

$$(4.1) \quad u(x, t) = \frac{1}{\sqrt{4\pi K_\gamma t^\gamma}} H_{11}^{10} \left[\frac{|x|}{\sqrt{K_\gamma t^\gamma}} \left| \begin{matrix} (1 - \gamma/2, \gamma/2) \\ (0, 1) \end{matrix} \right. \right].$$

In our numerical solution we used the boundary conditions $u(-L, t) = u(L, t) = 0$ with a sufficiently large L in order to avoid finite size effects. In Figure 4.1 we compare the numerical integration results with the exact solution (4.1) for $\gamma = 1/4, 1/2, 3/4, 1$ at $t = 10$. The time step used was $\Delta t = 0.01$ and $\Delta x = \sqrt{K_\gamma (\Delta t)^\gamma / S_\gamma}$ with $K_\gamma = 1$ and $S_\gamma = 0.28, 0.33, 0.4,$ and 0.5 . All these values of S_γ are just below the stability bound S_γ^\times (see (3.12)). The agreement is excellent except for $\gamma = 1/4$ and $x = 0$, but this minor discrepancy is surely due to the large spatial cell $\Delta x \simeq 1.06$ used in this case.

We have also considered a problem with absorbing boundaries, $u(0, t) = u(1, t) = 0$, and initial condition $u(x, t = 0) = x(1 - x)$, with $0 \leq x \leq 1$. The exact analytical solution of (1.2) is easily found by the method of separation of variables: $u(x, t) =$

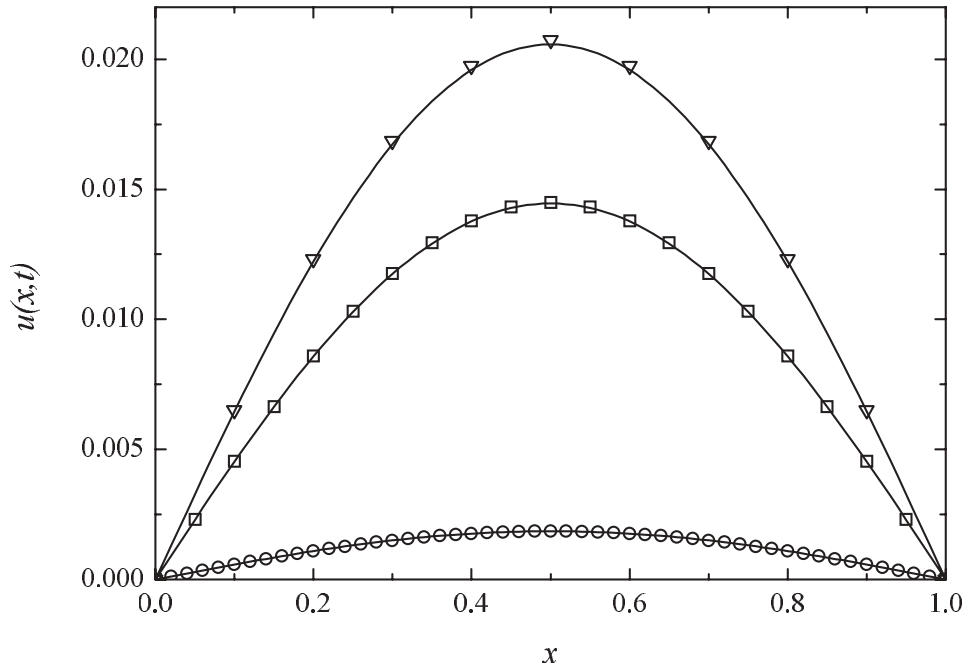


FIG. 4.2. Numerical solution of the subdiffusion equation for the problem with absorbing boundary conditions $u(0, t) = u(1, t) = 0$ and initial condition $u(x, 0) = x(1 - x)$, $0 \leq x \leq 1$, for $t = 0.5$. The solution $u(x, t)$ is shown for $\gamma = 0.5$ (triangles), $\gamma = 0.75$ (squares), and $\gamma = 1$ (circles). The lines correspond to the exact analytical solution.

