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Weighted average finite difference methods for fractional diffusion equations

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Abstract

A class of finite difference methods for solving fractional diffusion equations is considered. These methods are an extension of the weighted average methods for ordinary (non-fractional) diffusion equations. Their accuracy is of order $(\Delta x)^2$ and Δt, except for the fractional version of the Crank–Nicholson method, where the accuracy with respect to the timestep is of order $(\Delta t)^2$ if a second-order approximation to the fractional time-derivative is used. Their stability is analyzed by means of a recently proposed procedure akin to the standard von Neumann stability analysis. A simple and accurate stability criterion valid for different discretization schemes of the fractional derivative, arbitrary weight factor, and arbitrary order of the fractional derivative, is found and checked numerically. Some examples are provided in which the new methods' numerical solutions are obtained and compared against exact solutions.

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Keywords: Fractional diffusion equation; von Neumann stability analysis; Finite difference methods; Anomalous diffusion

1. Introduction

The number of scientific and engineering problems involving fractional calculus is already very large and still growing. The applications range from control theory to transport problems in fractal structures, from relaxation phenomena in disordered media to anomalous reaction kinetics of subdiffusive reagents [1–4]. Recently, fractional diffusion equations have been proposed to describe subdiffusive anomalous transport in the presence of an external field [3–6], ion channel gating dynamics in some proteins [7], tumor development [8], and dynamics of interfaces between nanoparticles and substrates [9], to name just a few. All these developments have stimulated the study of fractional differential equations, a topic that had for many years been a relatively arcane field of mathematics.

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The fractional diffusion equation for the force-free case is usually written in the following way [3,10–12]:

$$\frac{\partial}{\partial t}u(x,t) = K_0 D_t^{1-\gamma}\frac{\partial^2}{\partial x^2}u(x,t), \tag{1}$$

where ${}_0D_t^{1-\gamma}$ is the fractional derivative defined by the Riemann–Liouville operator,

$${}_0D_t^{1-\gamma}f(t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t \mathrm{d}\tau \frac{f(\tau)}{(t-\tau)^{1-\gamma}}, \tag{2}$$

K is the diffusion coefficient and $\gamma \in (0,1)$ is the anomalous diffusion exponent. The process is called subdiffusive because

$$\langle x^2(t)\rangle \sim \frac{2K}{\Gamma(1+\gamma)}t^{\gamma}, \quad t \to \infty \tag{3}$$

is the mean square displacement of a diffusive particle whose probability distribution is governed by (1), so that, when $0 < \gamma < 1$, the diffusion is anomalously slow (subdiffusive) compared to the normal diffusion behavior, $\langle x^2(t)\rangle \propto t$.

There are many analytical techniques for dealing with these fractional equations [3,4,13]. But, as also happens with ordinary (non-fractional) partial differential equations, in many cases the initial condition, the boundary conditions, and/or the external force are such that the only reasonable option is to resort to numerical methods. However, although there have been an increasing number of works on this topic during the last few years [14–27], this field of applied mathematics is by far much less developed and understood than its non-fractional counterpart. Many of the numerical methods for solving fractional partial differential equations that have been proposed differ essentially in the way in which the normal and fractional derivatives are discretized. Usually, the ordinary time-derivative $\partial u/\partial t$ is discretized using the backward Euler formula and the fractional derivative is discretized by means of convolution formulae [28], so that the resulting methods are implicit [14–19]. However, the method proposed in [27] is explicit because $\partial u/\partial t$ is discretized using the forward Euler formula. Another explicit method is discussed in Refs. [20,21], but for a fractional diffusion equation formally different from the one considered in this paper, Eq. (1). The fractional equations in [22,24,25] are also different from Eq. (1) because the fractional derivatives considered in those papers are *spatial* derivatives. The recent paper by Langlands and Henry [26] is special in the sense that the time fractional derivative is approximated using the L1 scheme instead of one of the usual convolution formulae [28].

This paper considers a class of numerical methods for solving fractional partial differential equations, which are very close to the weighted average (WA) methods for ordinary (non-fractional) partial differential equations. The fractional explicit method discussed in [27] is a member of this class. The explicit method is particularly interesting because its simplicity makes it well suited to theoretical approaches. Also, it can be trivially extended to d-dimensional problems, which is not such an easy task when implicit methods are considered. However, as also happens with its non-fractional counterpart, it has the problem that the integration timestep must be very small even for not too small values of the spatial mesh for the algorithm to be stable. This problem is especially acute far from the normal diffusion regime, i.e., for small values of γ, in which case the number of steps needed to reach even moderate times may become prohibitively large. Fortunately, we will see that some of the fractional WA methods proposed in this paper do not suffer from this drawback.

