

WEIGHTED AVERAGE FINITE DIFFERENCE METHODS FOR FRACTIONAL DIFFUSION EQUATIONS

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Abstract: Weighted averaged finite difference methods for solving fractional diffusion equations are discussed and different formulae of the discretization of the Riemann-Liouville derivative are considered. The stability analysis of the different numerical schemes is carried out by means of a procedure close to the well-known von Neumann method of ordinary diffusion equations. The stability bounds are easily found and checked in some representative examples.

Keywords: Fractional diffusion equation, Numerical solution, Stability analysis, Difference methods.

1. INTRODUCTION

The number of scientific and engineering problems involving fractional calculus is very large and 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. Recently, a fractional Fokker-Planck equation has been proposed to describe subdiffusive anomalous transport in the presence of an external field (Metzler *et al.*, 1999; Barkai *et al.*, 2000; Metzler *et al.*, 2000). For the force-free case, the equation becomes the fractional partial differential equation (Balakrishnan, 1985; Scalas *et al.*, 2004; Metzler *et al.*, 2000; Schneider *et al.*, 1988)

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

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

the diffusion coefficient and $\gamma \in (0, 1)$ is the anomalous diffusion exponent. There are many analytical techniques for dealing with these fractional equations. But, as also with ordinary (non-fractional) partial differential equations (PDEs), in many cases the initial and/or boundary conditions and/or the external force are such that the only reasonable option is to resort to numerical methods. However, these methods are not as well studied as their non-fractional counterparts.

In this communication, some numerical methods for solving fractional partial differential equations, which are very close to the well-known weighted average (WA) methods of ordinary (non-fractional) PDEs, are considered. It will be shown that the stability of the fractional numerical schemes can be analyzed very easily and efficiently with a method close to von Neumann's (or Fourier's) method for non-fractional PDEs.

2. FRACTIONAL DISCRETIZATION FORMULAE

Two main steps will be considered to build numerical difference schemes for solving fractional

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PDE's. In the first step one discretizes the ordinary differential operators $\partial/\partial t$, $\partial^2/\partial x^2$ as usual (Press *et al.*, 1992; Morton *et al.*, 1994). This will be done in Sec. 3. In the second step, one discretizes the Riemann-Liouville operator:

$${}_0D_t^{1-\gamma} f(t) = \frac{1}{h^{(1-\gamma)}} \sum_{k=0}^{\lfloor t/h \rfloor} \omega_k^{(1-\gamma)} f(t-kh) + O(h^p), \quad (2)$$

where $\lfloor t/h \rfloor$ means the integer part of t/h . This formula is not unique because there are many different valid choices for $\omega_k^{(\alpha)}$ (Lubich, 1986). Let $\omega(z, \alpha)$ be the generating function of the coefficients $\omega_k^{(\alpha)}$, i.e.,

$$\omega(z, \alpha) = \sum_{k=0}^{\infty} \omega_k^{(\alpha)} z^k. \quad (3)$$

If the generating function is

$$\omega(z, \alpha) = (1-z)^\alpha \quad (4)$$

then we get 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. These coefficients are $\omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ and can be evaluated recursively:

$$\omega_0^{(\alpha)} = 1, \quad \omega_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right) \omega_{k-1}^{(\alpha)}. \quad (5)$$

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

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

and

$$\omega(z, \alpha) = \left(\frac{11}{6} - 3z + \frac{3}{2}z^2 - \frac{1}{3}z^3\right)^\alpha \quad (7)$$

is the generating function for the backward difference formula of order $p = 3$ (BDF3). Generating functions for higher-order BDF formulae can be found in (Lubich, 1986; Podlubny, 1999). Another type of discretization formula is that of Newton-Gregory of order p (NG p) (Lubich, 1986) whose generating function is

$$\omega(z, \alpha) = (1-z)^\alpha \times [\Omega_0 + \Omega_1(1-z) + \dots + \Omega_{p-1}] \quad (8)$$

where the coefficients Ω_n are defined by

$$\sum_{n=0}^{\infty} \Omega_n (1-\xi)^n = \left(\frac{\ln \xi}{\xi-1}\right)^\alpha. \quad (9)$$

