Some partial differential Volterra equation problems arising in viscoelasticity

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1 Introduction

This paper is concerned with the modelling of problems involving viscoelastic materials which, even in their simplest form, exhibit behaviour characteristic of both classical Hookean solids and Newtonian fluids. The resulting effects are important when the material is deforming under an applied load. This load could, for example, be due to externally applied forces; internal deformation caused by a diffusing penetrant; or, constrained thermal expansion caused by temperature gradients. See for example [21, 6, 28]. Moreover, the material somehow keeps a record of its response history and, for this reason, viscoelastic materials are said to possess *memory*. This memory is manifest in the constitutive relationship between the stress and strain tensors, $\underline{\boldsymbol{\sigma}}$ and $\underline{\boldsymbol{\varepsilon}}$, and as a result mathematical models of viscoelastic behaviour take the form of partial differential Volterra (PDV) equation problems. The canonical forms of these equations are: the *elliptic Volterra* problem,

$$Au(t) = f(t) + \int_0^t B(t,s)u(s)\,ds; \tag{1}$$

the *parabolic Volterra* problem,

$$u'(t) + Au(t) = f(t) + \int_0^t B(t,s)u(s)\,ds; \tag{2}$$

and, the *hyperbolic Volterra* problem,

$$u''(t) + Au(t) = f(t) + \int_0^t B(t,s)u(s)\,ds. \tag{3}$$

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These are supplied with initial and/or boundary data as appropriate, and the dependence on the space variable $\boldsymbol{x}$ is suppressed. In these problems we use A and $B(t,s)$ to represent partial differential operators (acting only in the space variables) where, for example, we could have

$$A := -\nabla^2 \qquad \text{and} \qquad B(t,s) := -\nabla \cdot \phi(t,s)\nabla,$$

although for (1) and (3) the appropriate form for A is the linear elasticity operator—with $B(t,s)$ "similar".

The purpose of this article is to illustrate how the memory terms arise in these equations and also to summarize the various PDV equations used when modelling problems of *quasistatic* and *dynamic* viscoelasticity, and *non-Fickian* diffusion in polymers. We also indicate some of the numerical analysis work that has been carried out for these problems (but we do not claim to be exhaustive, for a fuller account see [39]).

Throughout, the positive real number T will denote a final time and we use $\mathcal{J} := [0,T]$ and $\mathcal{I} := (0,T]$ to denote time intervals. Also, for $n = 1, 2$ or 3 we consider $\Omega \subset \mathbb{R}^n$ to be an open bounded domain with boundary $\partial\Omega$. Furthermore, we consider $\partial\Omega$ in the form

$$\partial\Omega := \overline{\Gamma_D \cup \Gamma_N} \qquad \text{with} \qquad \Gamma_D \cap \Gamma_N = \emptyset,$$

where the closed set $\Gamma_D \subseteq \partial\Omega$ is called the *Dirichlet boundary* and is of positive measure so that

$$\int_{\Gamma_D} d\Gamma > 0.$$

We call the (possibly empty) open set $\Gamma_N \subset \partial\Omega$ the *Neumann boundary.* The reason for this terminology is the obvious one where we refer to the type of boundary condition specified on these subsets. We indicate vector-valued quantities with boldface so that, for example, we use $\boldsymbol{x} := (x_i)_{i=1}^n$ to indicate a point in $\mathbb{R}^n$. Tensors are indicated by a further underlining: $\underline{\boldsymbol{\sigma}} = (\sigma_{ij})_{i,j=1}^n$.

2 Hereditary constitutive relationships

Suppose that the interior of a compressible viscoelastic body $\mathcal{G}$ occupies Ω and that its surface coincides with $\partial\Omega$. If at a time t this body is subjected to a system of body forces $\boldsymbol{f} := (f_i(\boldsymbol{x},t))_{i=1}^n$, for $\boldsymbol{x} \in \Omega$, and surface tractions $\boldsymbol{g} := (g_i(\boldsymbol{x},t))_{i=1}^n$, for $\boldsymbol{x} \in \Gamma_N$, then the body $\mathcal{G}$ will deform from its equilibrium configuration. A material particle originally at the point $\boldsymbol{x}$ will move to the new time dependent location $\boldsymbol{x}+\boldsymbol{u}(\boldsymbol{x},t)$ where $\boldsymbol{u} := (u_i)_{i=1}^n$ denotes the displacement vector. In the linear theory these displacements define the symmetric strain tensor $\underline{\boldsymbol{\varepsilon}} := (\varepsilon_{ij})_{i,j=1}^n$ by the relationships:

$$\varepsilon_{ij}(\boldsymbol{u}) := \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{4}$$

In addition to this strain field there will also be induced in $\mathcal{G}$ a stress field described by the symmetric stress tensor $\underline{\boldsymbol{\sigma}} := (\sigma_{ij})_{i,j=1}^{n}$. This stress field rationalizes the internal force field which is set up within $\mathcal{G}$ to resist the external forces $\boldsymbol{f}$ and $\boldsymbol{g}$.

The stress field can be related to $\boldsymbol{u}$, $\boldsymbol{f}$ and $\boldsymbol{g}$ by Newton's second law of motion (see later in equation (19)) and so it is of interest to derive a *constitutive relationship* linking $\underline{\boldsymbol{\sigma}}$ and $\boldsymbol{u}$, or in practice, linking the tensors $\underline{\boldsymbol{\sigma}}$ and $\underline{\varepsilon}$.