No numerical algorithm can be considered seriously unless conditions under which it is stable, if any, are not stated. To study the stability of the WA methods presented in this paper I have resorted to the kind of fractional von Neumann stability analysis employed in Ref. [27]. I will show that this procedure is also suitable for fractional WA methods, and leads to very good predictions for the stability bounds.

The plan of the paper is as follows. In Section 2 some fractional formulae and, in particular, some discrete versions of the fractional derivative are given. The fractional weighted averaged methods are developed, and their stability and accuracy are discussed in Section 3. Numerical solutions and exact analytical solutions of a typical fractional diffusion problem are compared in Section 4. The stability condition obtained in Section 3 is also checked numerically in Section 4. The paper ends with some conclusions and remarks in Section 5.

2. Discretization formulae

In finite difference methods the space-time solution's domain is discretized. I shall use the habitual notation: Δt is the temporal mesh or timestep, Δx is the spatial mesh, the coordinates of the mesh points are $x_j = j\Delta x$ and $t_m = m\Delta t$, and the values of the solution $u(x,t)$ on these grid points are $u(x_j,t_m) \equiv u_j^{(m)} \simeq U_j^{(m)}$, where I denote by $U_j^{(m)}$ the numerical estimate of the exact value of $u(x,t)$ at the point (x_j,t_m).

Two main steps are considered to build the fractional WA difference schemes. In the first step, the ordinary differential operators are discretized using three-point centered difference formulae [29,30]

$$\left.\frac{\partial u}{\partial t}\right|_{x_j,t_m+\Delta t/2} = \delta_t u_j^{(m+1/2)} + \mathrm{O}(\Delta t)^2, \tag{4}$$

where

$$\delta_t u_j^{(m+1/2)} \equiv \frac{u_j^{(m+1)} - u_j^{(m)}}{\Delta t} \tag{5}$$

and

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_j,t_m} = \delta_{xx} u_j^{(m)} + \mathrm{O}(\Delta x)^2 \tag{6}$$

with

$$\delta_{xx} u_j^{(m)} \equiv \frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{(\Delta x)^2}. \tag{7}$$

In the second step, the Riemann–Liouville operator is discretized

$${}_0D_t^{1-\gamma} u(x,t)\big|_{x_j,t_m} = {}_0\delta_t^{1-\gamma} u_j^{(m)} + \mathrm{O}(h^p), \tag{8}$$

where

$${}_0\delta_t^{1-\gamma} u_j^{(m)} = \frac{1}{h^{(1-\gamma)}} \sum_{k=0}^{[t_m/h]} \omega_k^{(1-\gamma)} u(x_j, t_m - kh) \tag{9}$$

and $[t_m/h]$ means the integer part of t_m/h. This expression can be conveniently written in terms of $u(x,t)$ evaluated at the grid points if one chooses $h = \Delta t$

$${}_0\delta_t^{1-\gamma} u_j^{(m)} = \frac{1}{(\Delta t)^{(1-\gamma)}} \sum_{k=0}^{m} \omega_k^{(1-\gamma)} u_j^{(m-k)}. \tag{10}$$

This formula is not unique because there are many different valid choices for $\omega_k^{(\alpha)}$ [28,31]. Let $\omega(z,\alpha)$ be the generating function of the coefficients $\omega_k^{(\alpha)}$, i.e.,

$$\omega(z,\alpha) = \sum_{k=0}^{\infty} \omega_k^{(\alpha)} z^k. \tag{11}$$

If the generating function is

$$\omega(z,\alpha) = (1-z)^{\alpha} \tag{12}$$

then (10) leads to the backward difference formula of order $p = 1$ (BDF1). This is also called the backward Euler formula of order 1 or, simply the Grünwald–Letnikov formula. The corresponding coefficients $\omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ can be conveniently evaluated by means of the recursive formulae

$$\omega_0^{(\alpha)} = 1, \quad \omega_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right) \omega_{k-1}^{(\alpha)}. \tag{13}$$

The generating function for the backward difference formula of order $p = 2$ (BDF2) is

$$\omega(z,\alpha) = \left(\frac{3}{2} - 2z + \frac{1}{2}z^2\right)^{\alpha} \tag{14}$$

and the generating function for the backward difference formula of order $p = 3$ (BDF3) is

$$\omega(z,\alpha) = \left(\frac{11}{6} - 3z + \frac{3}{2}z^2 - \frac{1}{3}z^3\right)^{\alpha}. \tag{15}$$

Generating functions for higher-order BDF formulae (and other types of discretization formulae such as the Newton–Gregory) can be found in [28,31]. The BDF formulae of order p reduce to the usual $(p+1)$-point backward difference quotient when $\alpha = 1$.

For $\gamma = 1$ the operator ${}_0D_t^{1-\gamma}$ becomes the identity operator so that, the consistency of Eqs. (8) and (9) requires $\omega_0^{(0)} = 1$, and $\omega_k^{(0)} = 0$ for $k \geqslant 1$, which in turns means that $\omega(z,0) = 1$. One can easily check that this is true for all the generating functions given above.

