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Reduced Numerical Approximation of Fractional Derivative in Application to Creep

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Abstract

Fractional viscoelasticity offers an alternative approach to describe viscoelastic materials with the use of derivatives and integrals of non-integer order. The main disadvantage occurs in the numerical applications of this approach. Compared to standard finite-order derivatives, the numerical approximation of the fractional derivative is based on the nodal values of all previous time steps. Each of these values has a different weight when computing the next value in every subsequent step. This leads to high requirements on memory and computing time. This paper introduces several possible modifications to approximate the fractional derivative, which rely on the application of a reduced number of nodal values and thus reduce the complexity of the calculation.

Keywords: springpot, fractional viscoelasticity, viscoelastic response, fractional derivative, numerical approximation of fractional derivative, reduced approximation.

1 Introduction

Viscoelastic materials are commonly described by theoretical models using purely elastic springs and purely viscous dashpots connected together to form more complex models. Fractional viscoelasticity employs another approach based on the fractional calculus, the theory of integrals and derivatives of non-integer order.

On the basis of this theory, another rheological element, the springpot, can be introduced. The springpot element behaves as viscoelastic itself, and its behavior can be represented by the following constitutive law

$$\sigma(t) = E\tau_{\mathrm{c}}^{\alpha} D^{\alpha}\varepsilon(t), \tag{1}$$

where σ stands for the normal stress, ε for the normal strain and τ_{c} is a characteristic time defined as the ratio of viscosity η and Young's modulus of elasticity E. D^{α} denotes a fractional derivative.

In general, the fractional derivative can be of any non-integer order. However, describing viscoelastic behavior requires a closer specification of the parameter α. When setting $\alpha = 0$, the constitutive law can be simplified to $\sigma(t) = E\varepsilon(t)$, the well-known Hooke law, which describes the behavior of a purely elastic material. On the other hand, for $\alpha = 1$ the resulting expression $\sigma(t) = \eta\dot{\varepsilon}(t)$ is Newton's equation of viscosity used to describe purely viscous liquids. Since viscoelastic behavior is somewhere between purely elastic and purely viscous, the order of the fractional derivative in the springpot element should be found somewhere in the range $\alpha \in \langle 0; 1\rangle$.

2 Brief insight to fractional calculus

Fractional calculus is a branch of mathematics that generalizes integrals and derivatives to non-integer order. The formula for the fractional integral is derived from the Cauchy formula for n times repeated integration, which reads

$$I^{n} f(x) = \frac{1}{(n-1)!} \int_{0}^{x} (x-y)^{n-1} f(y)\mathrm{d}y, \tag{2}$$

where I^{n} denotes an integral operator of a natural order $n \in \mathbb{N}$. The Riemann-Liouville fractional integral I^{α} of non-integer order $\alpha \in \mathbb{R}$ is then provided by

$$I^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{0}^{x} (x-y)^{\alpha-1} f(y)\mathrm{d}y, \tag{3}$$

where $\Gamma(\alpha)$ is the gamma function, a generalization of the factorial function. From this definition of the fractional integral there is only a simple step to the definition of the fractional derivative, considering the inverse relation between derivation and integration. The two most commonly used definitions are the Caputo and the Riemann-Liouville fractional derivative.

The Caputo fractional derivative is defined as

$$D^{\alpha} f(x) = I^{\lceil \alpha \rceil - \alpha} \left[D^{\lceil \alpha \rceil} f(x) \right] \tag{4}$$

where D^{α} is the derivative operator of order α and $\lceil \alpha \rceil$ denotes the ceiling function. For example, to obtain the 0.6th derivative of the function $f(x)$ according to this formula, we take the first derivative and then integrate the result 0.4 times.

The Riemann-Liouville fractional derivative is prescribed as

$$D^{\alpha} f(x) = D^{\lceil \alpha \rceil} \left[I^{\lceil \alpha \rceil - \alpha} f(x) \right]. \tag{5}$$

Both of these definitions give the same final results. A broader insight into fractional calculus can be found, for example, in [1] or [2].

3 Numerical approximation of fractional derivative

The application of fractional derivatives to describe physical problems introduces fractional differential equations. As with standard differential equations, the solution of fractional differential equations cannot usually be performed analytically. Instead, it requires the use of numerical solvers. The equation is then numerically evaluated in steps.

One of the possible numerical approximations of the fractional derivative was introduced by [3] in the following form

$$D^{\alpha} f^{n} \approx \frac{1}{(\Delta t)^{\alpha}} \sum_{j=0}^{\mathrm{n}} w_j(\alpha) f^{n+1-j}, \tag{6}$$

where Δt denotes the magnitude of the time step and j marks the index of the node; $j = 0$ represents the most actual time at t^n while with increasing value of j we move retrospectively, $j = n$ then identifies the initial node t^0. Each of the nodal values is multiplied by the corresponding weight, which can be calculated as

$$w_0(\alpha) = 1, \qquad w_j(\alpha) = w_{\text{j-1}}(\alpha) \frac{j - 1 - \alpha}{j}. \tag{7}$$

It is obvious that setting the fractional derivative order as $\alpha = 1$ provides the well-known scheme for the forward approximation of the first-order derivative. Note that in the following text we refer to this approximation as the GL approximation.