In classical linear elasticity theory this relationship is provided by Hooke's law:

$$\sigma_{ij} = D_{ijkl}\varepsilon_{kl} \qquad \text{or} \qquad \underline{\boldsymbol{\sigma}} = \underline{\boldsymbol{D}}\,\underline{\varepsilon},$$

where $\underline{\boldsymbol{D}}$ is a positive-definite fourth-order tensor of elastic coefficients satisfying the symmetries

$$D_{ijkl} = D_{jikl}, \qquad D_{ijkl} = D_{ijlk}, \qquad \text{and} \qquad D_{ijkl} = D_{klij}.$$

The first two of these are implied by the symmetry of $\underline{\boldsymbol{\sigma}}$ and $\underline{\varepsilon}$ while the third follows from energy considerations. However, in viscoelasticity the third of these only applies when the material is isotropic, see [21, Equations (1.10) and (2.62)].

One way of deriving a constitutive relationship for viscoelastic materials is to assume that a Boltzmann superposition of stress increments can be applied where these stress increments are related by Hooke's law to corresponding strain increments. For example, suppose that $\mathcal{G}$ is quiescent for $t < 0$ so that $\underline{\varepsilon}(t) \equiv \underline{\mathbf{0}}$ for $t < 0$, and that at $t = 0$ the body undergoes a strain $\underline{\varepsilon}(0)$. Then for $t \geq 0$ the resulting stress is assumed to be given by

$$\underline{\boldsymbol{\sigma}}_0(t) = \underline{\boldsymbol{D}}(t)\underline{\varepsilon}(0),$$

where a time dependence has been introduced into the Hooke's tensor $\underline{\boldsymbol{D}}$. Physically we expect $\underline{\boldsymbol{D}}$ to be a smooth monotone decreasing function of t since it is unrealistic to expect $\underline{\boldsymbol{\sigma}}$ to grow over time for the fixed strain $\underline{\varepsilon}(0)$. (Where would the strain energy come from?) In fact experiments on polymers show that $\underline{\boldsymbol{D}}$ does in fact decrease and this phenomena is known as *stress relaxation*.

Now, let Δt be a small time interval and set $t_i := i\Delta t$. We approximate the strain evolution by the step function

$$\widetilde{\underline{\varepsilon}}(t) := \underline{\varepsilon}(t_i) \qquad \text{in } [t_i, t_{i+1}) \text{ for } i = 0, 1, 2, \ldots,$$

and then each strain increment,

$$\Delta\underline{\varepsilon}(t_{i+1}) := \underline{\varepsilon}(t_{i+1}) - \underline{\varepsilon}(t_i),$$

induces a stress increment according to Hooke's law:

$$\Delta\underline{\boldsymbol{\sigma}}_j(t_i) := \underline{\boldsymbol{D}}(t_i - t_j)\Delta\underline{\varepsilon}(t_j) \qquad \text{for } 1 \leq j \leq i.$$

Notice that each of these stress increments will also relax according to the time dependence of $\underline{\boldsymbol{D}}$. The total stress at time t_i is now given by superposition:

$$\underline{\boldsymbol{\sigma}}(t_i) \;\; := \;\; \underline{\boldsymbol{\sigma}}_0(t_i) + \sum_{j=1}^{i} \Delta\underline{\boldsymbol{\sigma}}_j(t_i),$$

$$= \quad \underline{\boldsymbol{D}}(t_i)\underline{\boldsymbol{\varepsilon}}(0) + \sum_{j=1}^{i} \underline{\boldsymbol{D}}(t_i - t_j)\Delta\underline{\boldsymbol{\varepsilon}}(t_j),$$

and by taking an appropriate limit we get the hereditary constitutive law as

$$\underline{\boldsymbol{\sigma}}(\boldsymbol{x}, t) = \underline{\boldsymbol{D}}(t)\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}(\boldsymbol{x}, 0)) + \int_0^t \underline{\boldsymbol{D}}(t-s)\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}'(\boldsymbol{x}, s))\, ds. \tag{5}$$

Since we are assuming that $\underline{\boldsymbol{D}}(t)$ is smooth we can arrive at an alternate form by partial integration,

$$\underline{\boldsymbol{\sigma}}(\boldsymbol{x}, t) = \underline{\boldsymbol{D}}(0)\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}(\boldsymbol{x}, t)) - \int_0^t \underline{\boldsymbol{D}}_s(t-s)\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}(\boldsymbol{x}, s))\, ds, \tag{6}$$

where the subscript s indicates partial differentiation with respect to the *history variable* s. Either of these may be used as the constitutive relationship, and each demonstrates clearly the role of memory in viscoelastic modelling.

To get a feel for the form of the time dependence of the stress relaxation tensor $\underline{\boldsymbol{D}}$ we can also quote a perhaps more intuitive method for deriving these constitutive relationships.

We start with the physical observation that viscoelastic materials display the characteristics of both elastic solids and viscous fluids. The kinetics of these type of substances are modelled respectively by the spring and the dashpot.