The coefficients $\omega_k^{(\alpha)}$ for BDFp formulae with $p \geqslant 2$ can be calculated using fast Fourier transforms [31]. It is important to note that the error estimate given in (8) is valid only if either $t/h \gg 1$ [31] or $u(x,t)$ is sufficiently smooth at the time origin $t = 0$ [32]. It is also important to realize that, as Diethelm et al. [33] have shown, the pth order fractional BDF when $p \geqslant 2$ may "work reasonably well for special choices of γ and moderately small step sizes, but in the general situation serious problems may be expected".

3. Fractional weighted average methods

In a weighted average method the diffusion equation (1) evaluated at the intermediate (off-lattice) point of the grid $(x_j, t_m + \Delta t/2)$

$$\left\{\frac{\partial}{\partial t}u(x,t) - K_0 D_t^{1-\gamma}\frac{\partial^2}{\partial x^2}u(x,t)\right\}_{x_j,t_m+\Delta t/2} = 0 \tag{16}$$

is approximated by means of difference formulae that involve $u(x,t)$ evaluated at the lattice points (x_j, t_m). The first-order time-derivative is replaced by the three-point centered formula (4) and the second-order space derivative is replaced by a weighted average of the three-point centered formula (6) evaluated at the times t_m and t_{m+1}

$$\delta_t u_j^{(m+1/2)} - \left[\lambda K_0 \delta_t^{1-\gamma}\delta_{xx}u_j^{(m)} + (1-\lambda)K_0\delta_t^{1-\gamma}\delta_{xx}u_j^{(m+1)}\right] = T_j^{m+1/2} \tag{17}$$

with λ being the weight factor. Of course, the above replacements give rise to an error, the truncation error, denoted here by $T_j^{m+1/2}$. Its value will be discussed in Section 3.2.

Neglecting the truncation error, one gets a computable difference scheme

$$\delta_t U_j^{(m+1/2)} - \left[\lambda K_0 \delta_t^{1-\gamma}\delta_{xx}U_j^{(m)} + (1-\lambda)K_0\delta_t^{1-\gamma}\delta_{xx}U_j^{(m+1)}\right] = 0 \tag{18}$$

that I call the fractional weighted average difference scheme. Expanding the difference operators by using Eqs. (5), (7), and (10), one gets

$$-\widetilde{S}U_{j-1}^{(m+1)} + (1+2\widetilde{S})U_j^{(m+1)} - \widetilde{S}U_{j+1}^{(m+1)} = R, \tag{19a}$$

where $\widetilde{S} = (1-\lambda)\omega_0^{(1-\gamma)}S$,

$$S = K\frac{(\Delta t)^{\gamma}}{(\Delta x)^2}, \tag{19b}$$

and

$$R = U_j^{(m)} + S\sum_{k=0}^{m}\left[(1-\lambda)\omega_{k+1}^{(1-\gamma)} + \lambda\omega_k^{(1-\gamma)}\right]\left[U_{j-1}^{(m-k)} - 2U_j^{(m-k)} + U_{j+1}^{(m-k)}\right]. \tag{19c}$$

Eq. (19) is the fractional weighted average difference scheme considered in this paper. This scheme is, in general, implicit. Fortunately, Eq. (19a) is a tridiagonal system that can be easily solved using the Thomas algorithm [29,30]. The scheme is explicit when $\lambda = 1$. Indeed, for this value of λ, one recovers the explicit method discussed in Ref. [27]. For $\lambda = 0$ the WA methods are called fully implicit. When $\lambda = 1/2$ one gets the fractional version of the Crank–Nicholson method.

3.1. Stability analysis

Ordinary WA methods are well-known and quite useful finite difference methods with well established stability conditions [29]: they are stable for all S when $0 \leqslant \lambda \leqslant 1/2$, and for $S \leqslant 1/[2(2\lambda - 1)]$ when $1/2 < \lambda \leqslant 1$. The purpose of this section is to find a generalization of these stability conditions for the fractional weighted averaged methods given by Eq. (19). In [27] a novel method was used to decide the stability of the fractional explicit scheme. The stability bounds were surprisingly accurate and easy to find. Thus, a natural question is whether the new stability procedure is able to cope with the general fractional difference scheme (19). We will see in this section that the answer is yes. This kind of von Neumann stability analysis has also been employed recently in Ref. [26].

