

# A numerical assessment of the free energy function for fractional-order relaxation

Andrea Burlon\*, Francesco P. Pinnola\*, Massimiliano Zingales\*<sup>†</sup>

\*Università degli Studi di Palermo - DICAM, Viale delle Scienze Ed.8, I-90128 Palermo, Italy  
a.burlon91@gmail.com, francesco.pinnola@unipa.it, massimiliano.zingales@unipa.it

<sup>†</sup>Laboratory of Biomechanics and Nanomechanics in Medical Sciences,  
Mediterranean Center of Human Health and Advanced Biotechnologies, Viale delle Scienze Ed. 18, I-90128, Palermo, Italy

**Abstract**—In this paper the authors discuss the free energy function of fractional hereditary materials. The evaluation of the free energy has been obtained from a mechanical model that represents, exactly, the power-law relaxation of the material. The mechanical model separates, exactly, the elastic and the viscous phases, yielding the stored energy of the material that corresponds to the Staverman-Schwarz stress based free energy. Some numerical approximations of the free energy function in terms of the discretized rheological model have been reported in the paper.

## I. INTRODUCTION

Many materials applied in various fields of engineering have a viscoelastic mechanical behavior well described by fractional laws [1]–[5]. Such materials involve fractional integration and/or derivation operators in the stress-strain relation because the creep/relaxation laws are of power-law type. These power-law creep/relaxation functions do not have a unique definition of free energy function. The aim of this article is the study of fractional hereditary materials from a thermodynamic point of view to find the correct definition of free energy of fractional hereditariness. There are various definitions of the free energy functional of hereditary systems based on relaxation stress measures. Indeed the evaluation at time  $t$  of the free energy based on measures of the applied stress/strain involves additional integration term depending upon the entire deformation (stress) histories for  $\tau \leq t$  [6]–[10]. However the definition of the free energy for an isothermal transform is unique as  $\dot{\psi}(t) = \dot{w}_{ext}(t) - D(t)$ , where  $w_{ext}(t)$  is the specific external power of the applied load and  $D(t)$  is the material dissipation rate due to irreversible thermodynamics transformation (entropy increments). It is known that for a simple Maxwell and Kelvin-Voigt material models the evolution of  $\dot{\psi}(t)$  is unique and it coincides with the elastic power stored in spring. In this prospective the power-law relaxation possesses an equivalent mechanical model made of elastic springs and viscous dashpots [11]–[13]. This model has been shown to yield the extension of the free energy in an unique form that coincides with the well-known Staverman-Schwarz free energy [14].

In this paper we will show that up to a specified time  $\bar{t}$  an appropriate approximation of the mechanical model may yield the correct value of the free energy with sufficient accuracy.

## II. FRACTIONAL CALCULUS

The fractional calculus is the natural extension of ordinary differential calculus. In fact, it extends the concepts of derivation and integration to non-integer and complex order. The fractional calculus was born in the 1695 when *G. W. Leibniz* introduced the half derivate concept in a note to *G. de l'Hôpital* [11]. Subsequent studies have focused by different mathematicians [12]: *J. B. J. Fourier*, *P. S. Laplace*, *L. Euler*, *S. F. Lacorix*, *N. H. Abel*, ect. The first definition of fractional operator is probably attributable to *J. Liouville*, who in 1832 gave the impulse to research by formulating the definition of fractional derivative of exponential function. In 1847, an important contribution was given by *G. F. B. Riemann*, who introduced their own definition of fractional integral. Following, *N. Ya. Sonin* unified formulations of Liouville and Riemann from multiple Cauchy integration formula [12], obtaining the following expression of fractional integral:

$$\left( I_{a+}^{\beta} f \right) (t) = \frac{d^{-\beta} f(t)}{d(t-a)^{-\beta}} = \frac{1}{\Gamma(\beta)} \int_a^t (t-\tau)^{\beta-1} f(\tau) d\tau \quad (1)$$

where  $\Gamma(\cdot)$  is the Euler-Gamma function, Eq. (1) is known in literature as a *fractional integral of Riemann-Liouville*, since  $\Re(\beta) > 0$ , and it is valid for  $\beta \in \mathbb{C}$ .

To obtain the *Riemann-Liouville fractional derivative* just think that the derivative of order  $n$  can be considered as the derivative of order  $n+m$  of the  $m^{th}$  primitive function, and then generalizing, we have:

$$\left( D_{a+}^{\beta} f \right) (t) = \frac{1}{\Gamma(n-\beta)} \left( \frac{d}{dt} \right)^n \int_a^t \frac{f(\tau)}{(t-\tau)^{\beta-n+1}} d\tau \quad (2)$$

valid for  $(n-1) < \Re(\beta) < n$ .

Another definition of fractional integro-differential operator was provided in 1967 by *M. Caputo* [15]. This definition is easier to handle for the solution of physical problems. The *Caputo fractional derivative* has the following expression:

$$\left( {}_C D_{a+}^{\beta} f \right) (t) = \frac{1}{\Gamma(n-\beta)} \int_a^t \frac{f^{(n)}(\tau)}{(t-\tau)^{\beta+1-n}} d\tau \quad (3)$$

the Eq. (3) is valid for  $(n-1) < \beta < n$ . The expression obtained is the result of an interpolation between the integer order derivatives, in fact, for  $\beta \rightarrow n$ , the expression becomes an  $n^{th}$  derivative of  $f(t)$ . It can be observed that the expressions (3) and (2) coincide if we start from initial conditions zero ( $f(a) = 0$ ).