Figure 1: A Hookean (linear) spring: $\sigma = E\varepsilon$; E is the spring stiffness

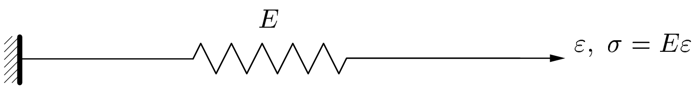
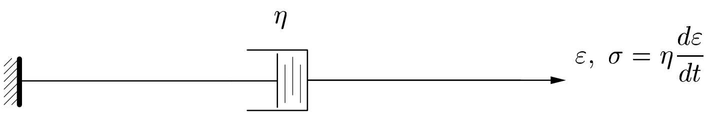


Figure 2: A Newtonian (linear) dashpot: $\sigma = \eta \dfrac{d\varepsilon}{dt}$; η is the viscosity



In these models the stress carried by the spring is proportional to the strain in the spring and is given by Hooke's law: $\sigma = E\varepsilon$. The stress carried in the dashpot is proportional to the strain rate and is given by Newton's law of viscosity: $\sigma = \eta\varepsilon'$.

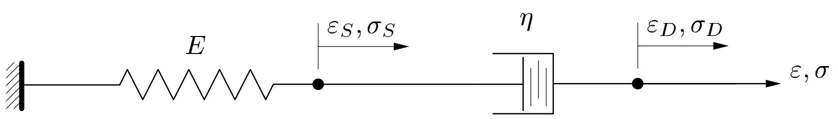
One then models a viscoelastic material by considering a notional system of springs and dashpots with independent stiffness and viscosity parameters.

There are essentially two ways to connect a spring to a dashpot: in *series* and in *parallel*. These are the building blocks and are named the "Maxwell" and "Voigt" models.

The Maxwell model

The Maxwell model is a series connection of a spring and dashpot.

Figure 3: THE MAXWELL MODEL



In this model ε_S and σ_S denote the strain and stress in the spring alone, and ε_D, σ_D denote those in the dashpot alone. The total stress is given by $\sigma = \sigma_S = \sigma_D$ and the total strain by $\varepsilon = \varepsilon_S + \varepsilon_D$. Differentiating and using Hooke's and Newton's laws yield

$$\frac{d\varepsilon}{dt} = \frac{1}{E}\frac{d\sigma_S}{dt} + \frac{\sigma_D}{\eta} \quad\Longrightarrow\quad \frac{d\sigma}{dt} + \frac{\sigma}{\tau} = E\frac{d\varepsilon}{dt}, \tag{7}$$

where $\tau := \eta/E$ is the so-called *relaxation time*. Using $\sigma(0) = E\varepsilon(0)$ this ODE is easily solved to give

$$\sigma(t) = Ee^{-t/\tau}\varepsilon(0) + E\int_0^t e^{-(t-s)/\tau}\varepsilon'(s)\,ds,$$

and this is essentially (5) with the scalar analogue of $\underline{\boldsymbol{D}}$ given by $D(t) = Ee^{-t/\tau}$.

The Voigt model

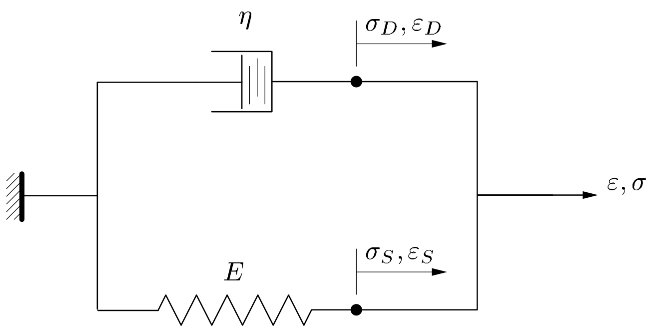
Connecting the spring and dashpot in parallel yields the Voigt model. This time $\varepsilon_S = \varepsilon_D = \varepsilon$ and equilibrium demands that $\sigma = \sigma_S + \sigma_D$, hence

$$\eta\frac{d\varepsilon}{dt} + E\varepsilon = \sigma \quad\Longrightarrow\quad \frac{d\varepsilon}{dt} + \frac{\varepsilon}{\tau} = \frac{\sigma}{\eta}.$$

This gives the constitutive law in hereditary form as

$$\varepsilon(t) = e^{-t/\tau}\varepsilon(0) + \frac{1}{\eta}\int_0^t e^{-(t-s)/\tau}\sigma(s)\,ds.$$

Figure 4: The Voigt model



The Maxwell solid

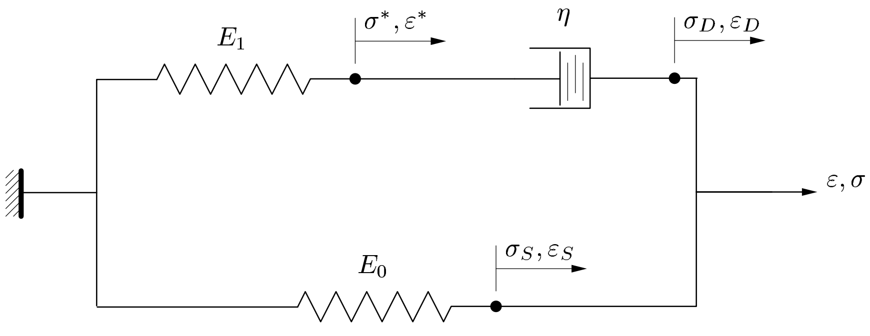
In his internal variable formulation A. Johnson, in for example [20], uses these basic building blocks in the Maxwell solid. Here E_0 and E_1 are spring stiffnesses and σ^*, ε^* are internal stress and strain variables. This time $\sigma^* = E_1\varepsilon^*$, $\varepsilon_D = \varepsilon - \varepsilon^*$ and $\sigma_S = E_0\varepsilon_S$. Also $\sigma^* = \sigma_D$ and this gives

$$E_1\varepsilon^* = \eta\frac{d}{dt}(\varepsilon - \varepsilon^*) \quad \Longrightarrow \quad \frac{d\varepsilon^*}{dt} + \frac{\varepsilon^*}{\tau} = \frac{d\varepsilon}{dt},$$

where now $\tau := \eta/E_1$. Solving this we get

$$\varepsilon^*(t) = e^{-t/\tau}\varepsilon(0) + \int_0^t e^{-(t-s)/\tau}\varepsilon'(s)\,ds. \tag{8}$$