As the sum in Eq. (6) indicates, the numerical approximation of the fractional derivative depends on all previous nodal values. Therefore, the number of values used for the approximation is not constant but increases in every subsequent step. This is different from approximating finite-order derivatives, where a constant number of nodal values is exploited. Also, when approximating the fractional derivative, each of the values is multiplied by the corresponding weight, which is different with every

subsequent step (the most actual value f^n is multiplied by weight w_0, the previous value f^{n-1} by weight w_1, etc.). This is the main disadvantage of using fractional derivatives in numerical calculations because computing the sum in Eq. (6) is requires more time and memory with each subsequent step. This complicates the use of fractional derivatives in large-scale problems.

Another possible approximation of the fractional derivative, introduced by Diethelm in [4] (referred to as the Diethelm approximation henceforth), is the approximation of the integral expression using the trapezoidal rule. This gives the following formula for the Caputo fractional derivative

$$D^\alpha f(\mathrm{n}\Delta t) \approx \frac{1}{(\Delta t)^\alpha \Gamma(2-\alpha)} \sum_{j=0}^{\mathrm{n}} a_{j,\mathrm{n}} f^{\mathrm{n}-j}, \tag{8}$$

where weights $a_{j,\mathrm{n}}$ are

$$a_{j,\mathrm{n}} = \begin{cases} 1, & \text{if } j = 0, \\ (j+1)^{1-\alpha} - 2j^{1-\alpha} + (j-1)^{1-\alpha}, & \text{if } 0 < j < \mathrm{n}, \\ (1-\alpha)\mathrm{n}^{-\alpha} - \mathrm{n}^{1-\alpha} + (\mathrm{n}-1)^{1-\alpha}, & \text{if } j = \mathrm{n}. \end{cases} \tag{9}$$

3.1 Numerical approximation of the springpot behavior

The numerical approximation of the fractional derivative given by Eq. (6) can be substituted into the constitutive law for the springpot element given by Eq. (1). The resulting expression can be then further adjusted considering $w_0(\alpha) = 1$ to get the following equation

$$\varepsilon^{n+1} = \frac{\sigma^n}{E} \left(\frac{\Delta t}{\tau_\mathrm{c}} \right)^\alpha - \sum_{j=1}^{\mathrm{n}} w_j(\alpha) \varepsilon^{n+1-j}, \tag{10}$$

which provides a numerical algorithm to compute the strain response of the springpot to the prescribed stress load. Similarly, an integrator based on the approximation (8) receives the form

$$\varepsilon^{n+1} = \frac{\sigma^n \Gamma(2-\alpha)}{E} \left(\frac{\Delta t}{\tau_\mathrm{c}} \right)^\alpha - \sum_{j=1}^{\mathrm{n}} a_{j,\mathrm{n}} \varepsilon^{\mathrm{n}+1-j}. \tag{11}$$

4 Reduced approximation of the fractional derivative

Both of the two numerical algorithms presented by Eqs. (10) and (11) include a sum of all previous strain nodal values, each of them multiplied by the corresponding weight. It was already mentioned that the computation of this sum has high requirements on memory and computing times. For this reason, neither of these two approximations seems to be suitable for use in large-scale numerical analyses. The objective thus

becomes to propose a potential modification to the original numerical schemes that reduces the computational and memory cost while maintaining sufficient accuracy.

To open this subject, first consider the approximation given by Eq. (10) with the weights computed according to Eq. (7). Focusing on the second term on the right-hand side of Eq. (10) we notice that the most actual nodal value is multiplied by the weight $w_0(\alpha) = 1$. The influence of older values is lower than that of the most recent ones, because the absolute value of the weights decreases with each following value. This phenomenon is shown in Fig. 1.

