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On three explicit difference schemes for fractional diffusion and diffusion-wave equations

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Abstract
Three explicit difference schemes for solving fractional diffusion and fractional diffusion-wave equations are studied. We consider these equations in both the Riemann–Liouville and the Caputo forms. We find that the Gorenflo *et al* (2000 *J. Comput. Appl. Math.* **118** 175) and the Yuste–Acedo (2005 *SIAM J. Numer. Anal.* **42** 1862) methods when applied to fractional diffusion equations are equivalent when BDF1 coefficients are used to discretize the fractional derivative operators, but that this is not the case for fractional diffusion-wave equations. The accuracy and stability of the three methods are studied. Surprisingly, the third method, that of Ciesielski–Leszczynski (2003 *Proc. 15th Conf. on Computer Methods in Mechanics*), although closely related to the Gorenflo *et al* method, is the least accurate, especially for short times. The stability analysis is carried out by means of a procedure close to the standard von Neumann method. We find that the stability bounds of the three methods are the same.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

The usefulness of the fractional derivative formalism, and in particular, of the fractional diffusion and fractional diffusion-wave equations, in addressing scientific problems is becoming ever more generally recognized in the scientific community as a consequence of the success of its application in fields as wide ranging as economics, biology, engineering, physics, etc. For example, one of the authors (SBY) has employed the fractional formalism to study the problem of the reaction kinetics when the reactive particles are subdiffusive [1–4]. Many more examples can be found in monographs [5–8].

The success of this formalism in practical applications depends strongly on the existence of exact or approximate solutions which can be calculated or computed efficiently. Fortunately, there exist many analytical methods of obtaining these solutions [7–13]. However, as also is the case in the non-fractional (classical) formalism, many problems can still only be suitably tackled by resorting to numerical methods. This makes the definition and evaluation of these methods of great importance. Although in the last few years many methods of solving fractional partial differential equations have been proposed and analyzed (see [14–23] and references therein), there is still much to be done, especially in evaluating and comparing their strengths and weaknesses. Here, we present results on three recently proposed explicit finite difference methods (the GMMP method [24], the CL method [25] and the YA method [26]) investigating their accuracy and stability. Explicit methods have some nice features that make them especially useful and widely employed [26, 27]: they are flexible, relatively simple and computationally undemanding, and can be easily generalized to spatial dimensions higher than one. However, in some cases, they can be unstable. This makes it crucial to ascertain under which conditions, if any, these methods are stable.

The equation we use as test bed is

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2}, \tag{1}$$

where

$$\frac{\partial^\gamma}{\partial t^\gamma} f(t) \equiv \frac{1}{\Gamma(n-\gamma)} \int_0^t \mathrm{d}\tau \frac{1}{(t-\tau)^{1+\gamma-n}} \frac{\mathrm{d}^n f(\tau)}{\mathrm{d}\tau^n}, \quad (2)$$
$$n-1 < \gamma < n, \quad (n = \text{integer})$$

is the fractional derivative in Caputo's sense. For $0 < \gamma \leqslant 1$ one has the fractional diffusion equation, or subdiffusion equation, in which we use the initial condition $u(x,0) = f(x)$. For $1 < \gamma \leqslant 2$ one has the fractional diffusion-wave equation for which we add the further initial condition: $\partial u(x,t)/\partial t|_{t=0} = g(x)$. It should be noted that although the GMMP and YA methods were originally designed for fractional diffusion equations, their extension to fractional diffusion-wave equations is straightforward.

Expressing the Caputo derivative in terms of the Riemann–Liouville derivative (which, for practical purposes, is valid under fairly general conditions; for more details see [7, 8, 28])

$${}_0D_t^\gamma f(t) \equiv \frac{1}{\Gamma(n-\gamma)} \frac{\mathrm{d}^n}{\mathrm{d}t^n} \int_0^t \mathrm{d}\tau \frac{f(\tau)}{(t-\tau)^{1+\gamma-n}}, \quad (3)$$
$$n-1 < \gamma < n, \quad (n = \text{integer})$$

one finds that the subdiffusion equation becomes

$$\frac{\partial}{\partial t} u(x,t) = {}_0D_t^{1-\gamma} \frac{\partial^2}{\partial x^2} u(x,t), \quad 0 < \gamma \leqslant 1, \quad (4)$$

whereas

$$\frac{\partial^2}{\partial t^2} u(x,t) = {}_0D_t^{2-\gamma} \frac{\partial^2}{\partial x^2} u(x,t), \quad 1 < \gamma \leqslant 2 \quad (5)$$

is another way of writing the subdiffusion-wave equation. The YA method was originally devised for equation (4), but can easily be extended to deal with equation (5).

