

Qualitative interpretation of creep and relaxation experimental data

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Abstract

Automated interpretation of experimental data is a necessary component in automated model building environments, i.e. tools capable to select a model which explains the observed behavior of a physical system. This paper describes an algorithm for the qualitative interpretation of experimental data whose goal is to single out the qualitative properties which characterize the behavior of a real physical system, and, consequently, to make a guess for a set of plausible candidate models of the phenomenon under study. We consider observations which are gathered from creep and relaxation experiments on visco-elastic materials. In this specific context, the interpretation problem consists in determining rules for the conversion of the numerical data into the specific qualitative properties which characterize the creep and relaxation response of the material. Such properties allow us to select within a library of mathematical models [4] of ideal materials a set of candidate models which describe, at least qualitatively, the behavior of the material.

1 Introduction

A major problem in the development of a computational environment that can reason about physical systems is its ability to formulate a model. The interpretation of observations is a necessary step in the model formulation process: the expert, given a set of observations, examines the shape of the plotted data and, on the basis of the highlighted properties, makes an initial guess for one or more models explaining the features of the data. In this paper, we describe a method to automate the visual interpretation skills performed by rheologists in the interpretation of numerical observations obtained by creep and relaxation experiments on visco-elastic materials [1, 7, 10]. Creep and relaxation tests are the most commonly performed because of the simplicity of their implementation with respect to the richness

of the captured information [11]. A *creep* experiment consists in applying an external force on the material and observing the caused deformation, whereas a *relaxation* test consists in imposing a deformation and measuring the corresponding produced stress. According to the input signal shape, we further distinguish static from dynamic experiments. Static tests involve the instantaneous imposition of a constant stress (or strain) and the observation of the subsequent evolution over time of the strain (or stress). Dynamic tests involve the application of an oscillatory input signal. Static experiments highlight the qualitative visco-elastic properties we are interested in better than dynamic tests, as in the former case the response of the material can be analyzed even in the very initial phase of the experiment, whereas in the latter one it provides useful information only after a transitory phase. For this reason, we only consider static tests.

For the sake of a clear explanation, let us focus our attention on creep data. In this specific context, the qualitative strain properties which may characterize the response of visco-elastic materials are *instantaneous elasticity*, *delayed elasticity* and *viscosity*. Therefore, the interpretation problem consists in determining conversion rules which specify which sets of numerical observations map into the three mentioned properties. More specifically, the analysis of creep experimental data obtained during the loading time $[t_0, t_1[$ allows us to identify the strain properties of the material: (1) a steep growth near t_0 may identify the presence of instantaneous elastic strain; in $]t_0, t_1[$, (2) a trend to increase according to a non-linear concave curve and (3) a trend to increase asymptotically as a straight line with positive slope may denote the presence of either delayed elasticity or viscosity, respectively.

Although our approach has been designed for interpreting data in a specific domain, it results to be a domain-independent technique as it is capable to transform a stream of observed data into a qualitative description of its shape, that is it highlights the qualitative properties of the numerical data such as monotonicity, convexity and linearity regions. Moreover, problems which make the data interpretation a difficult task and which are common to most experimental situations, such as the choice of a suitable scale of representation, have been considered.

The work here described is part of a research effort aimed at developing a comprehensive computational environment that automates all steps of formulation of the constitutive law of an actual visco-elastic material [2, 3, 4, 5]. The candidate models of the material are drawn out of a library of models in accordance with the qualitative match of the response of the material to standard experiments against the qualitative simulated behaviors associated with the models in the library. The model library includes both models of ideal materials and their qualitative response to standard experiments. The models are generated in two different formalisms (rheological formulae and Ordinary Differential Equations (ODE)), by following an enumerative procedure and an approach which is grounded both on a component-connection paradigm and on internal state variables. The ODE which best reproduces the behavior of a material is automatically selected within the set of plausible candidates by exploiting pieces of in-

formation captured by experimental data. The values of the parameters which appear in the equation, calculated through techniques of fitting of experimental data, characterize the actual material.

2 Qualitative interpretation of experimental data

To assess the mechanical properties of a visco-elastic material, standard experiments are usually performed. Such tests consist in recording the measurements associated with the mechanical behavior of the material in response to simple known loading functions. As we consider only creep static tests, the input signal shape is given by:

$$s(t) = s_0[H(t - t_0) - H(t - t_1)], \quad s_0 > 0 \text{ constant}, \quad H(t) = \begin{cases} 0 & t < 0 \\ 1 & t \geq 0 \end{cases},$$

where $s(t)$ is the stress.