Others definitions of fractional operators exist but are not reported for brevity sakes. For in-depth studies look at previous cited books and [16]–[21].

### III. POWER-LAWS RELAXATION: THE FREE ENERGY

In the subsequent derivations we recall that two hypotheses are considered while analyzing viscoelastic materials: *i*) invariance under time translation and *ii*) causality. With the first requirement we mean that time shift in the input is reflected as a same shift in the output; with the second we mean that the material response depends on previous histories only, reflecting hereditariness of such materials. The discussion about the power-law relaxation (creep) function in integral material hereditariness is reported in this section with regards to the issues: *i*) *Power-law relaxation (creep) functions* yielding the constitutive relations among the stress measure and the strain measure in terms of fractional-order operators. *ii*) *The free energy function of FHM* that represent a scalar measure of the stored material energy.

The section is devoted to the introduction of power-law relaxation/creep functions and their relations with fractional-order derivatives and integrals (sec. II). The definition of the material free energy and its relation with the stress measure is discussed in sec. III-B.

#### A. Power-law relaxation (creep) function : Fractional-order calculus

Let us assume, in this section, to deal with *virgin* materials, namely either the strain or the stress are known from the very beginning of the observation of their behavior, conventionally set at  $t = 0$ , and hence no past histories with respect to such a time need to be taken into account.

Creep and relaxation tests are performed to detect material hereditariness: in the first case, the stress is held constant and the strain is measured, whereas in the second one the strain is held constant and the stress is measured. Whenever either a unit stress or a unit strain is utilized, the creep compliance  $J(t)$  and relaxation modulus  $G(t)$  are found as the strain and stress response to the imposed unit stress and strain respectively, i.e.

$$\begin{aligned} \epsilon(t) = U(t) &\longrightarrow \sigma(t) = G(t) \\ \sigma(t) = U(t) &\longrightarrow \epsilon(t) = J(t) \end{aligned} \quad (4)$$

where  $U(\cdot)$  is the unit Heaviside step function. When either the creep or the relaxation function is known, the Boltzmann superposition principle allows for writing convolution-type Riemann-Stieltjes integrals to express the relationships between  $\sigma$  and  $\epsilon$ . Whenever either the strain or the stress are prescribed, the constitutive relations for the corresponding derived quantities read as follows:

$$\sigma(t) = \int_{0+}^t G(t-\tau) d\epsilon(\tau), \quad (5a)$$

$$\epsilon(t) = \int_{0+}^t J(t-\tau) d\sigma(\tau). \quad (5b)$$

Creep compliance and relaxation modulus are not independent. Indeed they are linked to each other by the relationship

$$\hat{J}_+(\omega) \hat{G}_+(\omega) = \frac{1}{(i\omega)^2}, \quad (6)$$

where the symbol  $\hat{\cdot}$  denotes the right-sided Fourier transform.

Experiments on polymeric materials performed [1]–[5] showed that their relaxation function is well fitted by power-laws, i.e.

$$G(t) = \frac{C_\beta}{\Gamma(1-\beta)} t^{-\beta}, \quad (7)$$

where  $C_\beta$  and  $\beta$  are characteristic constants of the material. The exponent  $\beta$  must be enclosed in the range  $0 < \beta < 1$  because of thermodynamics restrictions [22]. At the extrema of the range, asymptotic behaviors are obtained:  $\beta \rightarrow 0$  corresponds to purely elastic solid whereas  $\beta \rightarrow 1$  to purely viscous fluid. The values of  $0 < \beta < 1$  correspond to an intermediate behavior between elastic solid and viscous fluid, allowing for describing both complex-structured materials and soft matter. As we expect, the creep compliance of the given material can be determined through (6) from the relaxation modulus assumed in (7). Furthermore, the right Fourier transform of the relaxation function (7) yields

$$\hat{G}_+(\omega) = C_\beta (i\omega)^{\beta-1}, \quad (8)$$

that may be replaced in (6) yielding, after inverse transform:

$$J(t) = \frac{1}{C_\beta \Gamma(1+\beta)} t^\beta. \quad (9)$$

The constitutive equations of fractional hereditary materials may be obtained with the substitution of (7) and (9) into Boltzmann integrals in (5) yielding:

$$\sigma(t) = \frac{C_\beta}{\Gamma(1-\beta)} \int_{0+}^t \frac{\dot{\epsilon}(\tau)}{(t-\tau)^\beta} d\tau = C_\beta \left( {}_C D_{0+}^\beta \epsilon \right) (t) \quad (10a)$$

$$\epsilon(t) = \frac{(C_\beta)^{-1}}{\Gamma(1+\beta)} \int_{0+}^t (t-\tau)^\beta \dot{\sigma}(\tau) d\tau = \frac{1}{C_\beta} \left( I_{0+}^\beta \sigma \right) (t) \quad (10b)$$