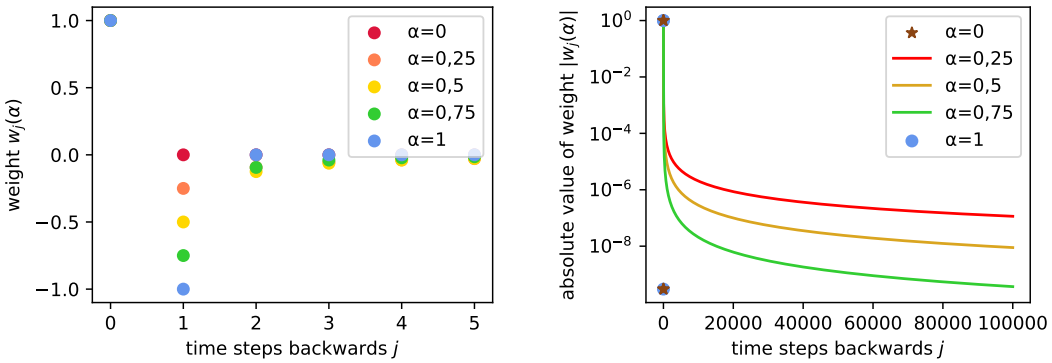

Figure 1: Weight function for different values of parameter α

Whether this observation can be exploited to adjust the available approximations is examined next. In particular, attention will be paid to the necessary number of m most recent values that should be kept in the approximation to maintain sufficient accuracy, provided the influence of older nodal values is reduced or totally neglected.

4.1 Suggested reduced approximations

Grounding on our extensive numerical study, we limit our attention to the three specific modifications denoted as:

- Simple cut method,
- Cut and average method,
- Bush cutting method.

Each method will be addressed in light of both the GL and Diethelm numerical schemes. The presented numerical simulations are limited to a simple creep test showing the variation of strain as a function of time due to the prescribed constant stress (Heaviside stress load) introduced at time $t = 0$. This simple loading case allows us to solve the response of the springpot analytically to be compared with the selected numerical approximations. The analytical solution has the following form

$$\varepsilon(t) = \sigma_0 \frac{1}{E\Gamma(\alpha+1)} \left(\frac{t}{\tau_c}\right)^{\alpha}, \tag{12}$$

where σ_0 denotes the prescribed value of the constant stress set equal to 1 hereinafter.

Simple cut method: This method simply reduces the number of adopted nodal values by keeping the contribution of the m most recent nodes only while totally neglecting the old ones.

Starting from the GL approximation, the original algorithm given by Eq. (10) applies to $n \leq m$, while for $n > m$ the algorithm is modified as

$$\varepsilon^{n+1} = \frac{\sigma^n}{E}\left(\frac{\Delta t}{\tau_c}\right)^{\alpha} - \sum_{j=1}^{\mathrm{m}} w_j(\alpha)\varepsilon^{n+1-j}. \tag{13}$$

The resulting response is shown in Fig. 2 for the selected number of nodal values m used in the approximation. The influence of the springpot parameter α is also examined. Recall that $\alpha = 0$ corresponds to a purely elastic response, whereas with increasing value $\alpha \to 1$ the behavior approaches a simple dashpot.