In the (fractional) von Neumann stability procedure, the stability of the fractional WA methods is decided by studying the stability of a single generic *subdiffusive* mode of the form $U_j^{(m)} = \zeta_m e^{iqj\Delta x}$. Inserting this expression into the WA difference scheme (19) one gets

$$\left[1 + 4(1-\lambda)S\omega_0^{(1-\gamma)} \sin^2\left(\frac{q\Delta x}{2}\right)\right]\zeta_{m+1} = \zeta_m - 4S\sin^2\left(\frac{q\Delta x}{2}\right)\sum_{r=0}^{m}\left[(1-\lambda)\omega_{r+1}^{(1-\gamma)} + \lambda\omega_r^{(1-\gamma)}\right]\zeta_{m-r}. \tag{20}$$

The stability of the mode is determined by the behavior of ζ_m. In the von Neumann method, the stability analysis is carried out using the amplification factor ξ defined by

$$\zeta_{m+1} = \xi\zeta_m. \tag{21}$$

Of course, ξ depends on m. But let us assume for the moment that, as in Ref. [27], ξ is independent of time. Then, inserting this expression into Eq. (20) one gets

$$\left[1 + 4(1-\lambda)S\omega_0^{(1-\gamma)} \sin^2\left(\frac{q\Delta x}{2}\right)\right]\xi = 1 - 4S\sin^2\left(\frac{q\Delta x}{2}\right)\sum_{r=0}^{m}\left[(1-\lambda)\omega_{r+1}^{(1-\gamma)} + \lambda\omega_r^{(1-\gamma)}\right]\xi^{-r}. \tag{22}$$

The mode will be stable as long as $|\xi| \leqslant 1$. Considering the time-independent limit value $\xi = -1$ one finds that the mode is stable when

$$\frac{1}{S\sin^2(q\Delta x/2)} \geqslant \frac{1}{S_m^{\times}}, \tag{23}$$

where

$$\frac{1}{S_m^{\times}} \equiv 2(2\lambda - 1)\sum_{r=0}^{m}(-1)^r\omega_r^{(1-\gamma)} + (-1)^m 2(\lambda - 1)\omega_{m+1}^{(1-\gamma)}. \tag{24}$$

Although $S_m^{\times}$ depends on m, it turns out that $1/S_m^{\times}$ tends quickly towards its limit value $1/S_{\times} \equiv \lim_{m\to\infty} 1/S_m^{\times}$. In this limit, the stability condition becomes

$$\frac{1}{S} \geqslant \frac{\sin^2(q\Delta x/2)}{S_{\times}}. \tag{25}$$

When $\lambda \neq 1/2$, one can write $S_{\times}$ in terms of the generating function $\omega(z, 1-\gamma)$ of the coefficients $\omega_m^{(1-\gamma)}$

$$\frac{1}{S_{\times}} = 2(2\lambda - 1)\omega(-1, 1-\gamma). \tag{26}$$

Note that $\omega(-1, 1-\gamma)$ is always positive (see Section 2). Because (26) is negative when $\lambda < 1/2$, then (25) holds for all S [S is always positive, see (19b)]. Therefore, any WA method with $\lambda < 1/2$ is stable. However, $1/S_{\times}$ is

positive and finite when $\lambda > 1/2$, so that Eq. (25) tells us that, for any WA method with $\lambda > 1/2$, there always exist values of S for which this WA method is unstable. Finally, from Eq. (24), $1/S_m^{\times} = (-1)^m 2(\lambda - 1)\omega_{m+1}^{(1-\gamma)}$ if $\lambda = 1/2$ (Crank–Nicholson method). But $\omega_m^{(1-\gamma)} \to 0$ for $m \to \infty$ so that $1/S_{\times} = 0$, and one concludes from Eq. (25) that the fractional Crank–Nicholson method is stable for all *finite* S.

Proceeding as usual in the von Neumann method, one can write a simpler and more conservative stability criterion than that given by Eq. (25) replacing $\sin^2(q\Delta x/2)$ by its highest value, i.e., making $\sin^2(q\Delta x/2) \to 1$. Then the stability conditions for the fractional WA difference scheme (19) can be summarized in the following way: a WA method with weight factor $0 \leqslant \lambda \leqslant 1/2$ is always stable; when $1/2 < \lambda \leqslant 1$, the method is stable if $1/S \geqslant 1/S_{\times}$, with $S_{\times}$ given by Eq. (26). Because S is always positive and $(2\lambda - 1)$ is negative for $0 \leqslant \lambda \leqslant 1/2$, the foregoing statements can summarized in this simpler way: A WA method, i.e., a difference scheme defined by (19), is stable if

$$\frac{1}{S} \geqslant \frac{1}{S_{\times}} \equiv 2(2\lambda - 1)\omega(-1, 1-\gamma). \tag{27}$$

These stability criteria are similar to those valid for ordinary WA methods mentioned at the beginning of this section. For $\gamma \to 1$ one recovers those non-fractional (ordinary) results because $\omega(-1,0) = 1$ (see end of Section (2)). For $\lambda = 1$ (explicit method) one recovers the result $1/S \geqslant 2\omega(-1, 1-\gamma)$ first obtained in [27].