Figure 5: The Maxwell solid



Now, defining the *stress relaxation function*

$$D(t) := E_0 + E_1 e^{-t/\tau}$$

as the scalar analogue to the tensor $\underline{\boldsymbol{D}}(t)$ in (5) and (6), and using this in (8) along with the relation

$$\sigma = \sigma_S + \sigma^* = E_0\varepsilon + E_1\varepsilon^* \qquad (\text{since } \varepsilon_S = \varepsilon),$$

gives

$$\begin{aligned}\sigma(t) &= E_0\varepsilon(t) + E_1 e^{-t/\tau}\varepsilon(0) + \int_0^t E_1 e^{-(t-s)/\tau}\varepsilon'(s)\,ds,\\ &= D(0)\varepsilon(t) - \int_0^t D_s(t-s)\varepsilon(s)\,ds.\end{aligned}$$

This is the scalar analogue of equation (6) and suggests that we model $\underline{\boldsymbol{D}}$ with the *Dirichlet-Prony series*,

$$\underline{\boldsymbol{D}}(t) = \varphi(t)\underline{\boldsymbol{D}}(0) \tag{9}$$

where $\varphi(t)$ is a generic stress relaxation function given by

$$\varphi(t) = \varphi_0 + \sum_{i=1}^{N} \varphi_i e^{-\alpha_i t}. \tag{10}$$

Here the (possibly $\boldsymbol{x}$ dependent) coefficients $\{\varphi_i\}_{i=0}^N$ are non-negative and normalized so that $\varphi(0) = 1$, and the (possibly $\boldsymbol{x}$ dependent) $\{\alpha_i\}_{i=1}^N$ are non-negative. More generally one could of course write

$$D_{ijkl}(t) := (D_{ijkl})_0 + \sum_{m=1}^{N_{ijkl}} (D_{ijkl})_m \exp(-(\alpha_{ijkl})_m t).$$

The Dirichlet-Prony series is an extremely convenient form to take for large scale computational approximations to problems (1), (2) and (3) since if

$$\psi(t) := e^{-\alpha t},$$

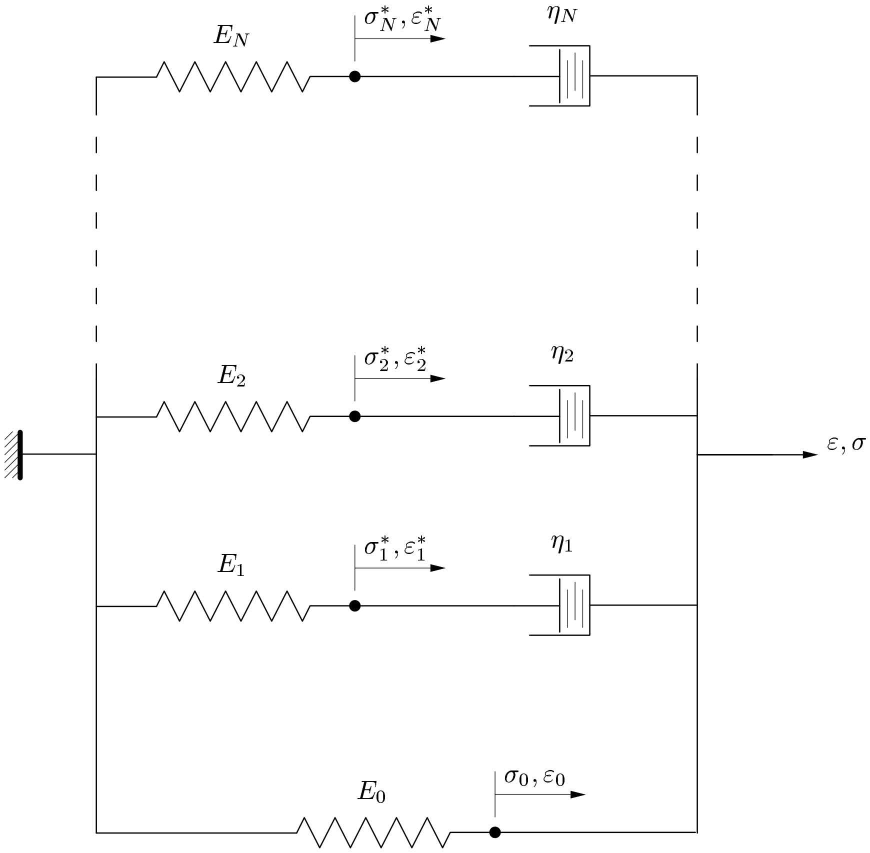
then one can exploit the simple recurrence

$$\psi(t+k) = e^{-\alpha k}\psi(t)$$

to update the history term arising from a discretization of the Volterra integral. For general Volterra problems one must usually store the entire solution history as the computation advances through the time levels and moreover, at each time level this history needs to be summed to approximate the integral. For such methods the number of operations required at time level N is of the order $O(N^2)$. The Dirichlet-Prony series provides a very useful short cut around this "N^2 problem". (In certain special cases one can also overcome this difficulty using other means, see for example [19, 16]).