In order to carry out the numerical comparisons, we will consider a problem defined in the interval $0 \leqslant x \leqslant \pi$, with absorbing boundary conditions, $u(x=0,t) = u(x=\pi,t) = 0$, and where the initial condition is $u(x,0) = f(x) = \sin x$ for the fractional diffusion problem, and $u(x,0) = f(x) = \sin x$ and $\partial u(x,t)/\partial t|_{t=0} = g(x) = 0$ for the diffusion-wave problem. This problem is chosen because its exact solution is known [10] and easy to calculate:

$$u(x,t) = E_\gamma(-t^\gamma)\sin(x), \quad (6)$$

where E_γ is the Mittag–Leffler function [7, 8].

2. The numerical methods

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

The GMMP and CL methods differ in the form in which they discretize the Caputo derivative, namely,

$$\left.\frac{\partial^\gamma f}{\partial t^\gamma}\right|_{t_m} \simeq (\Delta t)^{-\gamma} \sum_{r=0}^{m} \omega_r^\gamma \left[f(t_{m-r}) - f(0) - f'(0)t_m\right] \quad (7)$$

for the GMMP method, and

$$\left.\frac{\partial^\gamma f}{\partial t^\gamma}\right|_{t_m} \simeq (\Delta t)^{-\gamma} \sum_{r=0}^{m} \omega_r^\gamma f(t_{m-r}) - \frac{f(0)}{\Gamma(1-\gamma)} t_m^{-\gamma} - \frac{f'(0)}{\Gamma(2-\gamma)} t_m^{1-\gamma} \quad (8)$$

for the CL method [25, 29]. We shall use the notation $t_m = m\Delta t$. For the GMMP and CL methods, the subdiffusion case ($0 < \gamma < 1$) is recovered by deleting the term in which $f'(0)$ appears. In the fractional difference methods, the Riemann–Liouville derivative is approximated by using a discretization formula of order p:

$${}_0D_t^\gamma f(t_m) = (\Delta t)^{-\gamma} \sum_{r=0}^{m} \omega_r^\gamma f(t_{m-r}) + O(\Delta t)^p. \quad (9)$$

There are several valid sets of coefficients ω_k^γ: see [26, 30], for example. The BDF1 set, for which $p = 1$,

$$\omega_k^\gamma = (-1)^k \binom{\gamma}{k} \quad (10)$$

was the only one considered by Gorenflo *et al* in [24]. In this case, the equation (9) is known as the Grünwald–Letnikov formula.

Using (9) in equations (1), (4) and (5), and discretizing the second-order space derivative by the usual three-point centered formula

$$\frac{\partial^2}{\partial x^2} u(x_j, t_m) = \frac{u(x_{j+1}, t_m) - 2u(x_j, t_m) + u(x_{j-1}, t_m)}{(\Delta x)^2} + O(\Delta x)^2 \quad (11)$$

one obtains three difference schemes for subdiffusion equations with discretization errors of order $O(\Delta t)^p + O(\Delta x)^2$, namely:

- GMMP method:

$$\omega_0^\gamma U_j^{(m+1)} = S\left[U_{j-1}^{(m)} - 2U_j^{(m)} + U_{j+1}^{(m)}\right] - \sum_{k=1}^{m} \omega_k^\gamma U_j^{(m+1-k)} + U_j^0 \sum_{k=0}^{m} \omega_k^\gamma, \quad (12)$$

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

- CL method:

$$U_j^{(m+1)} = S\left(U_{j-1}^{(m)} - 2U_j^{(m)} + U_{j+1}^{(m)}\right) - \sum_{k=1}^{m+1} \omega_k^\gamma U_j^{(m+1-k)} + \left(\frac{1}{m+1}\right)^\gamma \frac{U_j^{(0)}}{\Gamma(1-\gamma)}. \quad (14)$$