3.2. Truncating error

From the definition of truncating error given by Eq. (17), one gets

$$T_j^{m+1/2} = \delta_t u_j^{(m+1/2)} - \frac{K}{h^{1-\gamma}} \sum_{k=0}^{m} \omega_k^{(1-\gamma)} \left\{ (1-\lambda)\delta_{xx} u_j^{(m+1-k)} + \lambda \delta_{xx} u_j^{(m-k)} \right\} - \frac{K}{h^{1-\gamma}} (1-\lambda)\omega_{m+1}^{(1-\gamma)} \delta_{xx} u_j^{(0)}. \tag{28}$$

But

$$\delta_{xx} u_j^{(m+1-k)} = u_{xx} + \frac{(\Delta x)^2}{12} u_{xxxx} + \frac{\Delta t}{2} \left[u_{xxt} + \frac{(\Delta x)^2}{12} u_{xxxxt} + \cdots \right] + \frac{(\Delta t)^2}{8} u_{xxtt} + \cdots \tag{29}$$

and

$$\delta_{xx} u_j^{(m-k)} = u_{xx} + \frac{(\Delta x)^2}{12} u_{xxxx} - \frac{\Delta t}{2} \left[u_{xxt} + \frac{(\Delta x)^2}{12} u_{xxxxt} + \cdots \right] + \frac{(\Delta t)^2}{8} u_{xxtt} + \cdots \tag{30}$$

where the partial derivatives are evaluated at the point $(x_j, t_{m-k} + \Delta t/2)$. Inserting these expressions into Eq. (28) and taking into account Eqs. (1), (8), and (9), one gets

$$\begin{aligned} T_j^{m+1/2} &= \mathrm{O}(h^p) - \left(\frac{1}{2} - \lambda\right) \Delta t K_0 D_{\tau}^{1-\gamma} u_{xxt} - \frac{(\Delta x)^2}{12} K_0 D_{\tau}^{1-\gamma} u_{xxxx} + \frac{(\Delta t)^2}{24} u_{ttt} \\ &\quad - \frac{(\Delta t)^2}{8} K_0 D_{\tau}^{1-\gamma} u_{xxtt} - K(1-\lambda) \frac{\omega_{m+1}^{(1-\gamma)}}{h^{1-\gamma}} \delta_{xx} u_j^{(0)} + \cdots \\ &= \mathrm{O}(h^p) + \left(\frac{1}{2} - \lambda\right) \mathrm{O}(\Delta t) + \mathrm{O}(\Delta t)^2 + \mathrm{O}(\Delta x)^2 + \frac{\omega_{m+1}^{(1-\gamma)}}{h^{1-\gamma}} \delta_{xx} u_j^{(0)} \end{aligned} \tag{31}$$

with $\tau \equiv t_m + \Delta t/2$, and where terms of order $\mathrm{O}[(\Delta t)^a (\Delta x)^b h^p]$ with $a + b + p > 2$ have not been included.

Some conclusions may be drawn from this expression. First, if $h = \Delta t$, it is useless to employ discretization formulae for the Riemann–Liouville derivative of order p higher than two because of the unavoidable presence of an $\mathrm{O}(\Delta t)^2$ term. Also, one notes that a low-order term proportional to Δt is present for all WA methods with $\lambda \neq 1/2$. Therefore, the choice of λ (as long as $\lambda \neq 1/2$) does not affect the precision of the WA method (although it matters for the stability of the numerical scheme, as we have seen in Section 3.1). The value $\lambda = 1/2$ is special because removes the $\mathrm{O}(\Delta t)$ term. I shall name the resulting method the fractional Crank–Nicholson method because for $\gamma = 1$ one recovers the usual Crank–Nicholson scheme. In sum, taking

$h = \Delta t$, the truncation error is of order $(\Delta x)^2$ and $(\Delta t)^q$ where $q = 1$ if $\lambda \neq 1/2$, and $q = 2$ if $\lambda = 1/2$ and a second-order (or higher-order) discretization scheme for the fractional derivative is used.

The last term in Eq. (31) does not appear in non-fractional discretization schemes: it is characteristic of fractional methods. It goes to zero for large m for any set of coefficients $\{\omega_m^\alpha\}$ because the series of Eq. (11) converges. For m large enough, the quantity $\omega_{m+1}^{(1-\gamma)}/h^{1-\gamma}$ becomes of order of, or smaller than, $O(\Delta t)^2$. The particular value of m for which this happens depends on the discretization formula of the Riemann–Liouville derivative that is used. However, for the first integration steps (m small) this term, and consequently, the truncation error, is large unless the initial curvature of $u(x,t)$, $\partial^2 u(x,t)/\partial x^2$, is small. These difficulties disappear for $\lambda = 1$, i.e., they are absent in the explicit method. This suggests that a practical integration procedure could be one in which the first integration steps were performed by means of the explicit method (see Ref. [27] for more details on this method), and the subsequent steps were carried out by means of, say, the fractional Crank–Nicholson method.