We now return to the Maxwell solid and generalize the conceptual spring and dashpot model in order to motivate the choice of the Dirichlet-Prony series

Figure 6: The generalized Maxwell solid.



for the relaxation function as given in (10). To begin with we assume again a state of uniaxial stress and strain.

The generalized Maxwell solid, shown in Figure 6, consists of a Hookean spring connected in parallel to a sequence of N spring-dashpot components. In this model

$$\varepsilon_0 = \varepsilon, \qquad \sigma_0 = E_0 \varepsilon, \qquad \text{and} \qquad \sigma_i^* = E_i \varepsilon_i^*.$$

Balancing the stresses carried by each of the spring-dashpot pairs we get for each $i \in \{1, \ldots, N\}$ that

$$\begin{aligned} & \frac{d\varepsilon_i^*}{dt} + \frac{\varepsilon_i^*}{\tau_i} = \frac{d\varepsilon}{dt}, \\ \Longrightarrow \qquad & \varepsilon_i^*(t) = e^{-t/\tau_i} \varepsilon(0) + \int_0^t e^{-(t-s)/\tau_i} \varepsilon'(s)\, ds, \end{aligned}$$

where now we have set $\tau_i := E_i/\eta_i$. The total stress carried by the assemblage is therefore given by:

$$\begin{aligned}
\sigma(t) &= \sigma_0(t) + \sigma_1(t) + \cdots + \sigma_N(t), \\
&= E_0\varepsilon(t) + E_1\varepsilon_1^*(t) + \cdots + E_N\varepsilon_N^*(t), \\
&= E_0\varepsilon(0) + E_0(\varepsilon(t) - \varepsilon(0)) \\
&\qquad + \sum_{i=1}^{N} \left(E_i e^{-t/\tau_i}\varepsilon(0) + \int_0^t E_i e^{-(t-s)/\tau_i}\varepsilon'(s)\,ds \right), \\
&= E(t)\varepsilon(0) + \int_0^t E(t-s)\varepsilon'(s)\,ds, \qquad (11)
\end{aligned}$$

where

$$E(t) := E_0 + \sum_{i=1}^{N} E_i e^{-t/\tau_i}.$$

The constitutive relationship (11) is the scalar analogue of (5) with the analogue of $\underline{\boldsymbol{D}}(t-s)$ given by $E(t-s)$, which itself is an example of the Dirichlet-Prony series given in (10). Note that if we set $E_0 := 0$ then this generalized Maxwell solid actually models a fluid since $\lim E(t) = 0$.

So much for uniaxial states of stress and strain. In fact it can be shown that for each *relaxation mode* (i.e. each spring-dashpot pair) there is an ODE governing the evolution of each of the internal strain tensor components. Thus we have

$$\frac{d(\varepsilon_{ij})_n^*}{dt} + \frac{(\varepsilon_{ij})_n^*}{\tau_n} = \frac{d\varepsilon_{ij}}{dt},$$

and for the details we refer to [20]. The significance of these internal variable formulations for the viscoelastic constitutive behaviour lies in the fact that it is possible to solve some kinds of viscoelasticity problems, when the relaxation functions are in the form of a Dirichlet-Prony series (10), using only a linear elasticity solver and an ODE solver. This obviates the need to create special software for quasistatic viscoelasticity problems. For more on this we refer again to [20] and also to [33]

The Dirichlet-Prony series is not however the only form used to model the stress relaxation functions, for example the authors of [1] use the *stretched* relaxation function

$$\varphi(t) = \varphi_0 \exp(-(\alpha t)^p) \qquad \text{for } p \in (0,1]. \qquad (12)$$

Obviously no simple recurrence exists for this form. Another popular choice for φ is the *power law* where

$$\varphi(t) = \varphi_0 t^{-p} \qquad \text{for } p \in (0,1), \qquad (13)$$

although from either of (5) or (6) this implies that either $\underline{\boldsymbol{\varepsilon}}(0)$ is zero irrespective of the magnitude of the load, or $\underline{\boldsymbol{\sigma}}(0)$ is infinite. Neither of these are physically realistic and so we would prefer to modify this law to

$$\varphi(t) = \varphi_0 (t + \varphi_1)^{-p} \qquad \text{for } p \in (0,1), \qquad (14)$$

where $\varphi_1 > 0$ in order to remove the non-physical behaviour. Nonetheless, it is instructive to see how one might "derive" the power law, and for this we borrow heavily from Chern's thesis [3] which exploits the fractional calculus.