that represents the constitutive relations in terms of fractional-order integrals and derivatives defined in the positive real axis  $[0, \infty[$ . In Eq. (10) the terms  $\left( {}_C D_{0+}^\beta \epsilon \right) (t)$  and  $\left( I_{0+}^\beta \sigma \right) (t)$  so-called Caputo's fractional derivative and Riemann-Liouville fractional integrals, respectively (see sec. II). We conclude that as soon as the creep and/or the relaxation function is assumed to be a power-law type, then the constitutive laws involves fractional operators. The constitutive equations in terms of fractional-order calculus assume, that the considered material is at rest for  $t = 0$  as the initial value a condition that is seldom available in engineering and physical applications. It has been shown in previous paper that the presence of an history of strain/stress undergone by the material up to the time instant  $\bar{t}$ , that is the initial time of the strain/stress process must be included in the constitutive equations to provide accurate estimations of the decaying and the force coefficients of the material, namely  $\beta$  and  $C_\beta$ .

#### B. The free energy functionals of FHM

The specific Helmholtz free energy  $\psi(\epsilon, \epsilon^t, T)$  with  $T$  the absolute temperature is, by definition, a thermodynamic state function whose gradient, with respect to the actual value of the deformation  $\epsilon$  yields the measured stress. Rate of increments of the material free energy is expressed in terms of the rate of increments of the specific internal energy  $\dot{u}$  and of the entropy production as:

$$\dot{\psi} := \dot{u} - T \dot{s} \quad (11)$$

where  $\dot{s}$  is the specific entropy production rate that must satisfy the thermodynamic restriction provided by the second principle of thermodynamics  $\dot{s} \geq \dot{q}/T$ , where  $\dot{q}$  is the rate of change of the specific thermal energy. The rate of change of the internal energy function is related to the specific mechanical work done on the system and to the thermal energy exchange as (first principle of thermodynamics)  $\dot{u} = \dot{w}_{ext} + \dot{q}$ . The free energy function in Eq. (11) may be reverted in a more explicit form as we introduce the entropy production rate due to irreversible transformations, namely  $\dot{s}^{(i)} \geq 0$  so that the second principle of thermodynamics may be written as:  $\dot{s} = \dot{q}/T + \dot{s}^{(i)}$  yielding, upon substitution in the expression of the free energy in Eq. (11)

$$\dot{\psi} = \dot{w}_{ext} - T\dot{s}^{(i)} = \dot{w}_{ext}(t) - D(t) \quad (12)$$

where we used the balance equation of the first principle and we introduced the specific dissipation rate  $D(t) = T\dot{s}^{(i)} \geq 0$  due to irreversible thermodynamical transformations in the material.

The free energy function  $\psi$  for simple hereditary material is function of the actual value of the strain and of the past history undergone by the material  $\psi(\epsilon(t), \epsilon^t(\tau))$  where  $\epsilon^t(\tau) = \epsilon(t - \tau)$  and  $\tau \leq t$  assuming isothermal processes. Under the assumption of linear hereditary behavior the stress value  $\sigma(t)$  at time instant  $t$  is provided by the Boltzmann-Volterra integral as reported in the first equality of Eq. (10). A general expression of the free energy functional explicitly dependent on the actual value of the strain as well as on the strain histories as:

$$\psi(\epsilon(t), \epsilon^t(\tau)) = \frac{1}{2}G(0)\epsilon(t)^2 + \epsilon(t) \int_0^\infty \dot{G}(\tau)\epsilon^t(\tau)d\tau + R(\epsilon^t(\tau)) \quad (13)$$

with  $R(\epsilon^t(\tau))$  an integration term, that must be a functional of the strain histories only. The presence of the functional  $R(\epsilon^t(\tau))$  is a source of indeterminacy for the free energy function that may be removed as a specific form for  $\psi(t)$  have been selected. In the following we refer to a specific functional class of the free energy in Eq. (13), assuming a linear material behavior yielding a quadratic functional of the strain measures for the free energy  $\psi(t)$  as [6]:

$$\psi_{ss}(t) = \frac{1}{2} \int_{-\infty}^t \int_{-\infty}^t G(2t - \tau_1 - \tau_2) \dot{\epsilon}(\tau_1) \dot{\epsilon}(\tau_2) d\tau_1 d\tau_2 \quad (14)$$

The observation of the energy rate reported in Eq. (12) shows that the dissipation rate associated to the free energy in Eq. (14) reads:

$$D(t) = -\frac{1}{2} \int_{-\infty}^t \int_{-\infty}^t \dot{G}(2t - \tau_1 - \tau_2) \dot{\epsilon}(\tau_1) \dot{\epsilon}(\tau_2) d\tau_1 d\tau_2 \quad (15)$$

that is a quadratic form of the strain histories with measure provided by the relaxation function  $G(t)$ . The explicit expressions of the free energy  $\psi(t)$  and of the dissipation rate of  $D(t)$ , in eqs.(14, 15) for the power-law relaxation function is

obtained as:

$$\begin{aligned} \psi_{ss}(t) &= \frac{C_\beta}{2\Gamma(1-\beta)} \int_{-\infty}^t \int_{-\infty}^t (2t - \tau_1 - \tau_2)^{-\beta} \dot{\epsilon}(\tau_1) \dot{\epsilon}(\tau_2) d\tau_1 d\tau_2 \\ D(t) &= \frac{\beta C_\beta}{2\Gamma(1-\beta)} \int_{-\infty}^t \int_{-\infty}^t (2t - \tau_1 - \tau_2)^{-1-\beta} \dot{\epsilon}(\tau_1) \dot{\epsilon}(\tau_2) d\tau_1 d\tau_2 \end{aligned} \quad (16)$$

