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The G^{α} -scheme for Approximation of Fractional Derivatives: Application to the Dynamics of Dissipative Systems

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Abstract: The Gear scheme is a three-level step algorithm, backward in time and second order accurate, for the approximation of classical time derivatives. In this article, the formal power of this scheme is used to approximate fractional derivative operators, in the context of finite difference methods. Numerical examples are presented and analyzed, in order to show the accuracy of the Gear scheme at the power α (G^{α}-scheme) when compared to the classical Grünwald-Letnikov approximation. In particular, the combined G^{α}-Newmark scheme is shown to be second-order accurate for a fractional damped oscillator problem.

Keywords: Fractional derivatives, viscoelasticity, multi-step scheme, linear dynamics

1. INTRODUCTION

The importance of fractional calculus for modeling viscoelastic materials has been recognized by the mechanical scientific community since the work of Bagley and Torvik (1983). The numerical approximation of such systems has been intensively studied since the late 1980s (Padovan, 1987). Meanwhile, the numerical community has also becoming interested in the approximation of fractional derivatives. Consider, for example, the pioneering theoretical work of Lubich (1986), and the state of the art as proposed by Diethelm et al. (2005). Most applications use the discrete convolution formula proposed by Grünwald and Letnikov. Another direction for recent research is autonomous systems, in the context of diffusive representations (Matignon and Montseny, eds., 1998; Trinks and Ruge, 2002; Yuan and Agrawal, 2002). In this work, we focus on the application of a numerical method based on the Gear scheme (called a G^{α} -scheme herein) to the approximation of fractional derivatives in linear dynamics. Note that preliminary tests of convergence have been performed, and are described elsewhere (Galucio et al., 2006). In what follows, we first describe the G^{α} -scheme. Two example applications are then presented and analyzed. The first of these studies a harmonic oscillator with fractional damping, in order both to validate the method and to derive an order of convergence. The use of the G^{α} -scheme is then extended to analysis of viscoelastic beams subjected to an applied time-dependent force.

2. THE G^{α} -SCHEME

We now introduce the G^{α} -operator, which is based in the Gear scheme, for use in the approximation of fractional derivatives

$$\mathbf{G}^{\alpha} = \frac{1}{\Delta t^{\alpha}} \left(\frac{3}{2}\right)^{\alpha} \left[I - \frac{4}{3}\delta^{-} + \frac{1}{3}(\delta^{-})^{2}\right]^{\alpha} \tag{1}$$

where Δt , which is assumed to be fixed, is the time step.

Let *u* be a time dependent function, known only by its discretized values u^n at each time t^n , where *n* is a positive integer. The function u^n is approximated by $u(t^n)$, where $t^n = n\Delta t$. The α -derivative of *u* at time t^n can be approximated using

$$(\mathbf{G}^{\alpha}u)^{n} = \frac{1}{\Delta t^{\alpha}} \left(\frac{3}{2}\right)^{\alpha} \sum_{j=0}^{\infty} g_{j+1}u^{n-j}$$
(2)

where g is a rational number. The calculation of these G^{α} -coefficients is a difficult task, because of the cumulative numerical errors. In order to overcome this difficulty, the method employed here requires analytical calculation of these coefficients (using Matlab symbolic toolbox, in our case). For illustrative purposes, the reader is referred to table 1, where the first ten G^{α} -coefficients are presented for three values of α : 1/3, 1/2, and 3/4.

3. THE FRACTIONAL DAMPED OSCILLATOR PROBLEM

Consider a fractional single degree of freedom system subjected to a constant step load f for t > 0 with zero initial conditions. The damping is taken into account by introducing a fractional damping term, or a *spring-pot* element in the formulation. The corresponding governing equation and initial conditions are

$$m\ddot{u} + c\tau^{\alpha} \mathcal{D}^{\alpha} u + ku = f, \quad t > 0$$

$$u(0) = \dot{u}(0) = 0$$
(3)

where *m* and *k* are mass and stiffness constants, respectively, and $c\tau^{\alpha}$ is a fractional damping constant formed using relaxation time τ and classical damping constant *c*.