4. Comparison with numerical results

In this section the WA difference scheme (19) with different values of λ is used to solve a fractional diffusion problem which has an analytical solution. The two solutions, numerical and analytical, will be compared for different values of S and γ. The problem considered is a typical (sub)diffusion problem on a line with absorbing boundaries

$$\frac{\partial}{\partial t}u(x,t) = K_0 D_t^{1-\gamma}\frac{\partial^2}{\partial x^2}u(x,t) \tag{32a}$$

with

$$u(0,t) = u(1,t) = 0, \tag{32b}$$

and initial condition

$$u(x, t=0) = x(1-x). \tag{32c}$$

The exact analytical solution of Eq. (1) is easily found by the method of separation of variables

$$u(x,t) = \frac{8}{\pi^3}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3}\sin[(2n+1)\pi x]E_\gamma[-K(2n+1)^2\pi^2 t^\gamma], \tag{33}$$

where E_γ is the Mittag–Leffler function [31].

All the numerical calculations in this paper were carried out using the BDF1 formula for the coefficients $\omega_k^{(\alpha)}$. There are three reasons for this: first, in contrast with other formulae, the BDF1 coefficients can be easily computed using the recursive relation (13); second, although this formula is only of order 1, this is not relevant because the truncation error has (except for $\lambda = 1/2$) a term of order Δt (see Eq. (31)); and, third, because second- and higher-order BDF formulae involve practical problems that in some cases may lead to completely useless results [33].

The stability limit $S_\times$ adopts an especially simple form when the BDF1 coefficients are used

$$S_\times = \frac{2^{\gamma-2}}{2\lambda - 1}, \tag{34}$$

because, from Eq. (12), $\omega(-1, 1-\gamma) = 2^{1-\gamma}$. Figs. 1–4 compare the exact solution (33) of problem (32) with the numerical solution obtained by means of different WA methods for several values of the anomalous diffusion exponent γ and, in all cases, for $\Delta x = 1/20$. In Fig. 1 the explicit method ($\lambda = 1$) for $\gamma = 3/4$ with $S = 0.4$ is used. Note that this value is smaller than $S_\times = 2^{-5/4} \simeq 0.4204\ldots$, so that according to Eq. (27) one expects, and Fig. 1 confirms, that the numerical scheme is stable. The results obtained using the fractional Crank–Nicholson method for $\gamma = 3/4$ are shown in Fig. 2. The next two figures, Figs. 3 and 4, show the numerical solutions obtained by means of the WA method with weight factor $\lambda = 0.8$, $\gamma = 1/2$, and two values of S. Note that in this case the stability bound is $S_\times = 5/6\sqrt{2} \simeq 0.589\ldots$ Fig. 3 corresponds to $S = 0.55 < S_\times$, and one sees that the numerical solutions are in excellent agreement with the exact results. However, Fig. 4 corresponds

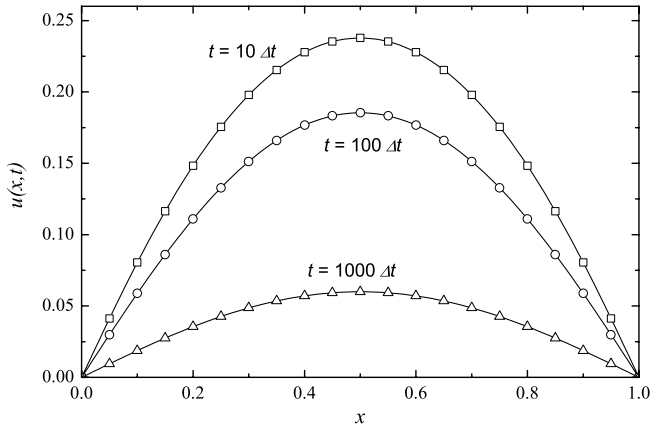

Fig. 1. Numerical solution of the fractional diffusion problem (32) by means of the fractional explicit method ($\lambda = 1$) for $\gamma = 3/4$ where $\Delta x = 1/20$, and $S = 0.4$. The solution is shown after 10 (squares), 100 (circles), and 1000 (triangles) timesteps. The lines correspond to the exact analytical solution.