2.1 The problem

A typical strain response of a visco-elastic material to a creep test is shown in Figure 1, and is here discussed.

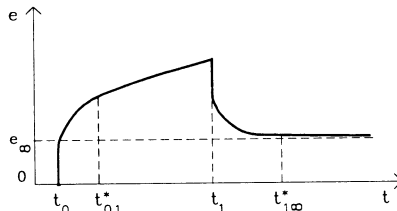


Figure 1: A typical strain response of a visco-elastic material to a creep test

When the load is applied, the material deforms. The evolution over time of the strain $e(t)$ characterizes the material ability at storing the deformation energy as potential energy, and, consequently, the material ability at releasing such energy as elastic energy in the recovery phase. Part of the produced deformation can occur instantaneously, at the loading instant $t = t_0$, and part can occur during the constant load interval $]t_0, t_1[$, with a rate which can eventually (in Figure 1, for $t > t_{01}^*$) get nearly constant. The presence of a constant deformation rate is explained by energy dissipation as viscous flow. When the load is removed, the instantaneous component of the produced strain is recovered, instantaneously as well, at time $t = t_1$; the remaining recoverable strain takes a longer time ($t > t_1$) to recover. However, some deformation may turn out to be permanent ($e(t) \approx e_{\infty} > 0$ for $t \in \tau_{\infty} =]t_{1\infty}^*, \infty[$) as a consequence of the material inability at storing all the deformation energy as potential energy.

Therefore, the strain response can be qualitatively described in terms of its instantaneous elastic (e_H), delayed elastic (e_K) and viscous (e_N) components, whose graphical characterization is summarized below. Denoting by T (True) and F (False) either the presence or absence of the

mentioned strain components, we can say that:

- (1) strain “jumps” at t_0 and t_1 denote *instantaneous elasticity* ($e_H=T$);
- (2) a non-linear concave curve in $t \in]t_0, t_1[$ or, equivalently, a non-linear convex curve for $t > t_1$ denote *delayed elasticity* ($e_K=T$);
- (3) an eventually “linear” growth at late loading ($t > t_{01}^*$) or, equivalently, a positive residual strain long after unloading ($t > t_{1\infty}^*$) denote *viscosity* ($e_N=T$).

2.2 The algorithm

The identification of the mechanical features that qualitatively characterize the behavior of a material is performed by an analysis of the experimental curve shape at significant “time points” and “time intervals”. Such an analysis combines techniques from both qualitative reasoning and pattern recognition.

The actual numerical values of the experimental data associated with different materials may differ by several orders of magnitude. To capture the shape features of the experimental curves we can associate with each curve a set of numerical descriptors. As data are affected by measurement errors, these descriptors cannot be “exact” values. For example, a horizontal straight line is characterized by a numerical descriptor (slope) whose numerical value is zero; but, in an experimental situation, straight lines whose numerical descriptor is smaller than a threshold can be considered to be horizontal. Of course, such a threshold is not fixed but depends on the material, i.e. on the order of magnitude of the measurements related to the material. Instead of associating with each material the set of its suitable threshold values for the numerical descriptors which describe the qualitative properties we are interested in, we fix the set of the threshold values and transform the data by suitable scaling factors. The scale factors are chosen so that the transformed data are plotted in the same reference coordinate window, where the quantitative numerical descriptors are calculated. In this window, data segmentation is performed, i.e. regions are identified which are homogeneous with respect to such graphical features as steepness, linearity, concavity, convexity: lines or curve segments are qualitatively characterized by mapping quantitative numerical descriptors to qualitative values.

2.2.1 Instantaneous elasticity Let us distinguish between *creep points* $(t_i^c, e_i^c)_{i=1, \dots, N_c}$, $t \in [t_0, t_1[$, and *recovery points* $(t_i^r, e_i^r)_{i=1, \dots, N_r}$, $t \in [t_1, +\infty[$. In order to reason about the instantaneous properties we should consider the data observed in t_0 and t_1 . Because of the measurement errors in these time-points, which are in part due to the instrumental inertia, we consider the experimental data in $\tau_0 = [t_1^c, t_1^c + \varepsilon]$ and $\tau_1 = [t_1^r, t_1^r + \varepsilon]$, neighbourhoods of t_0 and t_1 respectively. The qualitative strain rate of variation in τ_0 , $e'(\tau_0)$, can be estimated by the quantitative numerical descriptor $\alpha(\tau_0)$ which is the slope of the least squares line