Summing up, in this section we observed that the definition of the free energy in presence of material hereditariness is affected by a pathological drawback: The presence of an integration term that is not known by relaxation (or creep) measures. In this regard, the integration, residual term is related to the dissipation rate of the material during the strain history and, assuming a specific expression of the free energy functional it may be evaluated. Different kind of expressions of the dissipation rate may be obtained for the different expressions of the free energy functional each corresponding to the same measures of stress relaxation, thus providing a non-univoque relations among stress measures and the material dissipation.

#### IV. MECHANICAL DESCRIPTION OF POWER-LAW RELAXATION

In some previous studies [11]–[13] it has been shown that, from a mechanical prospective, it must be distinguished among values of order  $\beta = \beta_E \in [0, 1/2]$  and values of order  $\beta = \beta_V \in [1/2, 1]$ . Such a difference is reflected into the different mechanical models beyond  $\beta_E$  and  $\beta_V$ . In more details there are two different mechanical models that exactly reconstitute the stress-strain relation expressed in Eq. (10a). As  $0 \leq \beta = \beta_E \leq 1/2$  the mechanical model is a massless indefinite fluid column resting on a bed of independent springs as shown in Figure 1(a) and in this case is referred so elastoviscous material. If, instead,  $1/2 \leq \beta = \beta_V \leq 1$  the exact mechanical model is represented by indefinite massless shear-type column resting on a bed of independent dashpots as shown in Figure 1(b), this model is referred to visco-elastic material. The correspondence of these mechanical models and fractional order operators has been proved by introducing a  $z$  vertical axis as shown in Figure 1 and denoting  $\sigma(z, t)$  the shear stress (in the fluid or in the cantilever beam) and  $\gamma(z, t)$  the normalized displacement field [4]. Moreover let  $\sigma(0, t) = \sigma(t)$  and  $\gamma(0, t) = \gamma(t)$  the stress applied on the top of the model and the corresponding strain, respectively. The stress-strain relation in Eq. (10) is captured by the stress  $\sigma(t)$  on the upper lamina and its correspondent transverse displacement  $\gamma(t)$  (normalized displacement at the top). All the mechanical characteristics, viscosity of fluid  $c_E(z)$  and external stiffness  $k_E(z)$  for the model in Figure 1(a) ( $0 \leq \beta \leq 1/2$ ) as well as shear modulus  $k_V(z)$  and external viscous coefficient of external dashpots  $c_V(z)$  for the model in Figure 1(b) ( $1/2 \leq \beta \leq 1$ ), vary along the  $z$  axis with power-law.

In more details we define  $G_0$  and  $\eta_0$  the reference values of the shear modulus and viscosity coefficient. For the EV materials ( $\beta \in [0, 1/2]$ ) the stiffness and the viscous coefficients

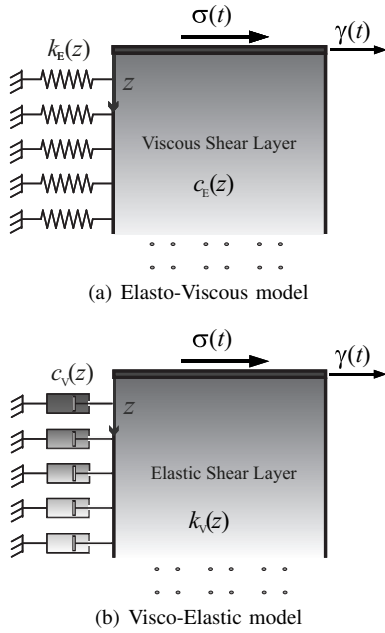


Figure 1. Continuous fractional models.

decay as:

$$k_E(z) = \frac{G_0}{\Gamma(1+\alpha)} z^{-\alpha}; \quad c_E(z) = \frac{\eta_0}{\Gamma(1-\alpha)} z^{-\alpha} \quad (17)$$

with  $0 \leq \alpha \leq 1$ , whereas the VE materials ( $\beta \in [1/2, 1]$ ) the mechanical characteristics of the model in Figure 1(b) reads:

$$k_V(z) = \frac{G_0}{\Gamma(1-\alpha)} z^{-\alpha}; \quad c_V(z) = \frac{\eta_0}{\Gamma(1+\alpha)} z^{-\alpha}. \quad (18)$$

The governing equation of the continuous model depicted in Figure 1(a) is written as:

$$\frac{\partial}{\partial z} \left[ c_E(z) \frac{\partial \dot{\gamma}(z, t)}{\partial z} \right] = k_E(z) \gamma(z, t) \quad (19)$$

while the equilibrium equation of the continuous model depicted in Figure 1(b) is written as:

$$\frac{\partial}{\partial z} \left[ k_V(z) \frac{\partial \gamma(z, t)}{\partial z} \right] = c_V(z) \dot{\gamma}(z, t). \quad (20)$$