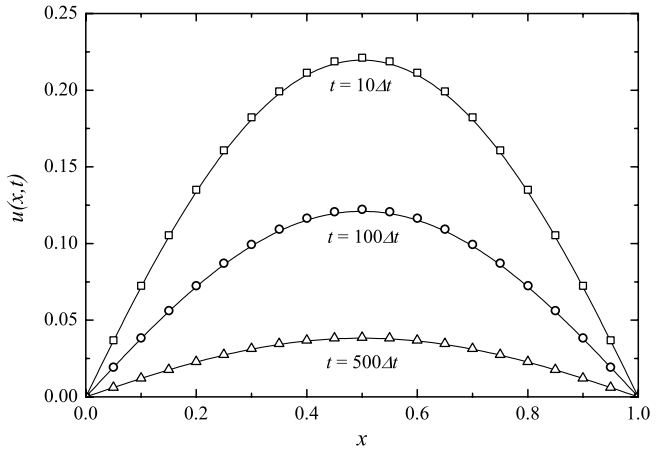

Fig. 2. Numerical solution of the fractional diffusion problem (32) by means of the fractional Crank–Nicholson method ($\lambda = 1/2$) for $\gamma = 3/4$, $\Delta x = 1/20$ and $S = 1$. The solution is shown after 10 (squares), 100 (circles) and 500 (triangles) timesteps. The lines correspond to the exact analytical solution.

to $S = 0.7 > S_\times$, a value that is well inside the unstable region. Now the solution is clearly wrong, showing the typical behavior that appears when unstable numerical schemes are used.

4.1. Numerical check of the stability analysis

Figs. 1–4 show some cases where the WA methods are stable and unstable according to the theoretical predictions of Section 3.1, cf., Eq. (27). Obviously, a more systematic check of this stability bound is desirable. To this end, the boundary problem (32) was solved by means of the WA scheme (19a) with five different values of the weight factor λ ($\lambda = 0.6, 0.7, 0.8, 1.0$), for values of γ spanning the interval $[0, 1]$, and for values of S given by $S = 0.95S_\times + 0.001n$ with $n = 0, 1, 2\ldots$ The WA scheme is considered unstable when u_j^{m-1}/u_j^m is negative or larger than 10 for some m with $m \leqslant 2000$ (the results do not change substantially for any other reasonable choices, although, as expected, they improve when the upper limit for m is increased). The smallest value of S for which the WA is unstable according to this criterion is denoted by $S_{\min}$. On the other hand, it is well known that for a lattice with $2N + 1$ points (including the absorbing boundaries) $\sin^2[(2N-1)\pi/(4N)]$ is the maximum value that $\sin^2(q\Delta x/2)$ can reach, so that, in this case, the stability condition Eq. (25) becomes

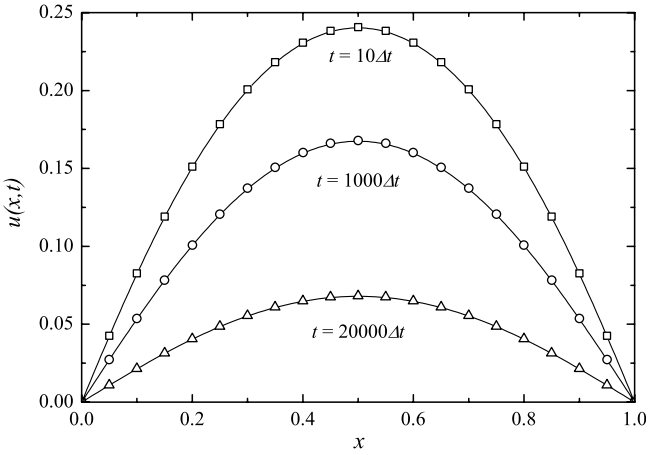

Fig. 3. Numerical solution of the fractional diffusion problem (32) by means of the fractional weighted-averaged method with $\lambda = 0.8$ for $\gamma = 1/2$, $\Delta x = 1/20$ and $S = 0.55$. The solution is shown after 10 (squares), 1000 (circles), and 20,000 (triangles) timesteps. The lines correspond to the exact analytical solution.

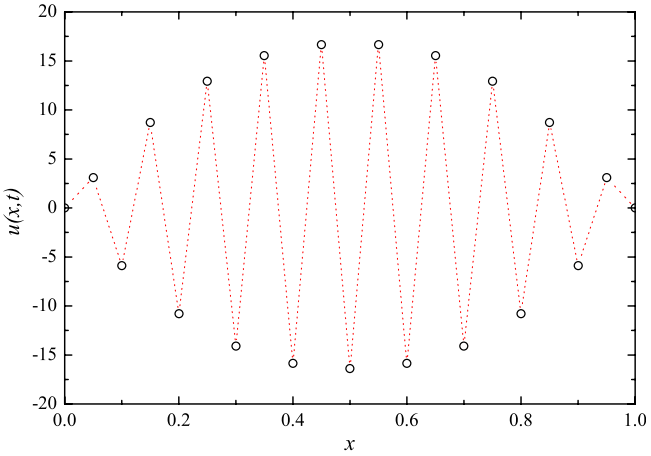

Fig. 4. The same as Fig. 3 but for $S = 0.7$. The solution after 100 timesteps is shown by circles. The dotted line is only to guide the eye.