3. FRACTIONAL DIFFERENCE SCHEMES

The notation $x_j = j\Delta x$, $t_m = m\Delta t$ and $u(x_j, t_m) \equiv u_j^{(m)} \simeq U_j^{(m)}$ will be used with $U_j^{(m)}$ being the numerical estimate of $u(x, t)$ at the point (x_j, t_m) . In the non-fractional weighted

average method, the diffusion equation is replaced by:

$$\begin{aligned} u_j^{(m+1)} &= u_j^{(m)} + \lambda S \left[u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)} \right] + \\ & (1-\lambda) S \left[u_{j-1}^{(m+1)} - 2u_j^{(m+1)} + u_{j+1}^{(m+1)} \right] + \\ & T(x, t), \end{aligned} \quad (10)$$

where λ is the weight factor, $T(x, t)$ the truncation error (Morton *et al.*, 1994), and $S = D\Delta t/(\Delta x)^2$. Similarly, the fractional equation is replaced by

$$\begin{aligned} u_j^{(m+1)} &= u_j^{(m)} + \lambda S \left[\dot{u}_{j-1}^{(m)} - 2\dot{u}_j^{(m)} + \dot{u}_{j+1}^{(m)} \right] + \\ & (1-\lambda) S \left[\dot{u}_{j-1}^{(m+1)} - 2\dot{u}_j^{(m+1)} + \dot{u}_{j+1}^{(m+1)} \right] + \\ & T(x, t), \end{aligned} \quad (11)$$

where $\dot{u}_j^{(m)} \equiv {}_0D_t^{1-\gamma} u(x_j, t_m)$. Inserting Eq. (2) into Eq. (11), neglecting the truncation error, and rearranging the terms, we finally get the fractional WA difference scheme

$$\begin{aligned} U_j^{(m+1)} &= U_j^{(m)} + \lambda S \sum_{k=0}^m \omega_k^{(1-\gamma)} \left[U_{j-1}^{(m+1-k)} - \right. \\ & \left. 2U_j^{(m+1-k)} + U_{j+1}^{(m+1-k)} \right] + (1-\lambda) S \times \\ & \sum_{k=0}^m \omega_k^{(1-\gamma)} \left[U_{j-1}^{(m-k)} - 2U_j^{(m-k)} + U_{j+1}^{(m-k)} \right], \end{aligned} \quad (12)$$

where

$$S = \frac{K\gamma\Delta t}{h^{1-\gamma}(\Delta x)^2}. \quad (13)$$

For $\lambda = 1$ we recover the fractional explicit method discussed in (Yuste *et al.*, 2003). The method is implicit for $\lambda \neq 1$. For $\lambda = 0$ one gets the (fractional) fully implicit method, and for $\lambda = 1/2$ the (fractional) Crank-Nicholson method. 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) 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,

$$S = K\gamma \frac{\Delta t^\gamma}{(\Delta x)^2}. \quad (14)$$

Before tackling Eq. (12) seriously, one must first know under which conditions, if any, the integration algorithm is stable.

4. STABILITY ANALYSIS

The stability analysis of the integration difference scheme (12) will be carried out by means of the method used in (Yuste *et al.*, 2003). Following the von Neumann ideas, one studies the stability of a single *subdiffusive* mode of the form $U_j^{(m)} = \zeta_m e^{iqj\Delta x}$. This mode will be stable as long as

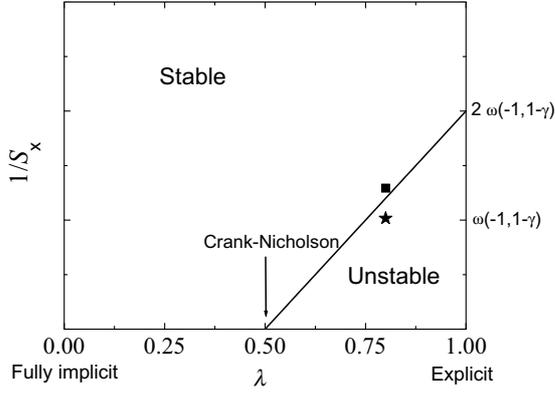


Fig. 1. Stability phase diagram for the weighted average methods versus the weight factor λ . The line corresponds to Eq. (15). The square corresponds to the case shown in Fig. 5 and the star corresponds to the cases shown in Figs. 6 and 7.