$X(x)T(t)$. We thus find $X_n(x) = \sin(n\pi x)$ and

$$(4.2) \quad \frac{dT}{dt} = -K_\gamma \lambda_n^2 {}_0D_t^{1-\gamma} T,$$

where $\lambda_n = n\pi$, $n = 1, 2, \dots$. The solution of (4.2) is found in terms of the Mittag-Leffler function [4]:

$$(4.3) \quad T_n(t) = E_\gamma(-K_\gamma n^2 \pi^2 t^\gamma).$$

Imposing the initial condition we obtain

$$(4.4) \quad u(x, t) = \frac{8}{\pi^3} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^3} \sin[(2n+1)\pi x] E_\gamma[-K(2n+1)^2 \pi^2 t^\gamma].$$

In Figure 4.2 we compare this exact solution with the results of the numerical integration scheme for $\gamma = 0.5$, $\gamma = 0.75$, and $\gamma = 1$ for $t = 0.5$ and $K_\gamma = 1$. The values of S_γ used were $S_\gamma = 0.33, 0.4$, and 0.5 with $\Delta x = 1/10, 1/20$, and $1/50$, respectively. The values of Δt for fixed S_γ and Δx stem from the definition of S_γ :

$$(4.5) \quad \Delta t = \left[\frac{S_\gamma (\Delta x)^2}{K_\gamma} \right]^{1/\gamma}.$$

Excellent agreement is observed for the three values of γ , it being slightly poorer for the smallest value, which is not surprising because in this case the mesh size $\Delta x = 1/10$ used is the largest.

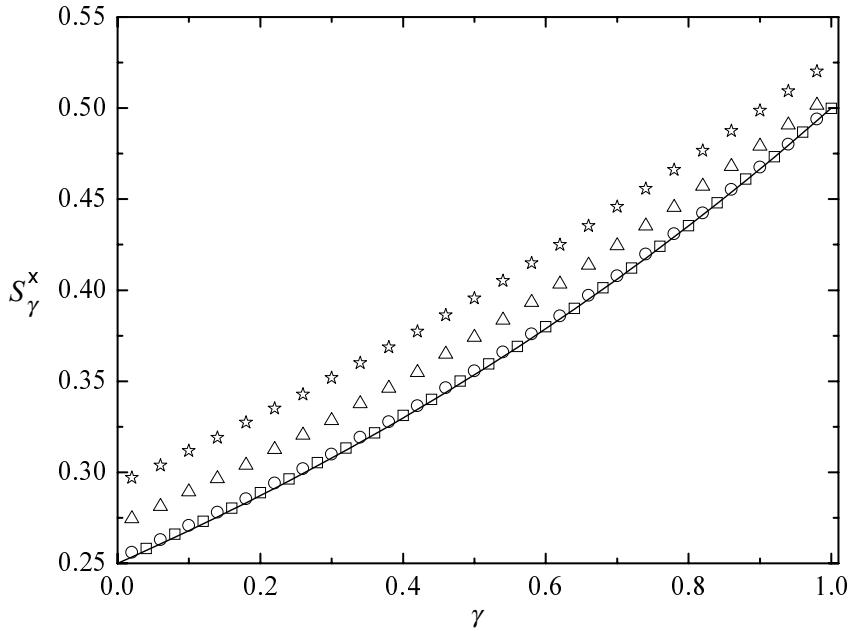


FIG. 4.3. Values of S_γ^x corresponding to the onset of instability versus the subdiffusion exponent γ . The solid line is the prediction of the Fourier-von Neumann analysis and the symbols denote the results of the numerical tests with the criterion in (4.6): stars, triangles, and squares for the absorbing boundary problem with $u(x, 0) = x(1 - x)$ with $M = 50, 100$ and 1000 , respectively, and circles for the propagator with $M = 1000$.