The formulation is based on the observed fact that viscoelastic materials behave in a way intermediate to that of solids and fluids. Interpreting this literally yields a constitutive law that contains fractional derivatives. Unfortunately we are unable here to give this interpretation the depth it deserves and instead try only to illustrate the main point. Recall that the stress in a solid is proportional to the strain while the stress in a fluid is proportional to the strain rate. Accepting the intermediate nature of viscoelastic materials the idea is to define the viscoelastic constitutive law as:

$$\underline{\boldsymbol{\sigma}}(t) = \underline{\boldsymbol{D}}^{(0)}\underline{\boldsymbol{\varepsilon}}(t) + \underline{\boldsymbol{D}}^{(1)}\partial_t^\alpha \underline{\boldsymbol{\varepsilon}}(t), \tag{15}$$

for constant fourth order tensors $\underline{\boldsymbol{D}}^{(0)}$ and $\underline{\boldsymbol{D}}^{(1)}$, and where $\alpha \in [0,1)$. The fractional derivative operator may be defined as:

$$\partial_t^\alpha \underline{\boldsymbol{\varepsilon}}(t) := \frac{\partial}{\partial t}\left(\frac{1}{\Gamma(1-\alpha)}\int_0^t (t-s)^{-\alpha}\underline{\boldsymbol{\varepsilon}}(s)\,ds\right), \qquad \text{for } \alpha \in [0,1). \tag{16}$$

(Note that α can be irrational, even though the word "fractional" is always used.) By firstly integrating by parts in (16) and then taking the differentiation through, Chern arrives at a constitutive law which is suitable for use within the standard finite element framework. Two solution schemes are considered: a solution in the Laplace transform domain and a direct time domain solution. However, in this case there is no efficient history storage and so the operation counts and computer memory requirement grow without bound as the time step is diminished.

The "justification" for the power law is as follows. Carrying out this integration-differentiation process gives

$$\partial_t^\alpha \varepsilon(t) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\varepsilon(0) + \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-s)^{-\alpha}\varepsilon'(s)\,ds, \tag{17}$$

and using this in the scalar analogue of equation (15) we now arrive at the constitutive law:

$$\sigma(t) = E_0\varepsilon(t) + \frac{E_1 t^{-\alpha}}{\Gamma(1-\alpha)}\varepsilon(0) + \frac{E_1}{\Gamma(1-\alpha)}\int_0^t (t-s)^{-\alpha}\varepsilon'(s)\,ds. \tag{18}$$

This seems to combine (5) and (6) when $\varphi(t)$ is given by the power law, (13).

We now have several candidates for the constitutive law and these may be used to generate a variety of differential equation problems. In the following pages we do just this and demonstrate how concrete forms of the abstract problems (1), (2) and (3), as well as some non-standard variants, can be derived to model viscoelastic behaviour.

3 Viscodynamics

To obtain the governing equations for the dynamic response of a viscoelastic body one uses Newton's second law to relate the stress field $\underline{\boldsymbol{\sigma}}$ and the forces $\boldsymbol{f}$ and $\boldsymbol{g}$ to the acceleration, or *inertia*, of the body $\mathcal{G}$. This process is familiar from linear elasticity theory and gives, with boundary and initial data, the following. For $i = 1, \ldots, n$:

$$\left.\begin{array}{rcll} \varrho u_i'' - \sigma_{ij,j} & = & f_i & \text{in } \Omega \times \mathcal{I}, \\ u_i & = & 0 & \text{in } \Gamma_D \times \mathcal{I}, \\ \sigma_{ij}\widehat{n}_j & = & g_i & \text{in } \Gamma_N \times \mathcal{I}, \\ u_i(\boldsymbol{x}, 0) & = & u_{i0} & \text{in } \Omega, \\ u_i'(\boldsymbol{x}, 0) & = & u_{i1} & \text{in } \Omega. \end{array}\right\} \tag{19}$$

Here: repeated indices imply summation; ϱ is the mass-density of $\mathcal{G}$; and, $\widehat{\boldsymbol{n}} := (\widehat{n}_i)_{i=1}^n$ is the unit outward directed normal to Γ_N.

Using (6) to substitute for the stress one arrives at the PDV problem: find $\boldsymbol{u}$ such that

$$\varrho u_i''(t) - \big(D_{ijkl}(0)\varepsilon_{kl}(\boldsymbol{u}(t))\big)_{,j} = f_i(t) - \int_0^t \left(\frac{\partial D_{ijkl}(t-s)}{\partial s}\varepsilon_{kl}(\boldsymbol{u}(s))\right)_{,j} ds,$$

in $\Omega\times\mathcal{I}$ with the indicated initial-boundary data. With an appropriate definition of A and $B(t,s)$ this is clearly a realization of the abstract problem (3). Note that it is "safe" to use the Dirichlet-Prony series (10) or modified power law (14) in this problem, but we may not use the power law (13) directly because we cannot then interpret $\underline{\boldsymbol{D}}(0)$.

In terms of existence, uniqueness and stability of solutions this problem has been studied in [9, 10, 24]. Numerical schemes are given in [12, 45, 29, 32].

One could also use the fractional calculus model to substitute for $\underline{\boldsymbol{\sigma}}$ in Newton's second law. This will yield a PDV equation of the form

$$\varrho u_i''(t) - \big(D_{ijkl}^{(0)}\varepsilon_{kl}(\boldsymbol{u}(t))\big)_{,j} = f_i(t) + \frac{D_{ijkl}^{(1)}}{\Gamma(1-\alpha)}\frac{\partial}{\partial t}\int_0^t (t-s)^{-\alpha}\varepsilon_{kl}(\boldsymbol{u}(s))\, ds.$$

On the other hand one could use (5) and then arrive at

$$\varrho u_i''(t) - \big(D_{ijkl}(t)\varepsilon_{kl}(\boldsymbol{u}(0))\big)_{,j} = f_i(t) + \int_0^t \big(D_{ijkl}(t-s)\varepsilon_{kl}(\boldsymbol{u}'(s))\big)_{,j}\, ds.$$