$S_\times \geqslant S\sin^2[(2N-1)\pi/(4N)]$. Because the BDF1 discretization formula is used in the numerical computations, $S_\times$ is given by Eq. (34), and the stability condition finally reads

$$2^{\gamma-2} \geqslant (2\lambda - 1)S\sin^2[(2N-1)\pi/(4N)]. \tag{35}$$

The numerical estimation of the right-hand side of this equation, $(2\lambda - 1)S_{\min}\sin^2[(2N-1)\pi/(4N)]$, is plotted in Fig. (5) and compared with the theoretical prediction $2^{\gamma-2}$ ($N = 10$ for all simulations, which corresponds to $\Delta x = 1/20$). The agreement is excellent, which confirms the validity of the Fourier–von Neumann type stability analysis of the WA integration schemes carried out in Section 3.1.

5. Conclusions and final remarks

A class of finite difference methods for solving fractional diffusion equations, akin to the well-known weighted average methods for ordinary diffusion equations, has been constructed. Each method is defined by the value of the weighting parameter λ. For $\lambda = 1$ one recovers the explicit method discussed in [27], and for $\lambda = 1/2$ one obtains a (fractional) generalization of the Crank–Nicholson method. The accuracy of these methods is of order $(\Delta x)^2$ and Δt, except for the (fractional) Crank–Nicholson method, where the

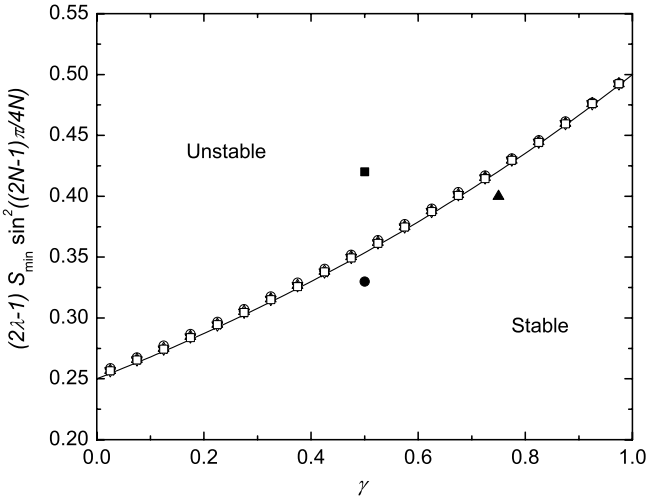

Fig. 5. Scaled numerical stability bounds $(2\lambda - 1)S_{\min}\sin^2[(2N - 1)\pi/(4N)]$ versus γ for several WA methods with different values of the weight parameter: $\lambda = 0.6$ (circles), $\lambda = 0.7$ (up triangles), $\lambda = 0.8$ (down triangles), $\lambda = 0.9$ (stars) and $\lambda = 1$ (squares). The solid line is the theoretical stability bound prediction $2^{\gamma-2}$ given by Eq. (35). The solid triangle corresponds to the case of Fig. 1, the solid circle corresponds to the case of Fig. 3, and the solid square corresponds to the case of Fig. 4.

accuracy with respect to the timestep can be of order $(\Delta t)^2$ if a second-order approximation to the fractional time-derivative is used. The stability of the weighted average methods presented in this paper depends strongly on the value of the weighting parameter λ: they are unconditionally stable for $0 < \lambda \leqslant 1/2$, and conditionally stable for $1/2 < \lambda \leqslant 1$. A very simple and accurate stability criterion, Eq. (27), valid for different discretization schemes of the fractional derivative, arbitrary weight factor λ, and arbitrary order of the fractional derivative γ, was provided. This criterion was obtained, following the von Neumann ideas, by assuming that the solution of the fractional diffusion problem can be decomposed into Fourier modes (subdiffusive modes), and analyzing the conditions under which every mode is stable.

The convenience of having unconditionally stable methods is especially relevant when integrating subdiffusion equations because otherwise the stability requirement limits the size of the timesteps to be of order $(\Delta x)^{2/\gamma}$, which, for small γ, can become extremely small. The fractional Crank–Nicholson method presented here is especially convenient because it is unconditionally stable, and its accuracy can be of order $(\Delta t)^2$ if a second-order approximation to the fractional time-derivative is used.

The success of the stability analysis employed in this paper prompts the question of whether its applicability extends to other difference schemes and other kinds of fractional partial differential equations, such as the fractional diffusion equation in the Caputo form [20,34], or the fractional diffusion-wave equation [12,35,36]. Preliminary results suggests that it does.

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