j	$\alpha = 1/3$	$\alpha = 1/2$	$\alpha = 3/4$	
0	1	1	1	
1	$-\frac{4}{9}$	$-\frac{2}{3}$	-1	
2	$-\frac{7}{81}$	$-\frac{1}{18}$	$\frac{1}{12}$	
3	$-\frac{104}{2187}$	$-\frac{1}{27}$	$-\frac{1}{108}$	
4	$-\frac{643}{19683}$	$-\frac{17}{648}$	$-\frac{1}{96}$	
5	$-\frac{4348}{177147}$	$-\frac{19}{972}$	$-\frac{7}{864}$	
6	$-\frac{92809}{4782969}$	$-\frac{59}{3888}$	$-\frac{193}{31104}$	
7	$-\frac{683552}{43046721}$	$-\frac{71}{5832}$	$-\frac{151}{31104}$	
8	$-\frac{5164958}{387420489}$	$-\frac{2807}{279936}$	$-\frac{5813}{1492992}$	
9	$-\frac{358288744}{31381059609}$	$-\frac{10627}{1259712}$	$-\frac{128713}{40310784}$	
10	$-\frac{2805807422}{282429536481}$	$-\frac{109159}{15116544}$	$-\frac{430313}{161243136}$	

Table 1. First ten coefficients g_{i+1} of formal power series.

The aim of this section is to solve set of equations (3) with a direct (Newmark) time integration method in conjunction with an approximation of the α -derivative $\mathcal{D}^{\alpha}u$ (G^{α}- or GL-scheme). In order to validate these combinations, the approximate solution produced is compared to an exact solution considered in earlier work (Galucio et al., 2006). Finally, error estimates in L^{∞} norm are performed. For a fixed time step $\Delta t = 1/2^m$, this error is computed as

$$e_{\infty}^{m} = \max\{|u(j\Delta t) - u^{j}|, j = 0, \cdots, 2^{m}\}$$
 (4)

where *m* is a positive integer.

3.1. Algorithm

As mentioned above, the average acceleration algorithm is used to solve equation 3. The displacement history arising from the α -derivative approximation (damping term) is shifted to the right-hand side of equation 3 (Galucio et al., 2004). Therefore, using equation 2, the governing equation can be written in its discretized form as

	$\alpha = 1/3$	$\alpha = 1/2$	$\alpha = 3/4$	
G ^α	1.99	1.96	1.90	
GL	1.00	0.99	0.99	

Table 2. Rates of convergence, computed using the L^{∞} norm, for three values of *a*.

$$m\ddot{u}^{n+1} + (k+\kappa)u^{n+1} = f^{n+1} + \phi^{n+1}$$
(5)

where the non-classical terms κ and ϕ arise from the approximation of the α -derivative:

$$\kappa = \frac{c\tau^{\alpha}}{\Delta t^{\alpha}} \left(\frac{3}{2}\right)^{\alpha} \tag{6a}$$

$$\phi^{n+1} = -\frac{c\tau^{\alpha}}{\Delta t^{\alpha}} \left(\frac{3}{2}\right)^{\alpha} \sum_{k=1}^{N} g_{k+1} u^{n+1-k}.$$
 (6b)

Note that the stiffness term κ is constant with time, depending only on the size of the time step, which is assumed to be fixed. The modified loading ϕ depends on the displacement history.

3.2. Results

In all calculations performed below, we assume that $m = k = \tau = f = 1$ in a suitable unit system. The results shown in table 2, and in Figures 1 to 2, assume that c = 1. Three different values of α are tested. The final time is chosen to be T = 15, for various values of the time step Δt .

It should be remembered that the error estimates in the L^{∞} norm are obtained using an exact solution, based on formal power series, as mentioned above.

Table 2 shows the error estimates in the L^{∞} norm. It can be seen that the combined G^{α} -Newmark scheme provides second-order accuracy for any value of α . However, the use of a GL-Newmark algorithm decreases the order of accuracy to 1.