4.2. Numerical check of the stability analysis. We checked the stability bound on the value of the S_γ given in (3.12) in the following way. For a set of values of γ in the interval $[0, 1]$, and for values of S_γ starting at $S_\gamma = 0.98S_\gamma^x$ (in particular, for $S_\gamma = 0.98/2^{2-\gamma} + 0.001n$, $n = 0, 1, 2, \dots$) we applied the fractional FTCS integration until step M . We say that the resulting integration for given values of γ and S_γ is unstable when the following condition is satisfied at any position j :

$$(4.6) \quad \left| \frac{u_j^{m-1}}{u_j^m} - \Xi \right| > \Xi \quad \text{for any } m = M - \Delta M, M - \Delta M + 1, \dots, M,$$

where $\Xi = 5$ and $\Delta M = 10$. This means that the numerical solution is considered unstable if the quotient u_j^{m-1}/u_j^m becomes negative or larger than 2Ξ at any of the last ΔM steps. (Of course, this criterion is arbitrary; however, the results do not change substantially for any other reasonable choice of Ξ and ΔM .) Let S_γ^{\min} be the smallest value of $S_\gamma = 0.98/2^{2-\gamma} + 0.001n$ that verifies the criterion (4.6). For the absorbing boundary problem we calculate these values using $\Delta x = 1/2N$ with $N = 5, M = 50, M = 100$, and $M = 1000$. For the propagator, we calculate S_γ^{\min} using $M = 1000$ and $\Delta t = 5 \times 10^{-4}$ in a lattice with absorbing frontiers placed at $x = -N\Delta x$ and $x = N\Delta x$ with $N = 50$. It is well known that for a lattice with $2N + 1$ points (including the absorbing boundaries) the maximum value of $\sin(q\Delta x/2)$ in (3.10) occurs for $q\Delta x = (2N - 1)\pi/(2N)$, so that in Figure 4.3 we plot $S_\gamma^{\min} \sin^2[(2N - 1)\pi/(4N)]$. We observe that for large M the stability bound predicted by (3.12) agrees with the result of the numerical test. The larger values obtained for smaller M mean that the method must