Note that $\boldsymbol{u}$ does not occur as a natural "unknown" in this problem and so it is possible to replace $\boldsymbol{u}$ with $\boldsymbol{u}'$ and arrive at the alternative problem: find $\boldsymbol{u}$ such that

$$\varrho u_i'(t) + \int_0^t \big(D_{ijkl}(t-s)\varepsilon_{kl}(\boldsymbol{u}(s))\big)_{,j}\, ds = f_i(t) - \big(D_{ijkl}(t)\varepsilon_{kl}(\boldsymbol{u}_0)\big)_{,j},$$

which makes sense if $\boldsymbol{u}_0$ is smooth enough. The initial datum for this problem is now $\boldsymbol{u}(0) = \boldsymbol{u}_1$. Properties of the solution of these type of problems are studied in [10, 24] and numerical analysis is given in [25, 23].

However, one must resist the temptation to interpret this as a parabolic problem for, in general, it is not. To see this use the power law (13) with (9) to obtain (with $\varrho = 1$ and $\underline{\boldsymbol{D}}$ not $\boldsymbol{x}$ dependent for simplicity):

$$u_i'(t) + D_{ijkl} \int_0^t (t-s)^{-p} (\varepsilon_{kl}(\boldsymbol{u}(s)))_{,j} \, ds = \widetilde{f}_i(t), \tag{20}$$

where $\widetilde{f}$ now incorporates the additional term in $\boldsymbol{u}_0$. In the case $p = \frac{1}{2}$ we find that the operator I defined by,

$$Iw(t) := \frac{1}{\sqrt{\pi}} \int_0^t (t-s)^{-\frac{1}{2}} w(s) \, ds$$

has the property,

$$I^2 w(t) \equiv I(Iw)(t) = \int_0^t w(s) \, ds,$$

and so may be regarded as the *square root* of the definite integral operator. Applying $\partial_t^{\frac{1}{2}}$ to both sides of (20) in the case $p = \frac{1}{2}$ we arrive at

$$\left(\frac{\partial}{\partial t} \right)^{\frac{3}{2}} u_i(t) + \sqrt{\pi} D_{ijkl} (\varepsilon_{kl}(\boldsymbol{u}(t)))_{,j} = \partial_t^{\frac{1}{2}} \widetilde{f}_i(t).$$

This equation is *half way* between being parabolic and hyperbolic. Similar manipulations are also possible in the case $p \neq \frac{1}{2}$, with the final time derivative being of order between 1 and 2. Numerical methods for fractional order differential equations are studied in [31, 22, 11].

For more detail on these type of problems see [27], as well as the other papers in that collection.

4 Viscostatics

Recall that the classical linear elasticity equations are "derived" from Newton's second law (19) by dropping the inertia term $\varrho \boldsymbol{u}''$. This corresponds to modelling the problem at times long after the load has been applied when the transient response has died out, and results in a very well-known elliptic problem. A similar approach can be adopted for viscoelastic response although this time it is a true approximation since the resulting problem is not time independent due to the persistence of the Volterra term. It seems that this approximation can be useful when the inertia term is negligible, which may occur when the load is smoothly and slowly applied (and non-oscillatory), or when it is the long-time *creep* response that is of interest. Since the time dependence persists we refer to the resulting problems as modelling *quasistatic* viscoelastic response.

The governing equations for these type of problem are obtained from (19) by setting $\varrho \boldsymbol{u}''(t) := 0$ and discarding the initial data. Thus, for $i = 1, \ldots, n$ we have

$$
\left.\begin{array}{rcll}
-\sigma_{ij,j} & = & f_i & \text{in } \Omega\times\mathcal{J}, \\
u_i & = & 0 & \text{in } \Gamma_D\times\mathcal{J}, \\
\sigma_{ij}\widehat{n}_j & = & g_i & \text{in } \Gamma_N\times\mathcal{J},
\end{array}\right\} \qquad (21)
$$

which are turned into differential equation problems for $\boldsymbol{u}$ by substituting for the stress using either of (5) or (6). These give respectively the PDV problems: find $\boldsymbol{u}$ such that for each $i\in\{1,\ldots,n\}$,

$$
-\int_0^t \big(D_{ijkl}(t-s)\varepsilon_{kl}(\boldsymbol{u}'(s))\big)_{,j}\,ds = f_i(t) + \big(D_{ijkl}(t)\varepsilon_{kl}(\boldsymbol{u}(0))\big)_{,j},
$$

and

$$
-\big(D_{ijkl}(0)\varepsilon_{kl}(\boldsymbol{u}(t))\big)_{,j} = f_i(t) - \int_0^t \left(\frac{\partial D_{ijkl}(t-s)}{\partial s}\varepsilon_{kl}(\boldsymbol{u}(s))\right)_{,j} ds.
$$

The first of these is essentially a Volterra first-kind equation for $\boldsymbol{u}'$, while the second is a second-kind equation for $\boldsymbol{u}$. In both cases one obtains $\boldsymbol{u}(0)$ by solving a linear elasticity problem.

Numerical schemes and *a priori* error estimates were first provided for both of these problems in [35]. Later and for the second-kind problem only, the estimates were improved (in terms of the size of the error constant) in [34]. These results depend on by-passing Gronwall's inequality and using more sensitive comparison results to obtain sharp data-stability estimates. These estimates have now been generalized in [40]. Also for the second-kind problem, *a posteriori* error estimates for a space-time finite element discretization of a model problem have been given in [38] and [42]. These results are based on the error estimates in [37] and are currently being generalized to the multidimensional problem described above in [41].