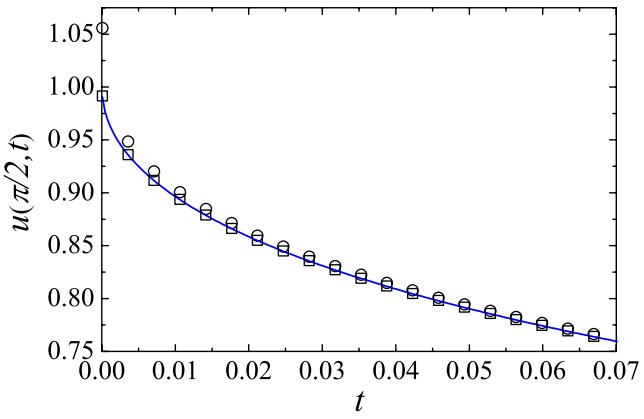

Figure 1. Solution at the mid-point $x = \pi/2$ of the fractional diffusion equation described in the main text for $\gamma = 1/2$. Line: exact solution, $u(\pi/2, t) = E_{1/2}(-t^{1/2})$; squares: numerical solution obtained with the GMMP and YA methods; circles: CL method. We have used $\Delta x = \pi/20$ and $\Delta t = 7.074 \times 10^{-5}$.

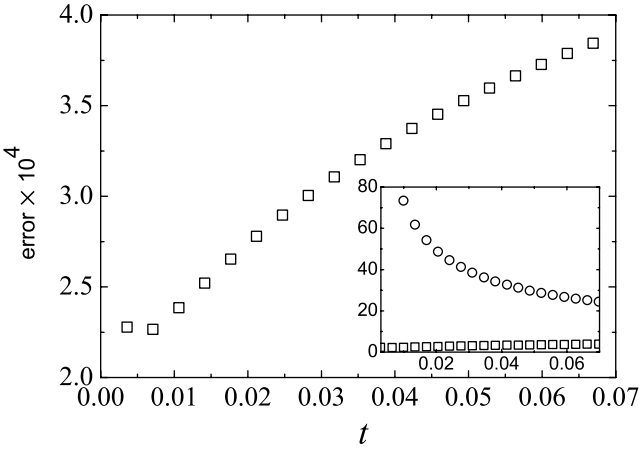

Figure 2. Error of the numerical methods for the problem considered in figure 1. Main panel: error for the GMMP and YA methods (squares). Inset: the same as in the main panel including the error corresponding to the CL method (circles).

- YA method:

$$U_j^{(m+1)} = U_j^{(m)} + S \sum_{k=0}^{m} \omega_k^{(1-\gamma)} \times \left[U_{j-1}^{(m-k)} - 2U_j^{(m-k)} + U_{j+1}^{(m-k)} \right]. \quad (15)$$

The difference schemes for fractional diffusion-wave problems ($1 < \gamma \leqslant 2$) can be deduced in a similar way:

- GMMP method:

$$\omega_0^{\gamma} U_j^{(m+1)} = S \left[U_{j-1}^{(m)} - 2U_j^{(m)} + U_{j+1}^{(m)} \right] - \sum_{k=1}^{m} \omega_k^{\gamma} U_j^{(m+1-k)} + U_j^0 \sum_{k=0}^{m} \omega_k^{\gamma} + U_j'^0 \Delta t \sum_{k=0}^{m+1} k \omega_k^{\gamma}. \quad (16)$$

Here $U'^{(0)}_j$ is the numerical value of the derivative of the exact solution at time $t = 0$.

- CL method:

$$U_j^{(m+1)} = S \left(U_{j-1}^{(m)} - 2U_j^{(m)} + U_{j+1}^{(m)} \right) - \sum_{k=1}^{m+1} \omega_k^{\gamma} U_j^{(m+1-k)} + \left(\frac{1}{m+1} \right)^{\gamma} \frac{U_j^{(0)}}{\Gamma(1-\gamma)} + \left(\frac{1}{m+1} \right)^{(\gamma-1)} \frac{U_j'^{(0)}}{\Gamma(2-\gamma)}. \quad (17)$$

- YA method:

$$U_j^{(m+1)} = 2U_j^{(m)} - U_j^{(m-1)} + S \sum_{k=0}^{m} \omega_k^{(2-\gamma)} \left[U_{j-1}^{(m-k)} - 2U_j^{(m-k)} + U_{j+1}^{(m-k)} \right]. \quad (18)$$