The solution of the differential equations in Eq. (19) and (20) can be solved by Laplace transform. In this way the solution  $\hat{\gamma}(z, s)$  in Laplace domain involves the modified first and second kind Bessel functions, denoted respectively with  $Y_\beta(\cdot)$  and  $K_\beta(\cdot)$ , in particular we obtain for EV case:

$$\hat{\gamma}(z, s) = z^\beta \left[ B_{E1} Y_\beta \left( \frac{z}{\sqrt{\tau_E(\alpha) s}} \right) + B_{E2} K_\beta \left( \frac{z}{\sqrt{\tau_E(\alpha) s}} \right) \right] \quad (21)$$

with  $\tau_E(\alpha) = -\eta_0 \Gamma(\alpha) / (\Gamma(-\alpha) G_0)$  and  $\beta = (1 - \alpha) / 2$ ; while for VE case we have:

$$\hat{\gamma}(z, s) = z^\beta \left[ B_{V1} Y_\beta \left( z \sqrt{\tau_E(\alpha) s} \right) + B_{V2} K_\beta \left( z \sqrt{\tau_E(\alpha) s} \right) \right] \quad (22)$$

with  $\tau_V(\alpha) = -\eta_0 \Gamma(-\alpha) / (\Gamma(\alpha) G_0)$  and  $\beta = (1 + \alpha) / 2$ . The constants of integration  $B_{Ei}$  and  $B_{Vi}$  with  $i = 1, 2$  are obtained by imposing the following pairs of boundary

conditions, for the EV and VE case respectively:

$$(EV) \begin{cases} \lim_{z \rightarrow 0} c_E(z) \frac{\partial \dot{\gamma}(z, t)}{\partial z} = \sigma(0, t) = \sigma(t), \\ \lim_{z \rightarrow \infty} \gamma(z, t) = 0 \end{cases} \quad (23a)$$

$$(VE) \begin{cases} \lim_{z \rightarrow 0} k_V(z) \frac{\partial \dot{\gamma}(z, t)}{\partial z} = \sigma(0, t) = \sigma(t), \\ \lim_{z \rightarrow \infty} \gamma(z, t) = 0 \end{cases} \quad (23b)$$

and by making the inverse Laplace transform we obtain the fractional stress-strain relation in Eq. (10), that is to say:

$$\gamma(t) = \frac{1}{C_E(\beta)} \left( I_{0+}^\beta \sigma \right) (t) \quad (EV) \quad (24a)$$

$$\gamma(t) = \frac{1}{C_V(\beta)} \left( I_{0+}^\beta \sigma \right) (t) \quad (VE) \quad (24b)$$

where the coefficients  $C_E(\beta)$  and  $C_V(\beta)$  are defined as:

$$C_E(\beta) = \frac{G_0 \Gamma(\beta) 2^{2\beta-1}}{\Gamma(2-2\beta) \Gamma(1-\beta)} (\tau_E(\alpha))^\beta, \quad 0 \leq \beta \leq 1/2 \quad (25a)$$

$$C_V(\beta) = \frac{G_0 \Gamma(1-\beta) 2^{1-2\beta}}{\Gamma(2-2\beta) \Gamma(\beta)} (\tau_V(\alpha))^\beta, \quad 1/2 \leq \beta \leq 1. \quad (25b)$$

At this point we observe that, if the boundary condition applied to the top layer of the model (see Eqs. (23a) and (23b)), respectively, for EV and VE materials, involves Dirichlet specifics, as:

$$\begin{cases} \lim_{z \rightarrow 0} \gamma(z, t) = \gamma(t), \\ \lim_{z \rightarrow \infty} \gamma(z, t) = 0. \end{cases} \quad (26)$$

The evaluation of the stress at the top lamina in terms of the transverse displacement field yields:

$$\sigma(t) = C_E(\beta) \left( {}^C D_{0+}^{\beta+\gamma} \right) (t) \quad (EV) \quad (27)$$

$$\sigma(t) = C_V(\beta) \left( {}^C D_{0+}^{\beta+\gamma} \right) (t) \quad (VE)$$

as reported in [11]–[13].

#### A. Discrete model

The discrete counterpart of the FHM model is described in this section. The mechanical representation of fractional order operators discussed in previous section may be used to introduce a discretization scheme that corresponds to evaluate fractional derivative.

The two cases corresponding to  $\beta \in [0, 1/2]$  and  $\beta \in [1/2, 1]$  will be analyzed in this subsection. The first one is the EV case. By introducing a discretization of the  $z$ -axis as  $z_j = j \Delta z$  into to the governing equation of the EV material in Eq. (19) yields a finite difference equation of the form:

$$\frac{\Delta}{\Delta z} \left[ c_E(z_j) \frac{\Delta \dot{\gamma}(z_j, t)}{\Delta z} \right] = k_E(z_j) \gamma(z_j, t) \quad (28)$$

so that, denoting  $k_{Ej} = k_E(z_j) \Delta z$  and  $c_{Ej} = c_E(z_j) / \Delta z$  the continuous model is discretized into a dynamical model constituted by massless shear layers, with horizontal degrees of freedom  $\gamma(z_j, t) = \gamma_j(t)$ , that are mutually interconnected by linear dashpots with viscosity coefficients  $c_{Ej}$  and resting on a bed of independent linear springs  $k_{Ej}$ . The stiffness coefficient

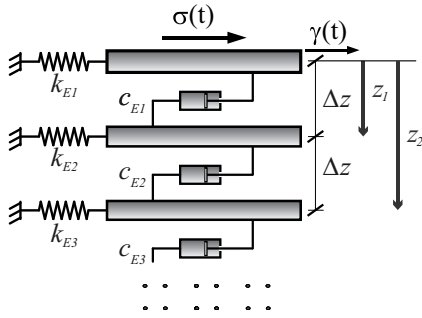


Figure 2. Discretized counterpart of the EV continuous model.

