Computational Materials Science 98 (2015) 287–296

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Comparison of approaches to model viscoelasticity based on fractional time derivatives

C. Zopf, S.E. Hoque, M. Kaliske *

Institute for Structural Analysis, Technische Universität Dresden, 01062 Dresden, Germany

ARTICLE INFO

Article history:
Received 8 July 2014
Received in revised form 5 November 2014
Accepted 8 November 2014

Keywords:
Inelastic material formulation
Fractional time derivative
Finite element simulation
Finite strains
Recursive formulation

ABSTRACT

Two approaches to describe a constitutive fractional Zener model at large strain are presented. Both viscoelastic Zener models consist of a nonlinear elastic spring and a fractional Maxwell element in parallel. The fractional Maxwell element represents the viscoelastic behaviour of the formulation. Here, development of a new fractional viscoelastic material model under consideration of finite strain theory is presented. Additionally, the constitutive equations based on two different algorithmic approaches to capture the fractional time integration within this material model are derived. The consideration of fractional elements enables the characterization of highly inelastic, time dependent materials with relatively few material parameters. For the fractional element, a material parameter α determines the transition of the rheological element's behaviour between spring ($\alpha = 0$) and dashpot ($\alpha = 1$). Accuracy and efficiency of a classical (non-recursive) and a new recursive algorithm to handle the fractional elements have been verified and validated by the comparison of several finite element (FE) simulations to material test results. The simulations found on finite strains and an implicit time integration scheme. Finally, a FE moulding simulation, found the extended constitutive model for the explicit time integration scheme has been carried out to illustrate the performance for large scale simulations in comparison to a real forming process and found to be quite efficient.

1. Introduction

The field of fractional calculus, which is devoted to the study and application of derivatives and integrals of arbitrary order (real or complex), can be dated back to 1695 when de L'Hospital and Leibniz were debating whether it make sense to define an operator d^n/dt^n for $n = 1/2$ [1].

Numerical methods [2–6] for the solution of fractional differential equations (FDEs) are of large importance because of their numerous fields of applications, e.g. electrochemical processes [7,8], dielectric polarization [9], coloured noise [10], chaos [11], bioengineering [12–14], to construct a transient probability density of non-linear systems [15] and others. Classical solution methods, proposed by e.g. Koh and Kelly [16], Zhang and Shimizu [17], Ruge and Wagner [18], Shokooh and Suarez [19], Trinks and Ruge [20], require large computational resources. Therefore, interest has grown to develop stable and efficient numerical techniques for the computation of FDEs (linear and nonlinear). A non-classical method for the numerical solution of FDE order $0 < \alpha \leq 1$ has been proposed by Yuan and Agrawal [21] (YA algorithm) which has been extended to $1 < \alpha \leq 2$ by Trinks and Ruge [20]. Diethelm revealed the reason of the slow convergence rate of the YA algorithm and proposed modifications which led to an improved performance [22,23]. A further modification has been suggested by Birk and Song [24] which overcomes the shortcomings of the YA algorithm and Diethelm's modified method.

In theory of viscoelasticity, fractional calculus has been used for several years to characterise complex phenomenological behaviour with less material parameters. Although the approaches are based on phenomenological observations, Bagley and Torvik [25,26] have shown that fractional calculus can be used to represent the mechanical behaviour in molecular theories. The same authors [27,28] as well as Koeller [29] made some fundamental contributions to the modelling of viscoelasticity using fractional calculus. Some further work on the application of fractional calculus in theory of viscoelasticity has been presented in [30–33]. In the last years, two articles dealing with fractional viscoelastic material models were published. Di Paola et al. [34] proposed a fractional relaxation and creep function for the description for linear viscoelastic behaviour. They showed the derivation of the fractional description by Laplace transformation and presented some analytical comparison to test results. This approach was extended by Di Paola et al. [35] to the analytical description of the behaviour

* Corresponding author.
E-mail address: michael.kaliske@tu-dresden.de (M. Kaliske).

http://dx.doi.org/10.1016/j.commatsci.2014.11.012
0927-0256/

of a Bernoulli beam. Furthermore, his group (Di Paola et al. [36] proposes a discretization scheme which bases on continuous mechanical models of fractional derivatives. This scheme is useful to obtain a mechanical description of fractional derivatives.

Polymeric and rubber-like materials are often subjected to large deformations in engineering applications which necessitates the development of nonlinear models for more precise analysis and design. Only very few articles Sjoeberg [37], Adolfsson and Enelund [38], Adolfsson [39], Lion and Kardelky [40], Sjoeberg [37], Müller et al. [41], Zopf and Kaliske [42], Müller et al. [43], Wollscheid and Lion [44] have been published on the application of fractional order operators in finite strain viscoelasticity. In this article, two fractional element based algorithms for viscoelastic material models are presented and compared. For both approaches, the symbolic rheology underneath is a fractional Zener model (see Fig. 1) and both consider large strain theory. Ala et al. [45] compared the behaviour of rheological elements which base on differential equations to electrical circuits. The derivation of the Zener model is following the derivation of the viscoelastic material model of Dal and Kaliske [46]. Another viscoelastic material formulation, presented by Boyce et al. [47], considers e.g. large strain theory, crystallisation and hardening. Pouriayevali et al. [48], Ayoub et al. [49] published similar approaches based on hyperelasticity with viscous behaviour and showed the ability to represent the real material behaviour of a wide range of rubber compounds under high rates.