Figures 1 and 2 show the evolution of the displacement for two values of α , and the associated error estimates for the L^{∞} norm, for both the G^{α}-Newmark and GL-Newmark schemes. In Figures 1(a) and 2(a), the exact solution of equation 3 is presented, along with its numerical approximations (using the GL and G^{α} methods), with a time discretization corresponding to 2⁶ = 64 time steps. It can be seen that the solution obtained using the G^{α}-scheme is very close to the exact solution, while using the GL-method gives in an overestimated result.

Error estimates in the L^{∞} norms are presented in Figures 1(b) and 2(b). In both cases, the combined G^{*a*}-Newmark scheme gives better accuracy than is achieved using GL-Newmark. The rates of convergence presented in table 2 are computed with 7–9 meshes, otherwise the slopes are wrongly estimated.

It should be emphasized that the order of the fractional derivative does not affect the rate of convergence (see table 2 and Figures 1 and 2) when using a Newmark integrator. The influence of α is exerted in the mechanical behavior of the fractional damped oscillator by



Figure 1. (a) Exact and approximate solutions of equation (3) for $\alpha = 1/3$ and $\Delta t = T/2^6$. (b) Error estimates in the L^{∞} norm.



Figure 2. (a) Exact and approximated solutions of equation (3) for $\alpha = 3/4$ and $\Delta t = T/2^6$. (b) Error estimates in the L^{∞} norm.



Figure 3. (a) Exact and approximate solutions of (3) for $\alpha = 1/2$ and $\Delta t = T/2^9$. (b) Error estimates in the L^{∞} norm.

Table 3. Rate of convergence computed using the L^{∞} norm for three values of *c*.

	c = 0.50	c = 1.00	c = 1.50	
Gα	1.98	1.96	1.93	
GL	0.96	0.99	1.00	

means of a damping factor. The result of this is that, when α decreases, the damping (and thus the time required to achieve the quasistatic time solution) increase.

In order to show the influence of added damping, the responses of the oscillator, computed using the G^{α}-Newmark scheme, are shown in Figure 3 (a) for three values of the damping constant: c = 0.5, c = 1.0, and c = 1.5 (see equation 3). These results, obtained for a semi-derivative problem, all use $\alpha = 1/2$; only the value of c varies. The corresponding error in the L^{∞} norm, for each result when compared to the exact solution, is shown in Figure 3 (b). The rate of convergence, as given in table 3 (see also table 2) remains the same for all three values of c. As in previous results, the results given by the combined G^{α}-Newmark algorithm are of about the second order of accuracy.

4. EXTENSION TO VISCOELASTIC BEAMS

4.1. Viscoelastic Constitutive Equations

The one-dimensional fractional Zener model is adopted to describe the behavior of a viscoelastic material (Bagley and Torvik, 1983) in this section

$$\sigma(t) + \tau^{a} \mathcal{D}^{a} \sigma(t) = E_{a} \varepsilon(t) + E_{\infty} \tau^{a} \mathcal{D}^{a} \varepsilon(t)$$
(7)

where σ and ε are the stress and strain, respectively, E_o and E_∞ are the relaxed and non-relaxed elastic moduli, and τ is the relaxation time.

In order to facilitate the numerical implementation of this model, we will introduce an internal variable as an "anelastic" strain function:

$$\varepsilon_{\alpha} = \varepsilon - \sigma / E_{\infty}. \tag{8}$$

This expression, when substituted into equation 7, gives an expression with only one fractional derivative operator.