$k_{Ej}$  and the viscosity coefficient  $c_{Ej}$  reads:

$$k_{Ej} = \frac{G_0}{\Gamma(1+\alpha)} z_j^{-\alpha} \Delta z; \quad c_{Ej} = \frac{\eta_0}{\Gamma(1-\alpha)} \frac{z_j^{-\alpha}}{\Delta z} \quad (29)$$

with  $\alpha = 1 - 2\beta$ . The equilibrium equations of the generic shear layer of the model read:

$$\begin{cases} k_{E0}\gamma_1(t) - c_{E0}\Delta\dot{\gamma}_1(t) = \sigma(t), \\ k_{Ej}\gamma_j(t) + c_{Ej-1}\Delta\dot{\gamma}_{j-1}(t) - c_{Ej}\Delta\dot{\gamma}_j(t) = 0 \end{cases} \quad (30)$$

where  $j = 1, 2, \dots, \infty$ ,  $\gamma_1(t) = \gamma(t)$  and  $\Delta\dot{\gamma}_j(t) = \dot{\gamma}_{j+1}(t) - \dot{\gamma}_j(t)$ . By inserting Eqs. (29) in Eqs. (30), at the limit as  $\Delta z \rightarrow 0$ , the discrete model reverts to Eq. (19). That is the discretized model presented in Figure 2 represents a proper discretization of the continuous EV counterpart.

As soon as  $z$  increase  $\gamma(z, t)$  decay and  $\lim_{z \rightarrow \infty} \gamma(z, t) = 0$  it follows that only a certain number, say  $n$ , of equilibrium equation may be accounted for the analysis. It follows that the system in Eqs. (30) may be rewritten in the following compact form:

$$p_E \mathbf{A} \dot{\boldsymbol{\gamma}} + q_E \mathbf{B} \boldsymbol{\gamma} = \mathbf{v} \sigma(t) \quad (31)$$

where:

$$p_E = \frac{\eta_0}{\Gamma(1-\alpha)} \Delta z^{-(1+\alpha)}; \quad q_E = \frac{G_0}{\Gamma(1+\alpha)} \Delta z^{1-\alpha}. \quad (32)$$

In Eq. (31):

$$\boldsymbol{\gamma}^T = [ \gamma_1(t) \quad \gamma_2(t) \quad \dots \quad \gamma_n(t) ]; \quad \mathbf{v}^T = [ 1 \quad 0 \quad \dots \quad 0 ] \quad (33)$$

where the apex  $T$  means transpose. The coefficient matrices  $\mathbf{A}$  and  $\mathbf{B}$  are given as:

$$\mathbf{A} = \begin{bmatrix} 1^{-\alpha} & -1^{-\alpha} & \dots & 0 \\ -1^{-\alpha} & 1^{-\alpha} + 2^{-\alpha} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & (n-1)^{-\alpha} + n^{-\alpha} \end{bmatrix} \quad (34)$$

$$\mathbf{B} = \begin{bmatrix} 1^{-\alpha} & 0 & 0 & \dots & 0 \\ 0 & 2^{-\alpha} & 0 & \dots & 0 \\ 0 & 0 & 3^{-\alpha} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & n^{-\alpha} \end{bmatrix}. \quad (35)$$

The matrices  $\mathbf{A}$  and  $\mathbf{B}$  are symmetric and positive definite (in particular  $\mathbf{B}$  is diagonal) and they may be easily constructed for an assigned value of  $\alpha$  (depending of the derivative order  $\beta$ ) and for a fixed truncation order  $n$ . Moreover Eq. (31) may

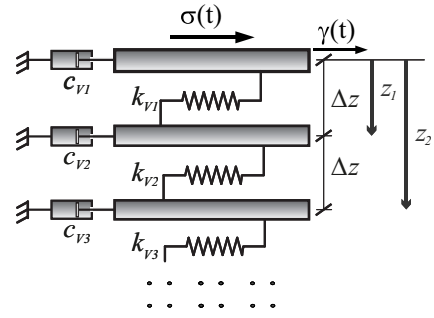


Figure 3. Discretized counterpart of the VE continuous model.

now be easily integrated by using standard tools of dynamic analysis how it will be shown later on.