Simply, the basic formulation shown subsequently could be expanded to a generalized fractional Maxwell model. The difference between the two approaches is the algorithmic computation of the fractional time derivative. For the first formulation, a classical treatment is used. Here, the authors follow the derivation of Schmidt and Gaul [50] in order to compute the fractional time derivative. Their material formulation is expanded in this article due to the fact that the small strain theory used by them is not permissible for the description of uncured rubber compounds which will be modelled in here. This classical approach requires the storage of the whole material history and, therefore, is quite storage and time consuming. Based on these findings, the authors developed a nonlinear large strain fractional derivative based constitutive description and derived the accompanying new algorithmic formulation by adapting the recursive algorithm for fractional derivatives of Birk and Song [24]. This derivation yields a more efficient algorithm and enables complex simulations.

2. Numerical computation of fractional time derivatives

In this section, the basic equations of the computation of fractional time derivatives of a function $z(t)$ are given for the classical Schmidt and Gaul [50] and for the new recursive approach (Birk and Song [24]). The operator $D_t^{\alpha}\{z(t)\}$ denotes a fractional time derivative of a function $z(t)$ of the order α.

2.1. Classical formulation of fractional derivatives

Different definitions of fractional derivatives are available. Among them, the Grünwald definition Grünwald [51], Schmidt and Gaul [52] involves the fewest restrictions on the functions to which it is applied and can be implemented into numerical algorithms in a practical way. Hence, the approach is used for the computational solution of fractional time derivatives. The shown derivation will be close to the publication of Schmidt and Gaul [50], where the general formula of a fractional derivative of integer order n is defined as

$$D_t^n\{z(t)\} = \frac{d^n z(t)}{dt^n} = \lim_{\Delta t \to 0}\left[(\Delta t)^{-n}\sum_{j=0}^{N}(-1)^j\binom{n}{j}z(t-j\Delta t)\right] \tag{1}$$

in dependency on the binomial coefficient (compare Oldham and Spanier [2]), which is defined by n and j. The product of the binomial coefficient and $(-1)^j$ can be expressed as

$$(-1)^j\binom{n}{j} = \binom{j-n-1}{j} \equiv \frac{\Gamma(j-n)}{\Gamma(-n)\Gamma(j+1)} =: GL_{j+1}(n), \tag{2}$$

in dependency on the gamma function Γ and the integer number j, which is also known as the Grünwald definition. If n is replaced by any real number α and the time step Δt by the ratio t/N, Eqs. (1) and (2) lead to

$$\frac{d^{\alpha}z(t)}{dt^{\alpha}} = \lim_{N\to\infty}\left[\left(\frac{t}{N}\right)^{-\alpha}\sum_{j=0}^{N-1}GL_{j+1}(\alpha)z\left(t-j\frac{t}{N}\right)\right]. \tag{3}$$

This equation represents the numerical solution of a real order time derivative, which is given as a series expansion. The numerical solution requires storage of the history for each time increment of the function z from time $t=0$ up to the current time t.

2.2. Recursive formulation of fractional derivatives

The approach presented in this section follows the description of Birk and Song [24]. As a starting point the definition of the fractional time derivative

$$D_t^{\alpha}\{z(t)\} = \frac{1}{\Gamma(\lceil\alpha\rceil-\alpha)}\int_0^t \frac{d^{\lceil\alpha\rceil}\{z(\tau)\}}{d\tau^{\lceil\alpha\rceil}}\frac{1}{(t-\tau)^{1+\alpha-\lceil\alpha\rceil}}d\tau, \tag{4}$$

explored by Diethelm [22], is given. The floor function $\lfloor\alpha\rfloor$ rounds down the argument α to the nearest integer and the ceiling function $\lceil\alpha\rceil$ rounds up the argument α to the following integer. These two functions are basic operations of this approach (e.g. in Eq. (4)). For the computation of the fractional derivative, a transformation into the frequency domain

$$\mathcal{F}\left\{D_t^{\alpha}z(t)\right\} = (i\omega)^{\alpha}Z(\omega) \tag{5}$$

is proposed. Here, a Fourier transformation is used and the power term $(i\omega)^{\alpha}$ results in

$$(i\omega)^{\alpha} = 2(-1)^{\lfloor\alpha\rfloor}\frac{\sin\pi\alpha}{\pi}\underbrace{\int_0^{\infty}\frac{(i\omega)^{\lceil\alpha\rceil}}{i\omega+p^2}p^{\bar{\alpha}}dp}_{I}, \tag{6}$$

where $\bar{\alpha} = 2\alpha - 2\lceil\alpha\rceil + 1$. The integral I of Eq. (6) is solved by a numerical approximation scheme. Therefore, the following substitutions

$$p = \frac{(1-\bar{q})^2}{(1+\bar{q})^2}, \quad \bar{q} = \frac{1-\sqrt{p}}{1+\sqrt{p}}, \quad \frac{dp}{d\bar{q}} = -4\frac{(1-\bar{q})}{(1+\bar{q})^3} \tag{7}$$

have been used in order to transform the limits of the integral I from $[0,\infty]$ to $[-1,1]$ yielding

$$I = (i\omega)^{\lceil\alpha\rceil}\int_{-1}^{+1}\frac{4(1-\bar{q})^{2\bar{\alpha}+1}(1+\bar{q})^{-(2\bar{\alpha}-1)}}{(1+\bar{q})^4\left(i\omega+\frac{(1-\bar{q})^4}{(1+\bar{q})^4}\right)}d\bar{q}. \tag{8}$$

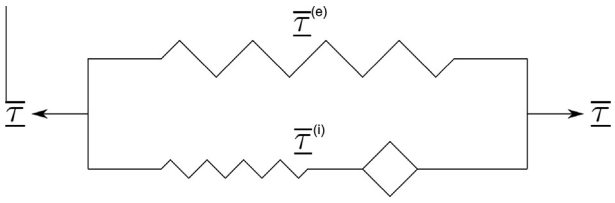

Fig. 1. Rheology of fractional Zener model.