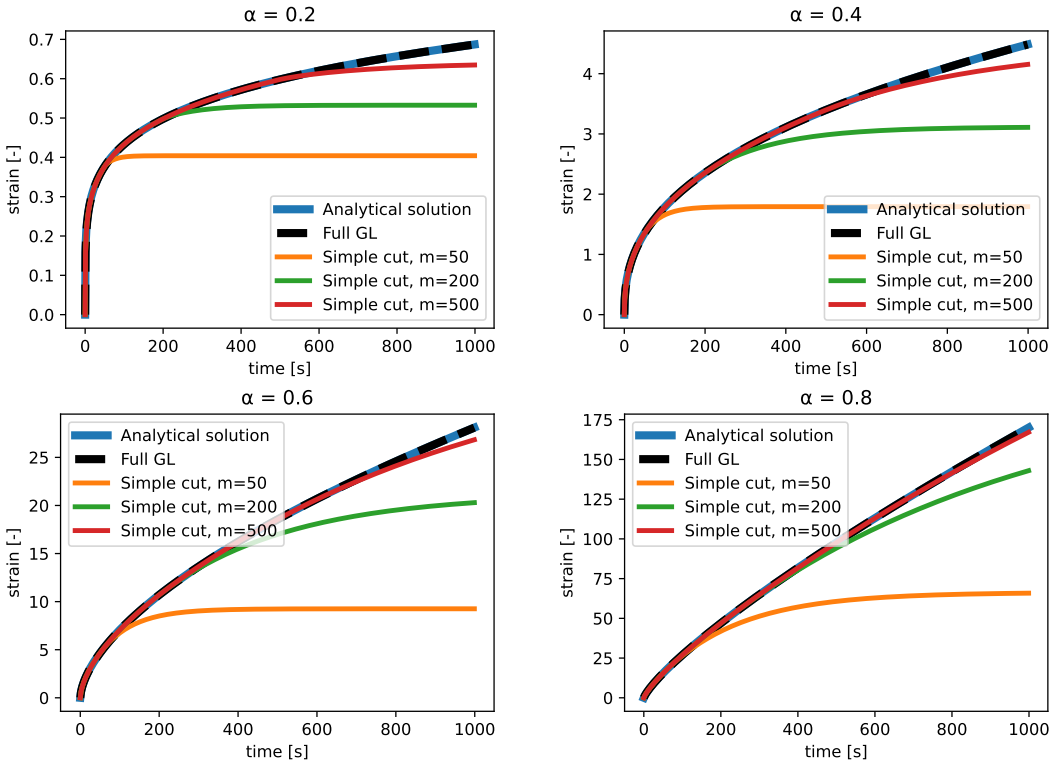

Figure 2: Simple cut method for the GL approximation

It is evident that the full GL approximation (black dashed line) that keeps all n nodal values matches the analytical solution (blue line) very well. As expected, the reduced approximation approaches the exact solution with increasing m. It is also seen that the closer the model is to the dashpot element, the less number of terms is needed to achieve a reasonable accuracy. For example, for $\alpha = 0.8$, it seems possible to reduce the number of values m to half of the total number of nodal values and still

get an approximation that meets the exact solution sufficiently. Unfortunately, this approximation cannot generally be accepted as sufficiently robust.

Similar conclusions can be drawn from the results presented in Fig. 3 attributed to the Diethelm method. In fact, the response generated by both methods is essentially identical. In other words, there is no obvious evidence that one method is superior to the other.

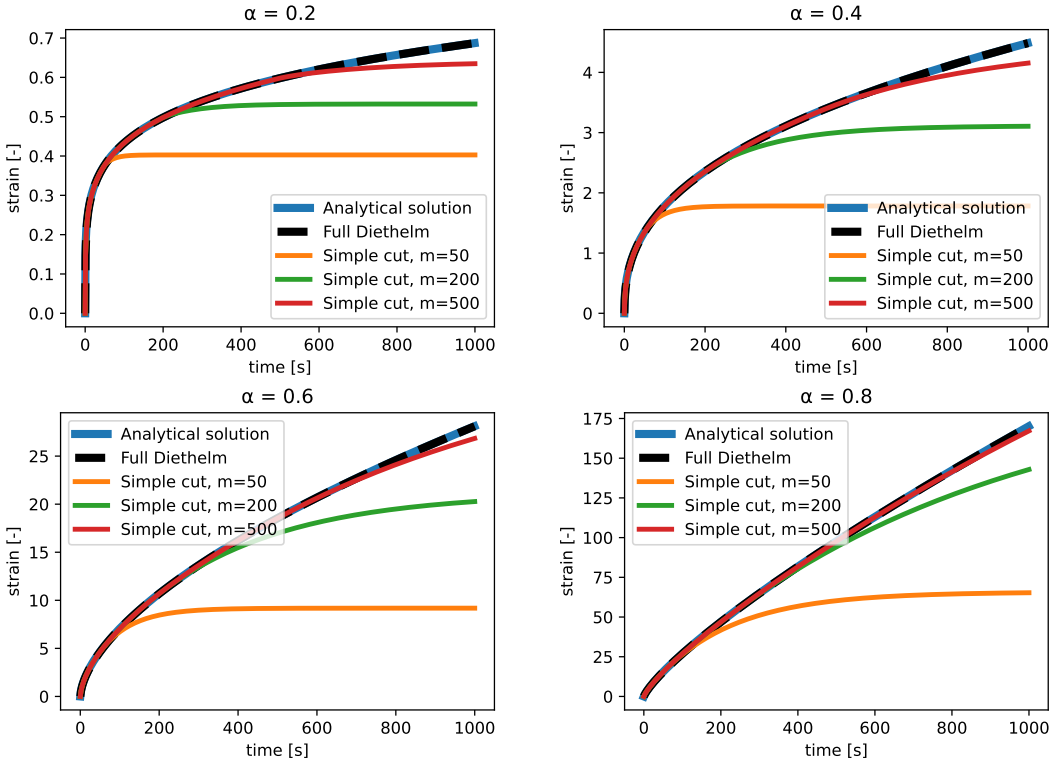

Figure 3: Simple cut method for the Diethelm approximation

Cut and average method: This second reduction method is based on the same idea of using m of the most actual nodal values, while to some extent exploiting the old ones. Here, it is proposed to account for the old values by their mean value which is multiplied by the sum of the remaining weights. Thus, similarly to the Simple cut method, the algorithm remains unchanged for $n \leq m$, whereas for $n > m$ it is adjusted as

$$\varepsilon^{n+1} = \frac{\sigma^n}{E}\left(\frac{\Delta t}{\tau_\varepsilon}\right)^\alpha - \sum_{j=1}^{\mathrm{m}} w_j(\alpha)\varepsilon^{n+1-j} - \frac{1}{n-m}\sum_{j=\mathrm{m}+1}^{\mathrm{n}} \varepsilon^{n+1-j} \sum_{j=\mathrm{m}+1}^{\mathrm{n}} w_j(\alpha). \quad (14)$$

The response is shown in Fig. 4 for the GL approximation and in Fig. 5 for the Diethelm approximation. Given the previous results, it is not surprising that both methods show identical performance. However, compared to the Simple cut method, the provided predictions are considerably improved. It is evident that considerably less

number of nodal values need to be adopted in order to arrive at reasonably accurate predictions. Even cutting the number of values of m down to 20% of the total number of steps still seems acceptable. Again, this also depends on the specific value of the parameter α.