The second case is that one where the fractional order derivative is  $\beta = \beta_V \in [1/2, 1]$  the mechanical description of the material is represented by the continuous model depicted in Figure 3 and ruled by Eq. (20). By introducing a discretization of the  $z$ -axis in intervals  $\Delta z$  in governing equation of the VE materials in Eq. (20) yields a finite difference equation of the form:

$$\frac{\Delta}{\Delta z} \left[ k_V(z_j) \frac{\Delta \gamma(z_j, t)}{\Delta z} \right] = c_V(z_j) \dot{\gamma}(z_j, t) \quad (36)$$

that corresponds to a discretized mechanical representation of fractional derivatives. The mechanical model is represented by a set of massless shear layers with state variables  $\gamma(z_j, t) = \gamma_j(t)$  that are mutually interconnected by linear springs with stiffness  $k_{Vj} = k_V(z_j, t)/\Delta z$  resting on a bed of independent linear dashpots with viscosity coefficient  $c_{Vj} = c_V(z_j, t)\Delta z$ . Springs and dashpots are given as:

$$k_{Vj} = \frac{G_0}{\Gamma(1-\alpha)} \frac{z_j^{-\alpha}}{\Delta z}; \quad c_{Vj} = \frac{\eta_0}{\Gamma(1+\alpha)} z_j^{-\alpha} \Delta z \quad (37)$$

with  $\alpha = 2\beta - 1$ . The set of equilibrium equations reads:

$$\begin{cases} c_{V0}\dot{\gamma}_1 - k_{V0}\Delta\gamma_1 = \sigma(t), \\ c_{Vj}\dot{\gamma}_j + k_{Vj-1}\Delta\gamma_{j-1} - k_{Vj}\Delta\gamma_j = 0, \quad j = 1, 2, \dots, \infty. \end{cases} \quad (38)$$

So that, accounting for the contribution of the first  $n$  shear layers the differential equation system may be written as:

$$p_V \mathbf{B} \dot{\boldsymbol{\gamma}} + q_V \mathbf{A} \boldsymbol{\gamma} = \mathbf{v} \sigma(t) \quad (39)$$

where:

$$p_V = \frac{\eta_0}{\Gamma(1+\alpha)} \Delta z^{1-\alpha}; \quad q_V = \frac{G_0}{\Gamma(1-\alpha)} \Delta z^{-(1+\alpha)}. \quad (40)$$

### B. The free energy approximation

The discretized models described in the previous subsection can be used to verify that the Staverman-Schwarzl formulation of free energy is still exact also for fractional hereditary systems. In this section a numerical application will be proposed in order to show the equivalence between  $\Psi_{SS}$  and the stored up springs energy of the discretized models. It will be presented for different values of  $\beta$  and a load history  $\sigma(t) = U(t)$ . For EV case materials ( $\beta \in [0, \frac{1}{2}]$ ) we selected  $n = 1500$  e  $\Delta z = 0.001$ , where  $\Delta z$  is the discretization step and  $n$  is the number of layers considered, moreover it

is assumed  $G_0 = 1$  e  $\eta_0 = 1$ . For VE case ( $\beta \in [\frac{1}{2}, 1]$ ) the discretization step  $\Delta z = 0.02$  and  $n = 1500$ . Perturbing the upper layer of the discretized models with a load history  $\sigma(t) = U(t)$  and denoting with  $\gamma_k$  the strain of the common layer, the springs energy of the model is determined :

*EV Model case*

$$\Psi(t) = \sum_{k=1}^n \left[ \int_0^{\gamma_k} k_{E_k} \gamma_k d\gamma_k \right] = \sum_{k=1}^n \left[ \frac{1}{2} k_{E_k} \gamma_k^2 \right] \quad (41)$$

$$\gamma_k(t) = k^{\frac{\alpha}{2}} \frac{1}{q_E} \sum_{j=1}^n \left[ \phi_{k,j} \phi_{1,j} \left( 1 - e^{-\frac{q_E t}{p_E \lambda(j)}} \right) \right] \quad (42)$$

*VE Model case*

$$\Psi(t) = \sum_{k=1}^{n-1} \left[ \frac{1}{2} k_{V_k} (\gamma_{k+1} - \gamma_k)^2 \right] + \frac{1}{2} k_{V_n} \gamma_n^2 \quad (43)$$

$$\gamma_k(t) = k^{\frac{\alpha}{2}} \frac{1}{q_V} \sum_{j=1}^n \left[ \frac{1}{\lambda(j)} \phi_{k,j} \phi_{1,j} \left( 1 - e^{-\frac{q_V t}{p_V \lambda(j)}} \right) \right] \quad (44)$$

From the first expression of (16) the free energy of the exact model:

$$\psi_{ss}(t) = \frac{C(\beta)}{2\Gamma(1-\beta)} \int_{-\infty}^t \int_{-\infty}^t (2t - \tau_1 - \tau_2)^{-\beta} \dot{\varepsilon}(\tau_1) \dot{\varepsilon}(\tau_2) d\tau_1 d\tau_2 \quad (45)$$

where:

$$\varepsilon(t) = \frac{t^\beta}{C(\beta)\Gamma(1+\beta)} \quad (46)$$

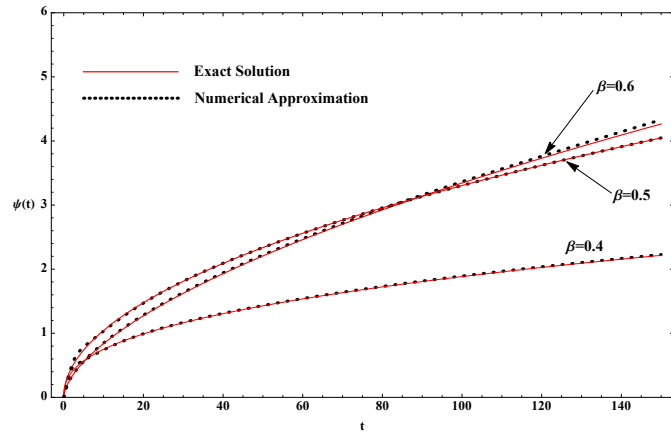


Figure 4. Comparison between the exact formulation of free energy and the approximated one