through $\{(t_i^c, e_i^c), t_i^c \in \tau_0\}$:

$$e'(\tau_0) = \begin{cases} +\infty & \alpha_{large} < \alpha(\tau_0) \\ +large & \alpha_{small} < \alpha(\tau_0) < \alpha_{large} \\ +small & \alpha_{null} < \alpha(\tau_0) < \alpha_{small} \\ 0 & -\alpha_{null} < \alpha(\tau_0) < \alpha_{null} \\ -small & -\alpha_{small} < \alpha(\tau_0) < -\alpha_{null} \\ -large & -\alpha_{large} < \alpha(\tau_0) < -\alpha_{small} \\ -\infty & \alpha(\tau_0) < -\alpha_{large} \end{cases}$$

where $\{-\infty, -large, -small, 0, +small, +large, +\infty\}$ are totally ordered qualitative values, and the positive constants α_{large} , α_{small} , α_{null} are the heuristically defined threshold values. The curve steepness in τ_1 can be qualitatively evaluated in a similar way. Instantaneous elasticity is then assessed according to the following rule:

$$e_H = T \Leftrightarrow \begin{cases} e'(\tau_0) = +\infty \wedge e'(\tau_1) \leq -large \\ e'(\tau_0) \geq +large \wedge e'(\tau_1) = -\infty \end{cases} \vee$$

2.2.2 Viscosity A quantitative descriptor suitable to capture linearity of data affected by noise is the linear correlation coefficient (r). Therefore, the presence of a linear growth region $[t_{01}^*, t_1]$ can be ascertained by computing r^2 on the late creep points and testing whether it takes a value sufficiently close to 1 ($r^2 > \bar{r}$, where $\bar{r} \approx 1$ is fixed).

More precisely, let $\mathcal{L}_p^c = \{(t_j^c, e_j^c), j = N_c - p, \dots, N_c\}$, with p great enough to ensure that a sufficient number of points is considered, and let $L^c = \cup_p \{\mathcal{L}_p^c \mid r^2(\mathcal{L}_p^c) > \bar{r}\}$. Then, we can define:

$$t_{01}^* = \begin{cases} t_1 & \text{if } L^c = \emptyset \\ \min_j \{t_j^c \mid (t_j^c, e_j^c) \in L^c\} & \text{if } L^c \neq \emptyset \end{cases}, \quad \tau_{01} = [t_{01}^*, t_1[,$$

and we might decide that if a region exists where the curve is characterized by linear growth at positive rate then there is viscosity:

$$L^c \neq \emptyset \wedge e'(\tau_{01}) > 0 \Rightarrow e_N = T$$

where $e'(\tau_{01})$ takes its qualitative value in accordance with the slope $\alpha(\tau_{01})$ of the least squares line through L^c .

The analysis of the recovery curve can corroborate conclusion about viscosity. Let us denote by c_∞ a numerical descriptor of the asymptotic strain e_∞ (e.g. obtained by exponential fitting of the late recovery points). The comparison of c_∞ with suitable threshold values allows us to assign a qualitative value $e(\tau_\infty) \in \{0, +small, +large\}$ to the asymptotic strain. Now, if $L^c(\bar{r}_1')$, $L^c(\bar{r}_2'')$ denote curve segments obtained as indicated above with respect to two different thresholds $\bar{r}_1'$, $\bar{r}_2''$ for r^2 , ($\bar{r}_2'' > \bar{r}_1'$), and

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τ'_{01} , τ''_{01} denote the corresponding time intervals, we can assess viscosity according to the following more comprehensive rule:

$$e_N = T \Leftrightarrow \left\{ \begin{array}{l} L^c(\bar{r}'') \neq \emptyset \wedge e'(\tau''_{01}) > 0 \wedge e(\tau_\infty) > 0 \\ L^c(\bar{r}') \neq \emptyset \wedge e'(\tau'_{01}) > 0 \wedge e(\tau_\infty) > +small \end{array} \right. \vee$$

2.2.3 Delayed elasticity To reason about delayed elasticity, the curve concavity must be studied. In absence of noise, a suitable quantitative descriptor could simply be the second strain derivative, but, since data are affected by noise, a different approach which emulates the subjective visual smoothing performed by the human expert has to be found.

A way to address the problem is to divide the time interval $[t_1^c, t_{N_c}^c]$ for creep curve analysis, $[t_1^r, t_{N_r}^r]$ for recovery) into subintervals τ^h , each containing a sufficient number of experimental points, and consider the frequencies of the sign of the second strain derivative e'' .