Bush cutting method: The last method presented here was originally introduced by Macdonald in [5]. This method relies on gradually increasing the time step by ignoring some of the older nodal values.

The method is better understood from the graphical representation shown in Fig. 6. It is suggested that only the red steps are considered when computing the sum in Eqs. (10) and (11), while the gray steps are ignored. Clearly, m most recent steps, i.e. $t \in (n-m, m)$ are all adopted. For $t \in (n-m, n-p); p = 1.5m$ only each second step is considered, and for $t \in (n-p, q)$ only each fourth step is taken into account. The steps for $t \in (q, 0)$ (we considered 5 steps) at the beginning of the time row are considered as usual.

It has already been suggested in the Cut and average method that with some of the values skipped, the weights need to be adjusted accordingly. This is achieved by multiplying the weights corresponding to a given region by specific coefficients. To this end, three particular choices are explored. The first one assumes that all coefficients are equal to 1. The second approach assumes the value of the multiplying coefficient equal to 1 only in the interval $t \in (n, m)$, while in the $t \in (m, p)$ and $t \in (p, q)$ regions the weights are multiplied by 2 and 4, respectively. The third approach modifies the previous one by raising the value of individual coefficients to the power of α. The results are plotted in Fig. 7. For illustration, only one particular value of $\alpha = 0.4$ is considered together with the Diethelm method.

Although the method offers some potential in reducing the computational and memory cost, the predictions in Fig. 7 clearly identify an obvious drawback of this method, which is the numerical stability. Note that the sum of weights in both the GL and Diethelm approximations approaches zero when the number of time steps goes to infinity. In other words, the sum of all values preceding the current time step with $w_0 = 1$ will eventually attain a value minus one. It has been confirmed for both the Simple cut and Cut and average methods that maintaining this condition generates stable solutions. Comparable behavior has also been observed for the Bush cutting method Fig. 7 when the multiplying coefficients are kept equal to 1. However, similarly to previous methods, the Bush cutting method underestimates the response for an insufficiently large value of m. On the other hand, with other choices of multiplying coefficients, an instability can occur, which is clearly evident for the case of $m = 50$ and coef = [1,2,4]. This is because the application of multiplying coefficients $2, 4$ and $2^\alpha, 4^\alpha$ causes the sum of weights to exceed 1 over time, which in turn is manifested by an exponential growth of strain over time. This method should therefore be approached with caution.

Thus, instead of using some ad hoc coefficients to multiply the weights corresponding to regions with reduced time steps, it appears more appropriate to use weights that maintain stability, i.e., their sum does not exceed the value -1. To this end, we pro-