## V. CONCLUSION

The power-law relaxation function of fractional hereditary material is an engineering measure of the stress decay that is easily evaluated by means of uniaxial tests. On the contrary, the evaluation of the material free energy, that is the stored elastic energy in FHM based on the only measure of stress relaxation is a formidable task and several free energies have been defined in scientific literature. In this paper the authors show that if the power-law relaxation is described by a mechanical model

separating the solid (elastic) and the fluid (viscous) phases in the material, then the free energy function may be directly evaluated on the mechanical model. In this regard it has been shown that the more appropriate form of the free energy that is the elastic energy stored in the material is the Staverman-Schwarz expression. Some numerical applications show that the discretization of the mechanical model corresponding to an approximation of the power-law yields a good representation of the Staverman-Schwartz energy.

## REFERENCES

- [1] P. G., Nutting, *A new general law of deformation*, Journal of the Franklin Institute, 191 (1921) 679-685.
- [2] A., Gemant, *A method of analyzing experimental results obtained from elasto-viscous bodies*, Physics, 7 (1936) 311-317.
- [3] M. Di Paola, A. Pirrotta, A. Valenza, *Visco-elastic behavior through fractional calculus: an easier method for best fitting experimental results*, Mechanics of Materials 43 (2011) 799-806.
- [4] S., Müller, M., Kästner, J., Brummund, V., Ulbricht, *A nonlinear fractional viscoelastic material model for polymers*, Computational Materials Science, 50 (2011) 2938-2949.
- [5] M., Di Paola, V., Fiore, F. P., Pinnola, A., Valenza, *On the influence of the initial ramp for a correct definition of the parameters of fractional viscoelastic materials*, Mechanics of Materials, article in press, 2014.
- [6] A. J., Staverman, F., Schwarzl, *Thermodynamics of viscoelastic behavior*, Verh. Akad. can Wet., 55 (1952) 474-485.
- [7] B., Coleman, *Thermodynamics of materials with memory*, Arch Rational Mech. Anal., 17 (1964) 1-47.
- [8] D., Graffi, *Sull'espressione dell'energia libera nei materiali viscoelastici lineari*, Annali di Matematica Pura ed Applicata, Series 4 98 (1974) 273-279.
- [9] M., Fabrizio, C., Giorgi, A., Morro, *Free energies and dissipation properties for system with memory*, Arch. Rational Mech. Anal., 125 (1994) 341-373.
- [10] L., Deseri, M., Fabrizio, M., Golden, *The concepts of a minimal state in viscoelasticity: new free energies and applications to PDEs*, Arch. Rational Mech. Anal., 181 (2006) 43-96.
- [11] M., Di Paola, M., Zingales, *Exact mechanical models of fractional hereditary materials*, Journal of Rheology, 56 (2012) 983-1004.
- [12] M., Di Paola, F. P., Pinnola, M., Zingales, *A discrete mechanical model of fractional hereditary materials*, Meccanica, 48 (2013) 1573-1586.
- [13] M., Di Paola, F. P., Pinnola, M., Zingales, *Fractional differential equations and related exact mechanical models*, Computers and Mathematics with Applications, 66 (2013) 608-620.
- [14] L., Deseri, M., Di Paola, M., Zingales, *Free Energy and States of Fractional-Order Hereditaryness*, Journal of Rheology, submitted, 2014.
- [15] M. Caputo, *Linear models of dissipation whose Q is almost frequency independent-II*, Geophysical J. Royal Astronomic Society, Vol. 13 (1967) 529-539. (Reprinted recently in: Fract. Calc. Appl. Anal., Vol. 11, No 1, pp. 3-14, 2008).
- [16] K. S. Miller, B. Ross, *An Introduction to the Fractional Calculus and Fractional Differential Equations*, Wiley-InterScience, New York, 1993.
- [17] G. S. Samko, A. A. Kilbas, O. I. Marichev, *Fractional Integrals and Derivatives: Theory and Applications*, New York (NY): Gordon and Breach: 1993.
- [18] A. A. Kilbas, H. M. Srivastava, J. J. Trujillo, *Theory and Applications of Fractional Differential Equations*, Elsevier, Amsterdam, 2006.
- [19] R. Hilfer, *Application of Fractional Calculus in Physics*, World Scientific, Singapore, 2000.
- [20] I. Podlubny, *Fractional Differential Equations*, Academic Press, San Diego, 1999.
- [21] K. B. Oldham, J. Spanier, *The Fractional Calculus: Theory and applications of differentiation and integration to arbitrary order*, Academic Press, New York, 1974.
- [22] R. L., Bagley, P. J. Torvik, *On the fractional calculus model of viscoelastic behavior*, Journal of Rheology, Vol. 30 (1986) 133-155.