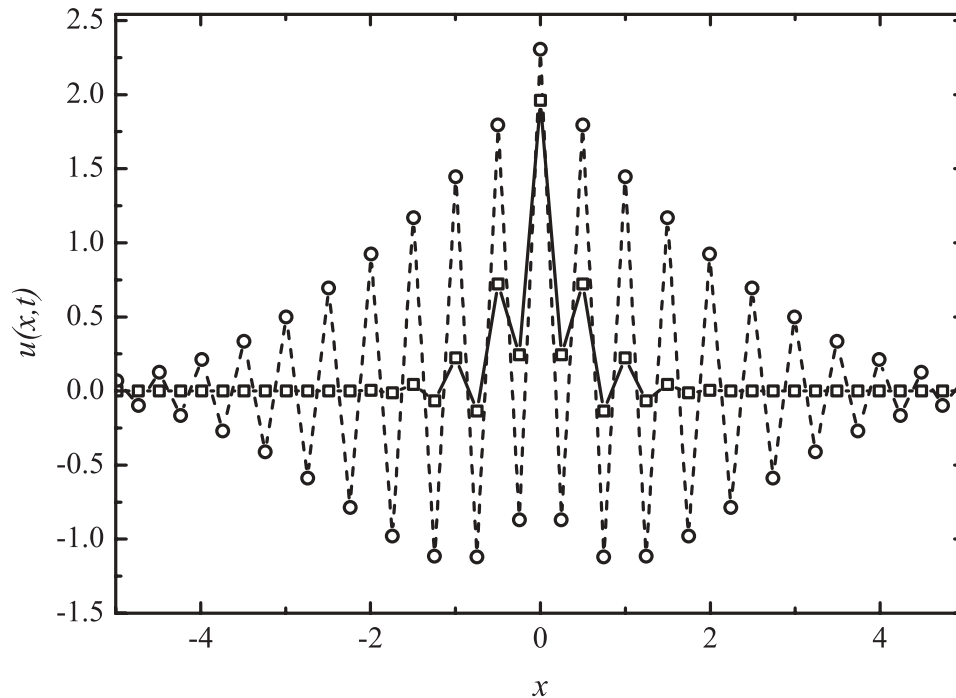


FIG. 4.4. Unstable numerical solution of the subdiffusion equation for the problem defined in the unbounded space with initial condition $u(x, t = 0) = \delta(x)$ for $\gamma = 1/2$, $K_\gamma = 1$, $S = 0.36$ and $t = 0.005$ (squares), and $t = 0.05$ (circles). The time step is $\Delta t = 0.0005$ and the spatial mesh Δx is obtained according to (4.5). The lines are plotted as a visual guide.

be “very unstable” to fulfill our instability criterion in so few steps. The success of the numerical test is truly remarkable and supports the application of our Fourier–von Neumann-type stability analysis to the fractional FTCS scheme made in section 3.1.

In Figure 4.4 we plot the numerical solution when $S_\gamma = 0.36 > S_\gamma^\times$ in the case of the propagator with $\gamma = 1/2$. This kind of awkward oscillatory behavior in the unstable domain is also typical for ordinary partial differential equations.

5. Concluding remarks. The availability of efficient numerical algorithms for the integration of fractional equations is important, as these equations are becoming essential tools for the description of a wide range of systems [3]. In this paper we have discussed a numerical algorithm for the solution of the fractional (sub)diffusion equation (1.2). Although we have dealt with this particular equation, our procedure could be extended to any fractional integrodifferential equation (for example, to fractional diffusion-wave equations) by means of an obvious combination of the Grünwald–Letnikov definition of the fractional derivative [1, 2, 4] with standard discretization algorithms used in the context of ordinary partial differential equations [26]. Furthermore, the method (given its explicit nature) can be trivially extended to d -dimensional problems, which is not such an easy task when implicit methods are considered.

In our numerical method the state of the system at a given time $t = m\Delta t$ is given explicitly in terms of the previous states at $t = (m - 1)\Delta t, \dots, \Delta t, 0$ by means of the FTCS scheme (3.3). We verified that for some standard initial conditions with exact analytical solution, namely, (a) the propagator in an unlimited

system with $u(x, t = 0) = \delta(x)$, and (b) a system with absorbing boundaries and $u(x, t = 0) = x(1 - x)$, the present algorithm leads to numerical solutions which are in excellent agreement with the exact solutions. Using a Fourier–von Neumann technique we have provided the conditions for which the fractional FTCS method is stable (cf. (3.10) and (3.11)). For $\gamma = 1$ the well-known bound $S = D\Delta t/(\Delta x)^2 \leq 1/2$ of the ordinary explicit method for the diffusion equation is recovered.

Concerning the implementation of the method, we must remark that the evaluation of the state of the system at a given time step $m\Delta t$ requires information about all previous states at $t = (m-1)\Delta t, (m-2)\Delta t, \dots, \Delta t, 0$ and not merely the immediately preceding state as in ordinary diffusion. This is a consequence of the non-Markovian nature of subdiffusion and implies the need for massive computer memory in order to store the evolution of the system, which is especially cumbersome in computations of long-time asymptotic behaviors. This could be palliated by using the “short-memory” principle [1] or the nested mesh procedure [30]. Another feature of the explicit numerical scheme is the interdependence of the temporal and spatial discrete steps for a fixed S_γ . If, as usual, one intends to integrate an equation with a given mesh Δx , then the corresponding step size Δt for a given $S_\gamma < S_\gamma^\times$ is of the order $(\Delta x)^{2/\gamma}$. As a consequence, Δt could become extremely small even for no too small values of Δx , especially when the problem is far from the diffusion limit, i.e., for small values of γ , so that the number of steps needed to reach even moderate times would become prohibitively large. In this case, resorting to other methods (e.g., implicit methods [14, 21, 22, 23, 24, 25]) that are stable for larger values of Δt is compulsory.

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