In figure 1, we compare the analytical solution and the numerical solutions obtained from these methods for the fractional diffusion equation defined in the interval $0 \leqslant x \leqslant \pi$ with $\gamma = 0.5$, $f(x) = \sin x$, and boundary conditions $u(0, t) = u(\pi, t) = 0$. The error of each method is shown in figure 2. One sees that the results given by the CL method are the poorest, and that those of the YA and GMMP methods are *exactly the same!* This is quite surprising because the CL and GMMP schemes are closely related (note that the only difference lies in their last term), whereas the YA and GMMP schemes appear to be completely different. Figure 3 shows the solution for a fractional diffusion-wave equation with $\gamma = 1.7$ in the interval $0 \leqslant x \leqslant \pi$ with $\gamma = 0.5$, $f(x) = \sin x$, $g(x) = 0$, and boundary conditions $u(0, t) = u(\pi, t) = 0$. We find again that the YA and GMMP results coincide and that the CL method gives even poorer results than for the case considered in figure 1. It is important to note that these numerical solutions have been obtained using the BDF1 coefficients (10). The fact that the YA and GMMP method lead to the same results is not casual. We discuss this issue further in section 4.

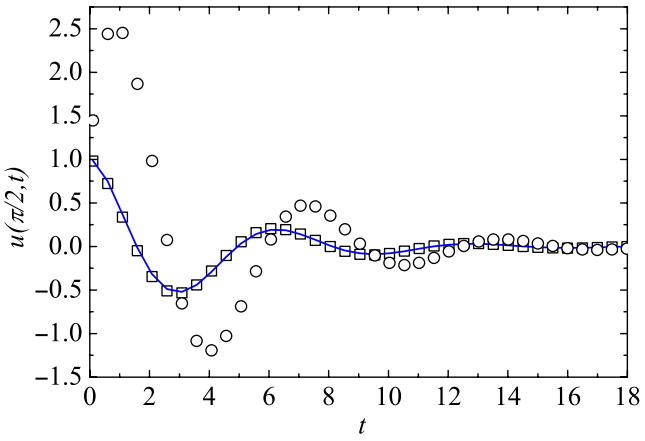

Figure 3. Solution at the mid-point $x = \pi/2$ of the fractional diffusion-wave equation described in the main text for $\gamma = 1.7$. Line: exact solution, $u(\pi/2, t) = E_{1.7}(-t^{1.7})$; squares: numerical solution obtained with the GMMP and YA methods; circles: CL method. We have used $\Delta t = 0.0994$ and $\Delta x = \pi/20$.

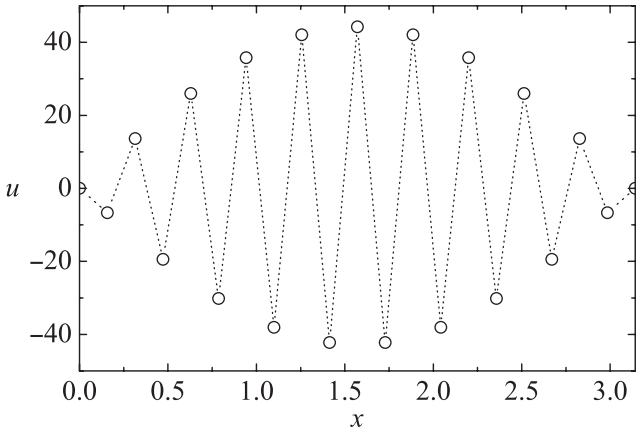

Figure 4. Numerical solution (circles) provided by the GMMP and YA methods for the fractional diffusion equation with $\gamma = 0.5$ and $f(x) = \sin(x)$ after 800 timesteps when $\Delta x = \pi/20$ and $S = (\Delta t)^\gamma/(\Delta x)^2 = 0.37$. Note that this value of S is larger than the stability bound $2^{-1.5} \simeq 0.3535\ldots$ provided by equation (20). The broken line is to guide the eye.