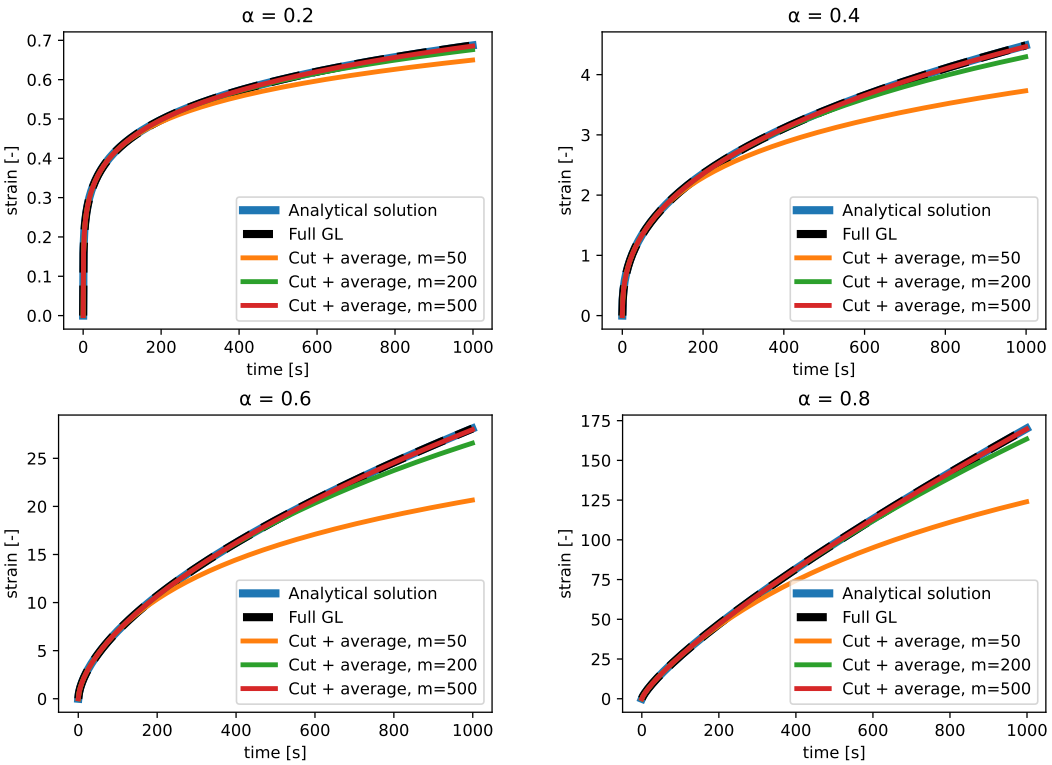

Figure 4: Cut and average method for the GL approximation

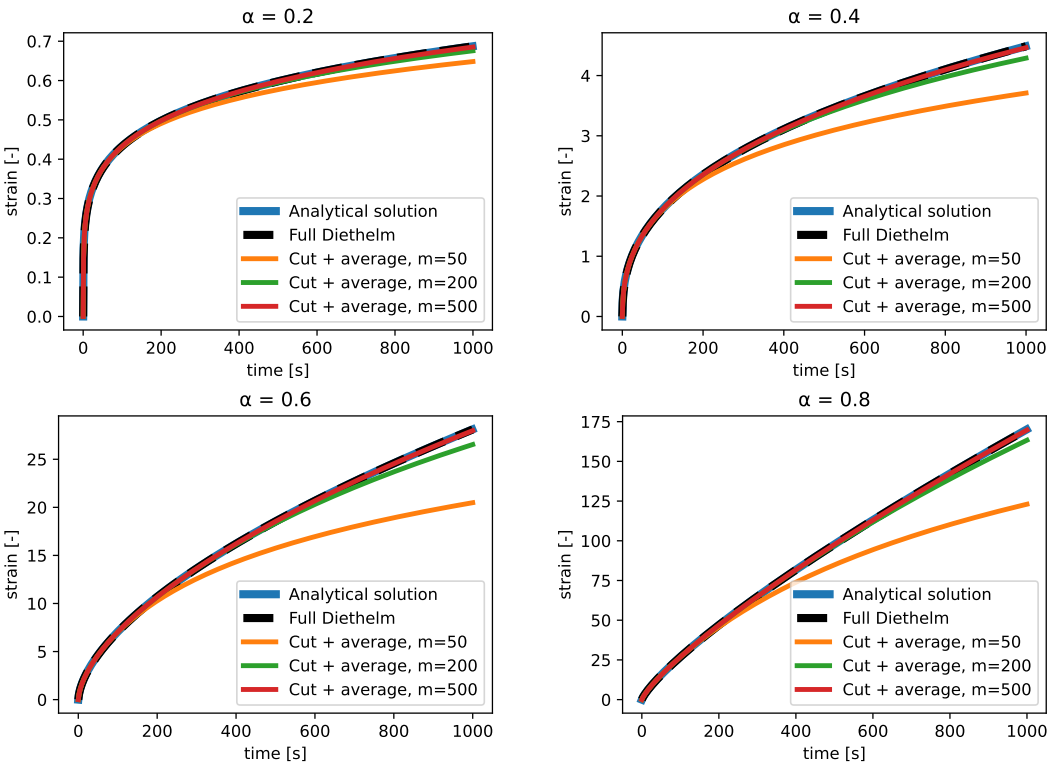

Figure 5: Cut and average method for the Diethelm approximation

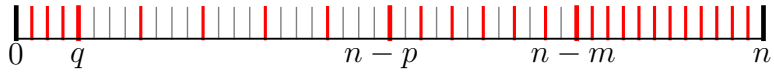

Figure 6: Numerical scheme for the step-skipping algorithm

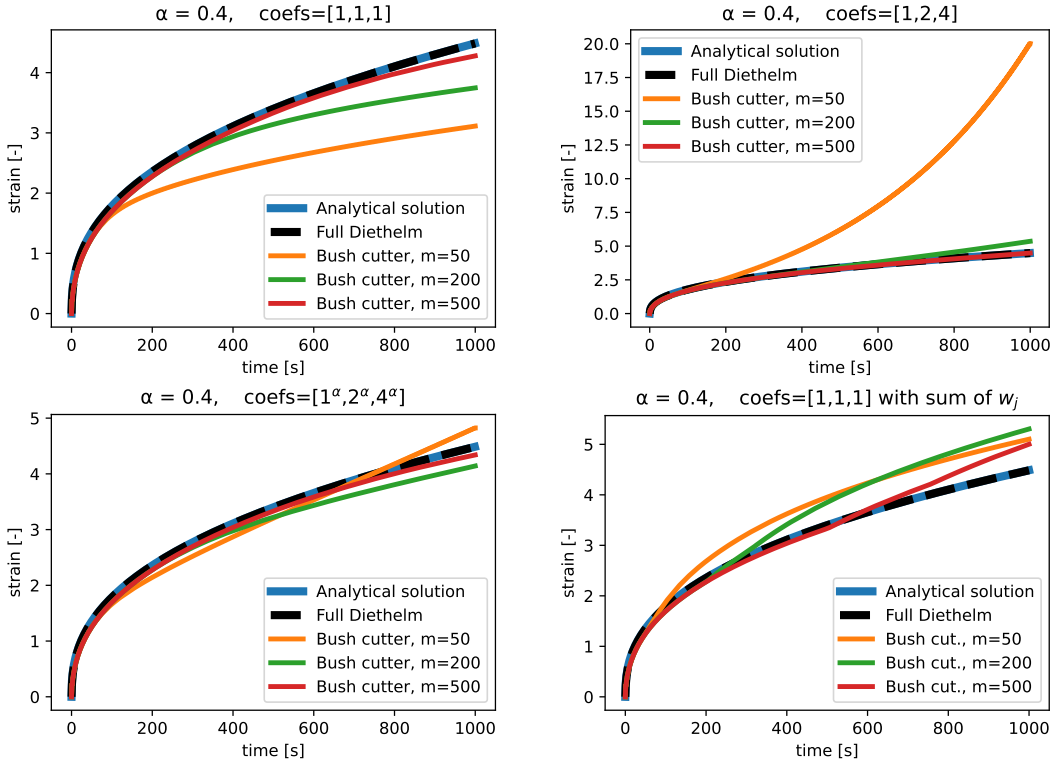

Figure 7: Bush cutting method for the Diethelm approximation – different multiplying coefficients

pose setting the value of the weight pertinent to a given interval of skipped time steps to the sum of some of the weights associated with these skipped values. For example, if we jump from the strain value ε^{n+1-i} to ε^{n+5-i}, thus skipping the time steps from $n+1-i$ to $n+5-i$, then the appropriate weight to multiply the strain ε^{n+5-i} will be set to $w_i + w_{i+1} + w_{i+2} + w_{i+3}$.

The corresponding response, termed Bush cutting and sum from now on, is compared first in Fig. 7 with the predictions attributed to the original format of the Bush cutting method. The influence of the parameter α is further examined in Figs. 8 and 9 to address again both types of approximation of the fractional derivative. As before, both approximations perform analogously. In addition, we see that the proposed approach does not qualitatively change the response and does not show instability and a transition to exponential growth. On the other hand, an apparent deviation from the exact solution occurs once we start to skip some old strains at a certain time. This is something one would expect because the strain value multiplying the sum of weights is, in this particular example of a simple creep, greater than the strain values associated with individual weight in the sum. Nevertheless, the solution still qualitatively