the ζ_m stay bounded for $m \rightarrow \infty$. Proceeding as (Yuste *et al.*, 2003) one finds that a fractional WA method is stable as long as $1/S \geq 1/S_x$ where

$$1/S_x = 2(2\lambda - 1)\omega(-1, 1 - \gamma). \quad (15)$$

This is the main result of the present work. From (15) one sees that a WA method is stable for any value of S if $\lambda \leq 1/2$ because the generating function $\omega(z, 1 - \gamma)$ for $z = -1$ is positive (S is always positive: see Eq. (13)). For $\lambda > 1/2$, S_x is positive, and there exist values of $1/S$ smaller than $1/S_x$, so that the fractional WA methods are unstable for these cases. Figure 1 shows the stability phase diagram for the WA methods. For $\lambda = 1$ one recovers the stability bound $1/S_x = 2\omega(-1, 1 - \gamma)$ for the fractional explicit methods discussed in (Yuste *et al.*, 2003). The stability bounds of these explicit methods versus the anomalous diffusion exponent γ for several Riemman-Liouville derivative discretization formulae are shown in Fig. 2. Note that the stability region shrinks when the order p of the discretization formula increases.

The fully implicit numerical method ($\lambda = 0$) and the Crank-Nicholson method ($\lambda = 1/2$) have been considered, together with their stability, by some authors (Sanz-Serna, 1988; López-Marcos, 2002; Lubichet *et al.*, 1996; McLean *et al.*, 1993; McLean *et al.*, 1996). However, their analysis is far more complex than that presented here. Also, to the best of my knowledge, neither generic implicit WA methods (arbitrary λ) nor the explicit method ($\lambda = 1$) have been considered previously. In this vein, it is interesting to note that an *explicit* method for solving the fractional diffusion equation written in the Caputo form has recently been proposed by Ciesielski and Leszczynski (Ciesielski *et al.*, 2003).

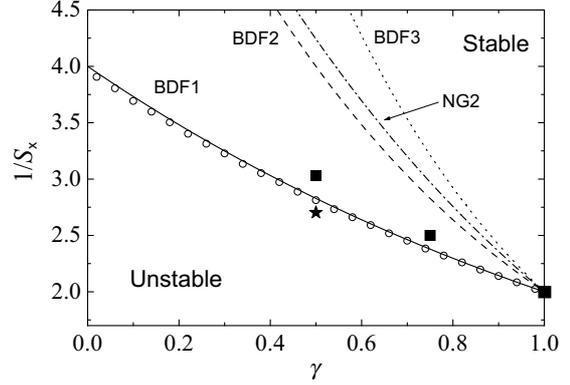


Fig. 2. Stability bound for the explicit method versus the anomalous exponent γ . The lines BDF1, BDF2, BDF3 and NG2 correspond to the theoretical stability bounds of the explicit method when the BDF1, BDF2, BDF3 and NG2 discretization formulae of the Riemann-Liouville derivative are used. The circles are numerical estimates of the BDF1 stability bound (Yuste *et al.*, 2003). The squares correspond to the cases shown in Fig. 3 and the star is the case of Fig. 4.

5. CHECK OF THE STABILITY BOUND

The stability of the fractional difference schemes of Sec. 3 will be checked here by applying them to solve Eq. (1) with the initial condition $u(x, t = 0) = x(1 - x)$ and the absorbing boundary conditions $u(0, t) = u(1, t) = 0$. The exact analytical solution of Eq. (1) is easily found by the method of separation of variables:

$$u(x, t) = \frac{8}{\pi^3} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^3} \sin[(2n+1)\pi x] \times E_{\gamma}[-K_{\gamma}(2n+1)^2 \pi^2 t^{\gamma}]. \quad (16)$$

where E_{γ} is the Mittag-Leffler function (Metzler *et al.*, 2000; Mainardi *et al.*, 2000). In Fig. 3 we compare this exact solution with the results provided by the BDF1 *explicit* integration scheme for anomalous diffusion exponents $\gamma = 0.5$, $\gamma = 0.75$, and $\gamma = 1$ for time $t = 0.5$ and $K_{\gamma} = 1$. The values of Δx used were $\Delta x = 1/10$, $1/20$, and $1/50$ with $S = 0.33$, 0.4 , and 0.5 , respectively. These values of S are marked by squares in Fig. 2. They are inside the stable region, which is confirmed by the well-behaved numerical solutions shown in Fig. 3. However, in Fig. 4 the BDF1-*explicit* numerical solution for $S = 0.37$ and $\gamma = 1/2$ shows a characteristic unstable behaviour. This is the expected behavior because $1/0.37$ is smaller than $1/S_x = 2\omega(-1, 1 - \gamma) = 2^{2-\gamma}$ for $\gamma = 1/2$. This case is marked by a star in Fig. 2.