More precisely, let e'_i , e''_i be the approximated values of e' and e'' in t_i^c . Let us consider only the subintervals τ^h where the qualitative value of $e'(\tau^h) < +large$. For each τ^h we define the qualitative value $e''(\tau^h) \in \{-, 0, +\}$ as the most frequent sign occurrence. Consequently, delayed elasticity can be assessed as follows:

$$e_K = T \Leftrightarrow [t_0, t_1] \setminus (\tau_{01} \cup \tau_0) \neq \emptyset \wedge e''(\tau^h) \leq 0 \forall h \wedge \exists \bar{h} : e''(\tau^{\bar{h}}) < 0$$

More comprehensively, the above rule can include clauses, based on quite a similar reasoning, on the curvature of the recovery curve.

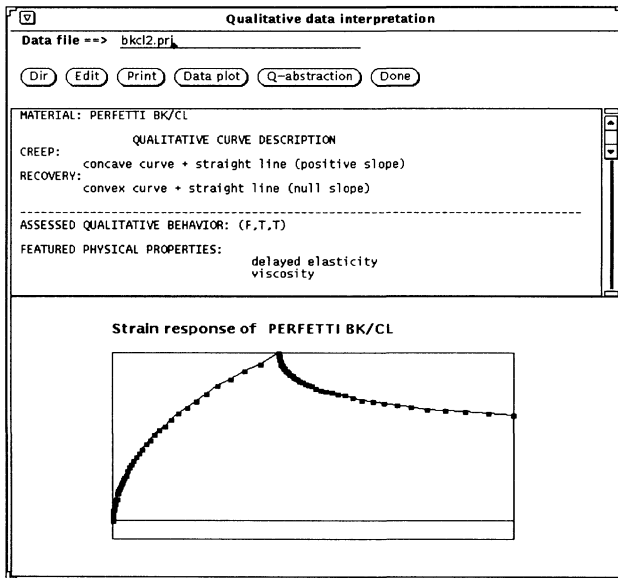


Figure 2: Qualitative interpretation of creep experimental data of a rubber-like material

2.2.4 An example As an example, let us consider the observed data from a creep experiment performed on a rubber-like material. Figure 2 is a screen dump from the implementation of the described algorithm. It displays a plot of the observations, the qualitative creep (concave curve + straight line with positive slope) and recovery (convex curve + positive horizontal straight line) curve description, and the featured physical properties attributed to the shape of the plot (delayed elasticity and viscosity). As a result of the match of the identified strain characteristics ($e_H = F$, $e_K = T$, $e_N = T$) against the qualitative simulated behaviors of ideal materials [4], plausible candidate mathematical models of the material can be automatically proposed. For the material in the example, 9 candidate models, whose equations are of the form $\sum_{i=0}^n a_i D^i s = \sum_{i=1}^{n+1} b_i D^i e$ (where $n = 1, \dots, 9$, D is the time derivative operator, a_i and b_i the parameters) are generated. Information on the number of retardation times will make it possible to select among the 9 proposed models the most appropriate one for the material.

3 Conclusion

Interpreting observations is a fundamental issue for the analysis of physical systems [6, 8, 9]. The presented implemented algorithm provides reasoning techniques to emulate the expertlike visual interpretation of rheological experimental data. We focussed on creep data as it has been easier to collect them than relaxation observations, but the same reasoning techniques are applied to identify the qualitative stress properties highlighted by relaxation experiments. Also in the latter case, the physical properties are characterized by the monotonicity regions of the curve associated with the data. The algorithm has been tested on experimental data related to different polymeric materials, such as inks, rubbers, and drugs (sodium carboxymethylcellulose) and its performance has been evaluated in accordance with the interpretation provided by the experts who supplied the data.

In spite of its simplicity, the algorithm provides also useful information about the adequacy of the models in the library to describe the behavior of the material under study: a possible convex shape of the data during the creep phase denotes that the linear theory of elasticity and viscosity we adopted to build the model library is inadequate to study such a material. Our future work will explore the possibility of enriching the library with non-linear models, which will be built starting from non-linear laws, e.g. $s(t) = k_1(\exp(k_2 e(t)) - 1)$, and $s(t) = k_1 \log(k_2 e'(t))$, for the elastic and viscous basic components, respectively. Another piece of work will deal with a more general and formalized version of the proposed algorithm, which will also deal with the statistical analysis of the measurement errors, so that it results to be a domain-independent tool for the qualitative interpretation of experimental data.

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