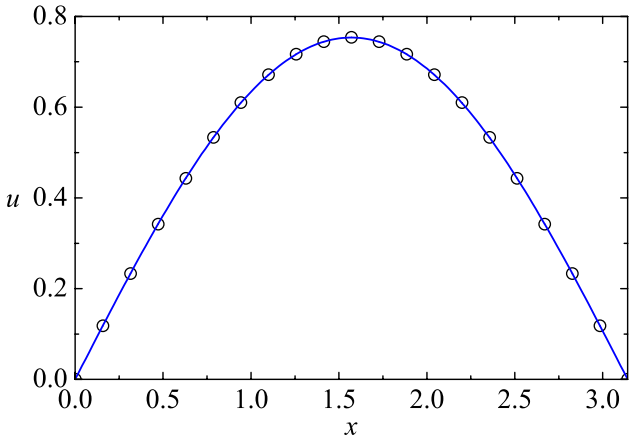

Figure 5. Numerical solution (circles) provided by the GMMP and YA methods for the fractional diffusion equation with $\gamma = 0.5$ and $f(x) = \sin(x)$ after 1000 timesteps when $\Delta x = \pi/20$ and $S = (\Delta t)^\gamma/(\Delta x)^2 = 0.35$. Note that this value is smaller than the stability bound $2^{-1.5} \simeq 0.3535\ldots$ provided by equation (20), so that we are inside the stability region. The solid line is the exact solution.

3. Stability

The explicit difference methods considered in section 2 are not always stable because for any given value of γ there are choices of Δx and Δt for which the numerical scheme becomes unstable, which leads to absurd numerical solutions (see an example in figure 4). Therefore, it is important to determine the conditions, if any, under which these explicit methods are stable. To this end, we use the fractional von Neumann stability analysis employed in [26, 31] for fractional diffusion equations. Their extension to fractional diffusion-wave equations is straightforward. Proceeding as in these references, one easily finds that the YA, GMMP and CL methods are stable if

$$\frac{(\Delta t)^\gamma}{(\Delta x)^2} \leqslant \frac{1}{4}\omega(-1, \gamma), \tag{19}$$

where $\omega(z, \gamma) = \sum_{k=0}^{\infty} \omega_k^\gamma z^k$ is the generating function for the ω_k^γ coefficients. If one uses the BDF1 coefficients (cf (10)), then the generating function is $\omega(z, \gamma) = (1 - z)^\gamma$ [30] and the stability bound becomes

$$\frac{(\Delta t)^\gamma}{(\Delta x)^2} \leqslant 2^{\gamma-2}. \tag{20}$$

Figures 4 and 5 show the numerical solution $u(x, t)$ for the same problem of figure 1 but for two values of S, respectively, larger and smaller than the stability bound provided by (20). One sees that the value of S is crucial: when this parameter is inside the 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.

4. Equivalence between the GMMP and YA methods

In section 2, it was seen that the numerical results obtained with the YA method were identical to those obtained by means of the GMMP method. This result seemed surprising given the quite different structure of the two algorithms (cf equations (15) and (12)). However, this is not just a coincidence since it is possible to prove that the two methods are equivalent (see below) if and only if the following relationship involving the generating functions of the coefficients ω_k^γ holds:

$$\omega(z; \gamma)\omega(z; 1 - \gamma) = 1 - z. \tag{21}$$

A similar result is also valid for diffusion-wave equations: as long as $\partial u(x, t)/\partial t|_{t=0} = g(x) = 0$, the two methods are equivalent if and only if

$$\omega(z; \gamma)\omega(z; 2 - \gamma) = (1 - z)^2. \tag{22}$$

4.1. Equivalence of the GMMP and YA methods for fractional diffusion equations

It is easy to see from (15) and (12) that the value for $U_j^{(1)}$ provided by the two methods is the same if $\omega_0^{(1-\gamma)}\omega_0^\gamma = 1$. In the same way, it is easy to prove that the two methods lead to the same value for $U_j^{(2)}$ if $\omega_0^\gamma\omega_1^{(1-\gamma)} + \omega_1^\gamma\omega_0^{1-\gamma} = -1$. In general, it is possible to prove by induction after some lengthy algebra that for $k \geqslant 2$ the two methods lead to the same value $U_j^{(k)}$ if, and only if,

$$\omega_0^\gamma\omega_0^{1-\gamma} = 1, \tag{23}$$

$$\omega_1^\gamma\omega_0^{1-\gamma} + \omega_1^{1-\gamma}\omega_0^\gamma = -1, \tag{24}$$

$$\sum_{n=0}^{k} \omega_n^{1-\gamma}\omega_{k-n}^\gamma = 0, \quad k \geqslant 2. \tag{25}$$

But

$$\omega(z; \gamma)\omega(z; 1 - \gamma) = \sum_{m=0}^{\infty}\sum_{r=0}^{m} z^m\omega_{m-r}^\gamma\omega_r^{1-\gamma}. \tag{26}$$

Therefore, inserting equations (23)–(25) into (26) one gets (21). Note that this equation is satisfied trivially if one uses the BDF1 coefficients in the YA and GMMP methods because, for these coefficients, $\omega(z; \gamma) = (1 - z)^\gamma$.