Figures 5, 6, and 7 show the numerical integration results for the WA implicit method with $\lambda = 0.8$, $\gamma = 1/2$ and two values of S . For $S = 0.55$ one has $1/S > 1/S_x = 1.2 \times 2^{1/2}$ (this case corresponds

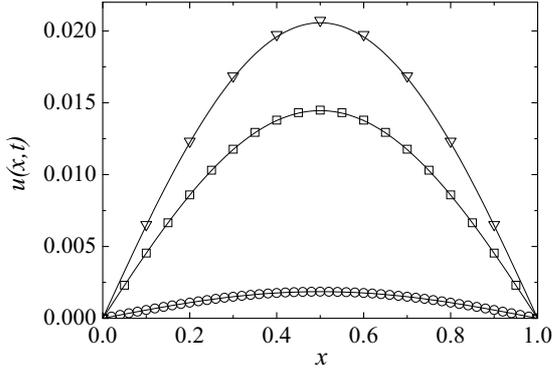


Fig. 3. Solution of the subdiffusion equation (1) with absorbing boundary conditions $u(0,t) = u(1,t) = 0$ and initial condition $u(x,0) = x(1-x)$. The symbols correspond to the BDF1-explicit numerical solution and the lines correspond to the exact analytical solution. The solution is shown for the time $t = 0.5$ for $\gamma = 0.5$ (triangles), $\gamma = 0.75$ (squares) and $\gamma = 1$ (circles). These cases are marked by squares in Fig. 2

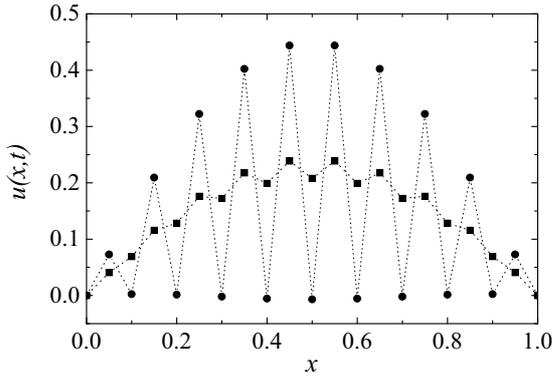


Fig. 4. BDF1-explicit numerical solution $u(x,t)$ for the same problem as in Fig. 3 but with $\gamma = 1/2$, $K_\gamma = 1$, $S = 0.37$, and $\Delta x = 1/20$ after 150 time steps (squares) and 200 time steps (circles). The lines are plotted as a visual aide. This case corresponds to the point marked by a star in Fig. 2.

to the square in Fig. 1) and the WA method must be stable. This is confirmed in Fig. 5. However, $1/S < 1/S_x = 1.2 \times 2^{1/2}$ for $S = 0.7$ so that the WA method must be unstable in this case, which is confirmed in Figs. 6 and 7 (this case is marked by a star in Fig. 1).

6. FINAL REMARKS

The truncation error $T(x,t)$ of Eq. 11 can be estimated in the same way as for non-fractional equations (Morton *et al.*, 1994). One gets:

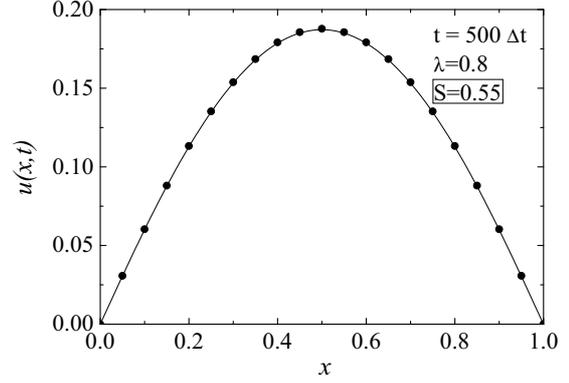


Fig. 5. Numerical solution $u(x,t)$ obtained by means of the weighted average method with weight factor $\lambda = 0.8$ for the same problem as in Fig. 3 but with $\gamma = 1/2$, $K_\gamma = 1$, $S = 0.55$, and $\Delta x = 1/20$ after 500 time steps (circles). The line is the exact analytical result. This case corresponds to the point marked by a square in Fig. 1.