4.2. Algorithm

For the sake of brevity, finite element considerations are not presented in this investigation. For full details, the reader is referred to the description in a previous work (Galucio et al., 2004). The governing equation to be solved takes the form

$$\begin{cases} \mathbf{M}\ddot{\mathbf{q}}^{n+1} + (\mathbf{K} + \mathcal{K})\mathbf{q}^{n+1} = \mathbf{F}^{n+1} + \mathbf{\Phi}^{n+1} \\ \mathbf{q}^0 = \dot{\mathbf{q}}^0 = \mathbf{0} \end{cases}$$
(9)

where **M** and **K** are the mass and stiffness matrices, **q** the degree-of-freedom vector, and **F** a mechanical load. \mathcal{K} and Φ are the terms arising from the viscoelastic behavior of the beam such that

$$\mathcal{K} = c_{\alpha} \frac{E_{\infty} - E_o}{E_o} \mathbf{K}$$
(10a)

$$\mathbf{\Phi}^{n+1} = -c_{\alpha} \frac{E_{\infty}}{E_o} \mathbf{K} \sum_{k=1}^{N} g_{k+1} \mathbf{q}_{\alpha}^{n+1-k}$$
(10b)

where $c_{\alpha} = \tau^{\alpha}/(\tau^{\alpha} + \Delta t^{\alpha})$. Note that, as in the single degree of freedom problem, the added stiffness matrix \mathcal{K} does not depend on time, while the dissipative force Φ depends on the history of "anelastic" displacements, which are updated at each time step as follows:

$$\mathbf{q}_{\alpha}^{n+1} = (1 - c_{\alpha}) \frac{E_{\infty} - E_o}{E_{\infty}} \mathbf{q}^{n+1} - c_{\alpha} \sum_{k=1}^{N} g_{k+1} \mathbf{q}_{\alpha}^{n+1-k}.$$

It is important to understand that the introduction of \mathbf{q}_{α} in the formulation does not imply an augmentation of the system. Instead, \mathbf{q}_{α} can be considered as an intermediate variable in the time scheme (see Galucio et al., 2004). As in the previous example, the average acceleration algorithm is used to solve equation 9.



Figure 4. Damped responses of the viscoelastic beam: (a) Tip displacement versus time; and (b) phase-space diagram.

4.3. Results

Consider a viscoelastic cantilever beam of length L = 150 mm, width b = 25 mm, and thickness h = 5 mm, discretized with 5 finite elements. The mechanical characteristics of the fictitious viscoelastic material are: Density $\rho = 1000$ kg/m³, Poisson's ratio $\nu = 0.5$, relaxed elastic modulus $E_o = 1$ MPa, non-relaxed elastic modulus $E_{\infty} = 50$ MPa, relaxation time $\tau = 1$ ms, and order of the fractional derivative $\alpha = 0.5$. The beam is subjected to a transverse load at its free end such that

$$F(t) = \begin{cases} F_o t/t_1, & 0 \le t \le t_1 \\ F_o, & t \ge t_1 \end{cases}$$

where $F_o = 0.01$ N, $t_1 = 50$ ms, and T = 1 s. The time step used is $\Delta t = 2$ ms, and the whole time history of "anelastic" displacements is used in the calculations.

Figure 4, shows the transient responses of the damped viscoelastic beam. The evolution of the tip displacement, and the phase-space diagram are plotted in Figure Figures 4(a) and (b), respectively. As expected, we observe that the oscillations of the viscoelastic beam are damped. It should be pointed out that these preliminary results show the versatility of the G^{α} -scheme, since it is implementation is easy, and there are no additional costs relative to the GL-scheme.

5. CONCLUSIONS

A numerical method based on the Gear scheme for approximation of fractional derivatives is used here to model damping in linear dynamics. This G^{α} -scheme is written in terms of a formal power series, the coefficients of which have to be calculated. The numerical evaluation of G^{α} -coefficients is delicate, as a result of bad conditioning of the recurrence formula. However, with the help of formal calculus, cumulative numerical errors are avoided.

Two examples are presented and analyzed. In both cases, the average-acceleration algorithm is used to integrate the governing equation. The first example concerns a single degree of freedom oscillator, with fractional damping. In order to validate the presented approach, numerical results for the method proposed are compared to an exact solution for the single degree of freedom problem under a constant load (Galucio et al., 2006). The second example deals with the finite element implementation of a viscoelastic beam subjected to a mechanical load. The combined G^{α} -Newmark algorithm seems a promising tool for dynamic problems, as second-order accuracy is obtained in the solutions to both problems.

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