5 Non-Fickian diffusion

In classical diffusion theory the gradient of the concentration u of an active agent (the penetrant) diffusing through a carrier medium is related to the mass flux by Fick's law: $\boldsymbol{J} = -\lambda\nabla u$, where λ is the diffusivity of the carrier substance. Conservation of mass then demands that $u' = -\nabla\cdot\boldsymbol{J}$ which yields the familiar heat equation,

$$
u'(t) = \nabla\cdot\lambda\nabla u.
$$

If we define $M(t)$ as the total mass of penetrant absorbed by the carrier per unit area at time t then it is well known (from similarity solutions) that $M(t)\sim t^{\frac{1}{2}}$ for Fickian diffusion.

Diffusion in rubbery polymers, those well above their glass transition temperature (GTT), is according to Durning in [13] adequately described by Fick's law, but the situation is much more complicated for glassy polymers, those near but above their GTT. As the penetrant moves through the polymer it can force a phase change and so leave behind it the polymer carrier in its rubbery state. The stiffness and relaxation properties of the polymer change abruptly by orders of magnitude across this phase change (see for example [15]), and as a result a differential stress is set up across the penetrant boundary. Moreover, because the carrier is viscoelastic this stress is described by a hereditary constitutive law and this behaviour provides a mechanism for the observed non-Fickian effects. Workers in the field make the following very rough classification.

Case I diffusion: standard Fickian diffusion where $M(t) \sim t^{\frac{1}{2}}$, applies to polymers in the rubbery state high above the GTT.

Case II diffusion: non-Fickian diffusion, $M(t) \sim t^{\alpha}$ where $\frac{1}{2} < \alpha \leq 1$, applies to glassy polymers near to but above the GTT.

There is also a "Super Case II" category corresponding to $\alpha > 1$, see [5]. For Case II sharp fronts (rather like shocks) may appear as the penetrant diffuses through the carrier. This front moves initially at a constant speed and then slows down, [7], and this explains why $M(t)$ is almost linear, and thus $M'(t)$—the rate of absorbtion—is almost constant. By contrast $M'(t)$ for Case I is, in the words of Cox in [7], "delta-function-like", and this property of glassy polymers has an interesting application in the area of controlled drug delivery products. Cox gives a nice example.

An active agent (the drug) is embedded into a polymer through which it cannot diffuse. This may for example be a tablet which is to be swallowed. When the carrier is invaded by a solvent, such as digestive fluid, the drug can then diffuse out of the polymer through the solvent in a non-Fickian way. Since $M'(t)$ is almost constant, this allows a controlled, constant-rate delivery of the drug to the body for several hours.

The polymer doesn't have to be a tablet. In fact, according to Cohen and White in [5] (who also describe other applications of non-Fickian diffusion), such "smart" pharmaceutical products can be designed to be "swallowed, smelled, surgically implanted, rubbed on, taped on, strapped on", and can in effect be applied to any part of the body. There is an extensive literature on this science and in addition to those already cited we refer also to [17, 6, 14].

To get a flavour of the mathematical modelling that these people employ we borrow from [4] and consider the modelling of one-space dimensional diffusion through a glassy polymer. Our development yields a linear model, but it is unlikely that this will reproduce the sharp fronts characteristic of polymer diffusion. The references cited deal with realistic nonlinear models.

To account for the differential stress set up at the penetrant front Fick's law is modified to include a stress dependence in the following way:

$$J = -(\lambda u_x + \kappa \sigma_x).$$

Here u is the concentration, λ the usual (Fickian) diffusion constant, and κ is a proportionality constant. Conservation of mass again demands that $u' = -J_x$ and this gives

$$u' = \lambda u_{xx} + \kappa \sigma_{xx}.$$

The stress is viscoelastic and the usual approach is to adopt the Maxwell model, given earlier in (7), with the assumption that u depends linearly on strain rate ε' (in order to get true Case II behaviour—see [8]). Thus

$$\frac{\partial \sigma}{\partial t} + \frac{\sigma}{\tau} = \mu u,$$

where μ is a proportionality constant. In the nonlinear theory the dependence of τ on u is crucial, but here we shall assume that τ is constant. Integrating we get

$$\sigma(t) = \mu e^{-t/\tau} u(0) + \mu \int_0^t e^{-(t-s)/\tau} u(s)\, ds.$$

Eliminating the stress from the transport equation and using mass conservation gives the single differential-Volterra equation,

$$u'(t) = \lambda u_{xx} + \kappa \mu e^{-t/\tau} u_{xx}(0) + \kappa \mu \int_0^t e^{-(t-s)/\tau} u_{xx}(s)\, ds.$$

Assuming for simplicity that $u(0) = 0$ we can generalize this to a multidimensional model and obtain the PDV equation,

$$u'(t) = \nabla \cdot \lambda \nabla u + \nabla \cdot \left(\kappa \nabla \int_0^t \mu e^{-(t-s)/\tau} u(s)\, ds \right).$$

This is a concrete realization of the abstract problem (2).

Equations of this nature have been studied in [26] and [18], and some numerical analysis is given in [45, 2, 43, 30, 44]. Also, *a priori* and *a posteriori* error estimates for a finite element discretization of a scalar prototype ODE with memory, of the type that arises after spatial finite element semi-discretization of this problem, are provided in [36].

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