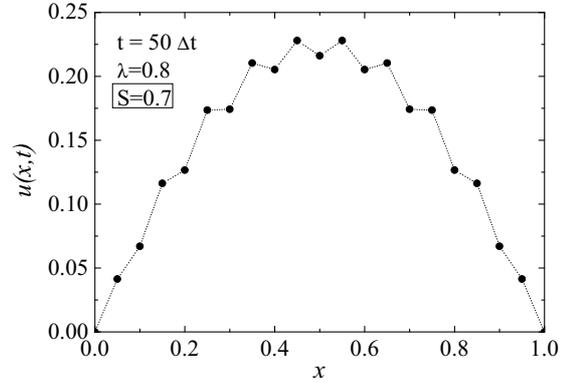


Fig. 6. Numerical solution $u(x,t)$ for the same problem as in Fig. 3 obtained by means of the weighted average method with weight factor $\lambda = 0.8$ for $\gamma = 1/2$, $K_\gamma = 1$, $S = 0.7$, and $\Delta x = 1/20$ after 50 time steps. The lines are plotted as a visual aide. This case corresponds to the point marked by a star in Fig. 1.

$$T_j^m = O(h^p) + O(\Delta t)^2 + (\Delta x)^2 + \left(\frac{1}{2} - \lambda\right) O(\Delta t) + (1 - \lambda) O\left(\frac{\omega_{m+1}^{(1-\gamma)}}{h^{1-\gamma}}\right) \frac{\partial^2}{\partial x^2} u(x_j, t_{1/2}) \quad (17)$$

where T_j^m is the truncation error at x_j and $t_m + \Delta t/2$: $T_j^m \equiv T(x_j, t_{m+1/2})$. From this expression some conclusions may be drawn:

- 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 $O(\Delta t)^2$ term.
- The undesirable low-order term proportional to Δt is present for all WA methods with $\lambda \neq 1/2$. Therefore, the chosen value of λ (as long as $\lambda \neq$

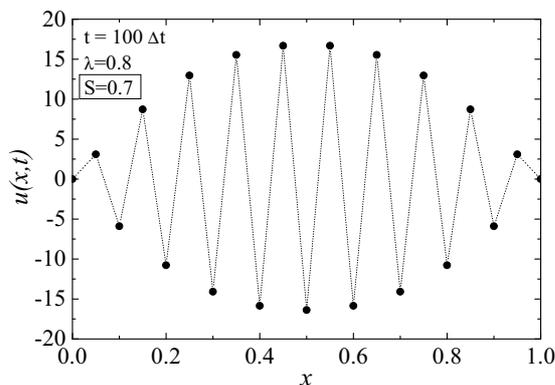


Fig. 7. Numerical solution $u(x,t)$ for the same problem as in Fig. 3 obtained by means of the weighted average method with weight factor $\lambda = 0.8$ for $\gamma = 1/2$, $K_\gamma = 1$, $S = 0.7$, and $\Delta x = 1/20$ after 100 time steps. The lines are plotted as a visual aide. This case corresponds to the point marked by a star in Fig. 1.

1/2) does not improve the precision of the WA method (although it matters for the stability of the numerical scheme). The value $\lambda = 1/2$ is special because it removes the $O(\Delta t)$ term. It leads to the (fractional) Crank-Nicholson method.

- The last term does not appear for non-fractional discretization schemes: it is characteristic of fractional methods. It becomes negligible for large m . In fact, 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. 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 a practical integration procedure in which the first integration steps are performed by means of the explicit method, and the subsequent steps are carried out by means of, say, the fractional Crank-Nicholson method.

Of the numerical integration schemes for fractional PDE's considered here, the Crank-Nicholson method appears to be the most promising because it is always stable and is second order accurate in Δt and Δx (provided that the discretization formula for the Riemann-Liouville derivative is second order accurate in $h = \Delta t$).

It has been shown that the stability of the WA methods can be studied by means of a on-Neumann-type stability analysis that is surprisingly simple and accurate. The fractional integration schemes and stability analysis discussed here can be easily extended to d -dimensional fractional diffusive equations and fractional wave equations.

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