4.2. Equivalence of the GMMP and YA methods for fractional diffusion-wave equations

Let us start by comparing the first value $U_j^{(1)}$ provided by the YA and GMMP methods. According to the YA method,

$$U_j^{(1)} = 2U_j^{(0)} - U_j^{(-1)} + S\omega_0^{(2-\gamma)}\left[U_{j-1}^{(0)} - 2U_j^{(0)} + U_{j+1}^{(0)}\right]. \quad (27)$$

The 'ghost' value $U_j^{(-1)}$ can be obtained from the boundary condition $\partial u(x,t)/\partial t|_{t=0} = g(x) = 0$:

$$U_j^{(-1)} = sU_j^{(0)} - g_j\Delta t \quad (28)$$

so that

$$U_j^{(1)} = U_j^{(0)} + g_j\Delta t + S\omega_0^{(2-\gamma)}\left[U_{j-1}^{(0)} - 2U_j^{(0)} + U_{j+1}^{(0)}\right]. \quad (29)$$

On the other hand, for the GMMP method one gets

$$\omega_0^\gamma U_j^{(1)} = S\left(U_{j-1}^{(0)} - 2U_j^{(0)} + U_{j+1}^{(0)}\right) + \omega_0^\gamma U_j^0 + g_j\Delta t\omega_1^\gamma. \quad (30)$$

Thus ones sees that the two methods lead to the same value $U_j^{(1)}$ if, and only if,

$$\omega_0^{(2-\gamma)}\omega_0^\gamma = 1, \quad (31)$$

$$\omega_1^\gamma = -\omega_0^\gamma. \quad (32)$$

But this last equation is not verified by the BDF1 set of coefficients, nor by any other set of known coefficients [30]. Therefore, we have to conclude that, in general, the YA and GMMP methods are not equivalent. However, note that if $g(x) = 0$, then the condition (32) is no longer necessary, and the two methods provide the same value $U_j^{(1)}$ if the BDF1 coefficients are used. In fact, it is possible to prove that the two methods lead to the same value $U_j^{(m)}$ for all m as long as the following equations hold:

$$\omega_0^\gamma\omega_0^{2-\gamma} = 1, \quad (33)$$

$$\omega_0^\gamma\omega_1^{2-\gamma} + \omega_1^\gamma\omega_0^{2-\gamma} = -2, \quad (34)$$

$$\omega_0^\gamma\omega_2^{2-\gamma} + \omega_1^\gamma\omega_1^{2-\gamma} + \omega_2^\gamma\omega_0^{2-\gamma} = 1, \quad (35)$$

$$\sum_{n=0}^{k}\omega_n^{1-\gamma}\omega_{k-n}^\gamma = 0, \quad k \geqslant 3. \quad (36)$$

Note that these equations imply (22), which is only satisfied by the generating function of the BDF1 coefficients.

5. Conclusions

We have considered three explicit methods (GMMP, YA and CL methods) for solving fractional diffusion and diffusion-wave equations. As the GMMP and YA methods were not originally developed for fractional diffusion and diffusion-wave equations, we have generalized them to cope with this class of equations. Regarding the accuracy, we found that the CL method is the poorest of the three methods considered, especially for short times. Initially, we found empirically that, when using BDF1 discretization coefficients, the YA and GMMP methods *always* lead to the same results for the fractional subdiffusion problem, and for the fractional diffusion-wave problem as long as the initial time derivative is zero. We proved that this is no coincidence: the two methods are equivalent if and only if the BDF1 discretization coefficients are used. The nonequivalence of the CL and GMMP methods and the equivalence of the YA and GMMP methods is quite remarkable: it is a nice example of how two almost identical algorithms obtained from the very same equation (the CL and GMMP schemes) are really different, and how two seemingly quite different algorithms obtained from two different forms of an equation (the YA and GMMP schemes) turn out to be identical. Finally, by means of a von Neumann stability analysis we obtained the stability conditions for the three methods and for both the fractional diffusion and diffusion-wave equations. We found that the three methods have the same stability.

Acknowledgments

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