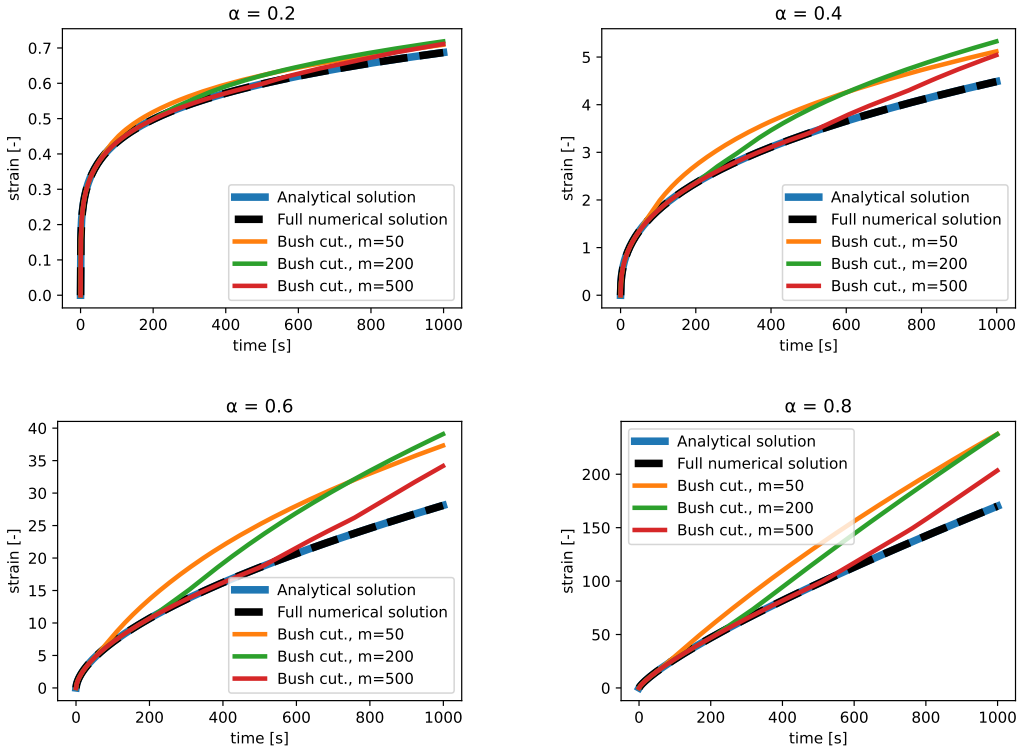

Figure 8: Bush cutting and sum method for the GL approximation

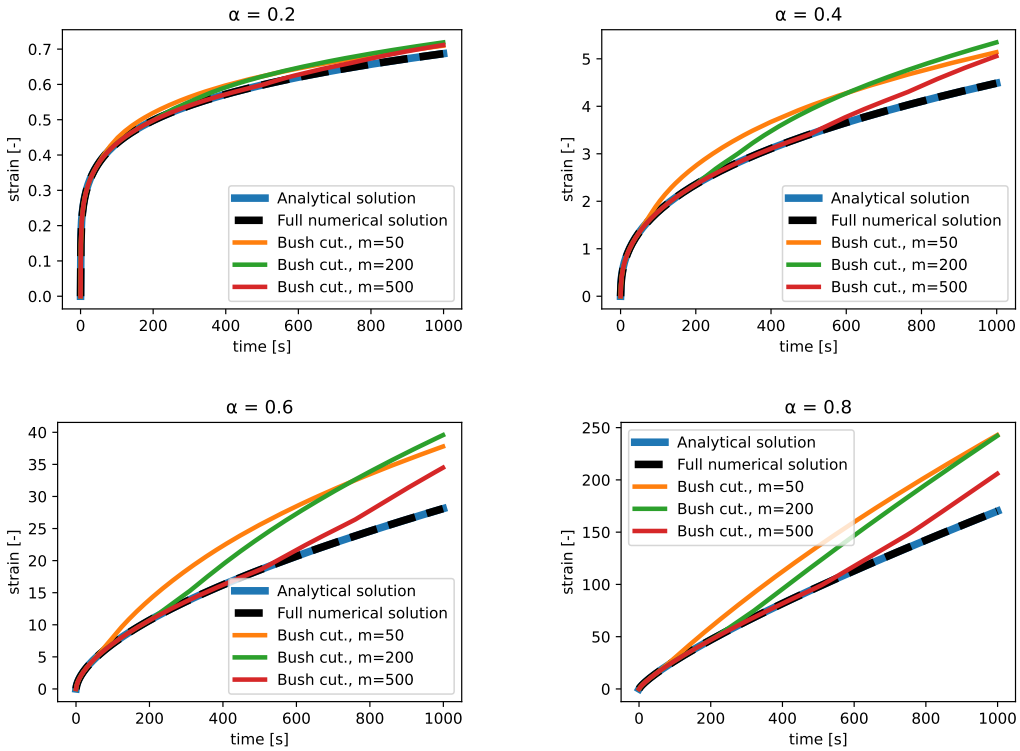

Figure 9: Bush cutting and sum method for the Diethelm approximation

preserves the actual response even in long times. For example, for the GL approximation for $\alpha = 0.6$ with $m = 50$, the response has lower accuracy, but the stability of the method is not compromised. The qualitative shape of the diagram is preserved.

A potential remedy is seen in the combination of the Bush cutting method with the Cut and average method applied within larger time steps. However, this approach is still under investigation.

5 Conclusions

Fractional calculus provides a strong tool for describing viscoelastic materials. For simple models and simple loading cases, the response can be solved analytically. However, if the fractional differential equation that describes the problem is too complex, the analytical solution cannot be obtained. Instead, a numerical algorithm is needed. In comparison to standard derivatives of integer order, the numerical approximations of the fractional derivative are based on nodal values obtained in all previous time steps. Since each of the values has a different weight in every subsequent step, the computation becomes significantly time- and memory-consuming.

This paper presents two possible approximations of the fractional derivative. For both of them, several possible modifications are presented. These modifications aim to reduce the number of values used in the approximation. From the presented options, the Cut and average and the Bush cutting and sum methods seem to be applicable as sufficient accuracy is maintained while the number of values included in the calculation could be significantly reduced.

However, neither of these two methods can fully comply with the analytical solution of the examined simple creep problem. Intuitively, a potential method of attack appears in their combination. However, this needs further study. The same applies to more complex models and loads.

Acknowledgements

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