# Automated modelling of visco-elastic materials *

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**Abstract.** To build model-based systems capable of emulating the scientist's or engineer's way of reasoning about a given physical domain requires methods for automating the formulation or selection of a model, which adequately captures the knowledge needed for solving a specific problem. To find and exploit such models requires the use and integration of different kinds of knowledge, formalisms and methods. This paper describes a system which aims at reasoning automatically about visco-elastic materials from a mechanical point of view. It integrates both domain specific and domain independent knowledge in order to classify and analyse the mechanical behaviours of materials. The classification task is grounded on qualitative knowledge while the analysis of a material is performed at a quantitative level and is grounded on numerical simulation. The key ideas of our work are: to generate automatically a library of models of ideal materials and their corresponding qualitative responses to standard experiments, to classify an actual material by selecting within the library a class of models whose simulated qualitative behaviours to standard loads match the observed ones, to identify a quantitative model of the material, and then to analyse the material by simulating its behaviour upon any load. Each model in the library is automatically generated in two different forms: at the lowest level, as a symbolic description and then, at a mathematical level, as an ordinary differential equation. This paper mainly concentrates on the methods and algorithms of model generation and of qualitative simulation.

## 1. Introduction

This paper describes some work being carried out within the framework of Qualitative Physics research ([4], [12], [28]) with the goal of building systems that are capable of emulating the scientist's or engineer's way of reasoning about a given physical domain when performing problem-solving activity. More precisely it deals with an on-going programme of research whose long-term goal is the realization of a system capable of automating the engineer's way of reasoning about materials from different perspectives according to the class of problems to be solved. The basic steps the engineer performs in the study of materials may be identified as:

1. Choice of the perspective (e.g. chemical, electro-magnetic, thermodynamic, mechanical, thermo-mechanical) and consequently of the physical variables (e.g. volume, electric current, temperature, stress, strain) which are relevant for the specific problem;
2. Interpretation of the observations gathered through ad hoc designed experiments on the studied material, and a first rough classification of the material based on heuristic knowledge according to the pointed out properties;
3. Formulation of a mathematical model, guided by domain specific knowledge and past experience in modelling;
4. Validation of the model obtained at step 3 through the identification of its parameters, and therefore derivation of a quantitative model for the material;
5. Simulation of the dynamic behaviour of the material under different conditions by using numerical methods.

This reasoning scheme is obviously not peculiar to the materials science but is applied in many other physical contexts. The variables definition, the interpretation and modelling steps mainly take place at a symbolic and qualitative level, while the parameters identification and simulation steps are mainly numeric. The formulation of an accurate model explaining the observed behaviour (step 3) is the primary and most difficult activity. The initial guess for the model is heuristically approached in the light of accumulated experience; detected inconsistencies between the model predictions and the observations may suggest a model revision. It is evident that the model formulation process requires skilled and experienced engineers. Therefore, making it automatic is a fundamental step towards building intelligent problem-solving systems. Some methods for the automation of the modelling process have been recently proposed by several researchers (e.g. [1], [13], [15], [21], [27]).

* A more complete version of this paper will appear in the *Intelligent Systems Engineering Journal*

The system here described currently aims at reasoning automatically about materials from a mechanical point of view. From this perspective, an important problem to be solved is to predict how the mechanical properties of materials are affected by complex loading histories and how this behaviour in turn affects the performance of composite structures. In this context the state variables are stress and strain, and the main goal is to associate each material with its constitutive law, that is with the relationships between stress, strain and their time dependencies. The adopted method for building models able to predict the behaviour of materials when they are subject to external forces is that of rheology, whose matter of study is the investigation, at a macroscopic level, of the different kinds of deformation in relation to the stresses by which they are accompanied. Despite large differences in the microscopic structure of materials, there is a similarity displayed in their macroscopic behaviour. With different order of magnitude, mechanical fundamental properties like elasticity, viscosity, plasticity can be associated with all materials. This justifies the approach to the mechanics of materials taken by rheology ([22], [29]) which, postulating a direct cause-effect relation between stress and strain, allows the construction of models to be independent of the internal structure of materials. By this approach, the models of the materials are built by analogy with mechanical models using a component-connection paradigm. An analogical model is an assembly of mechanical components reproducing the fundamental mechanical properties, so arranged, in parallel or in series, that the overall system behaves analogously to a real material, although the components themselves may have no direct analogues in the material. A model of a material, at the lowest level, is given by the symbolic description (rheological formula) of its corresponding analogical structure. By exploiting suitable connection rules, the mathematical model of the structure as a whole is derived from the models of its basic components, which are expressed as functional relationships (in our case ordinary differential equations. ODE) between internal state variables.

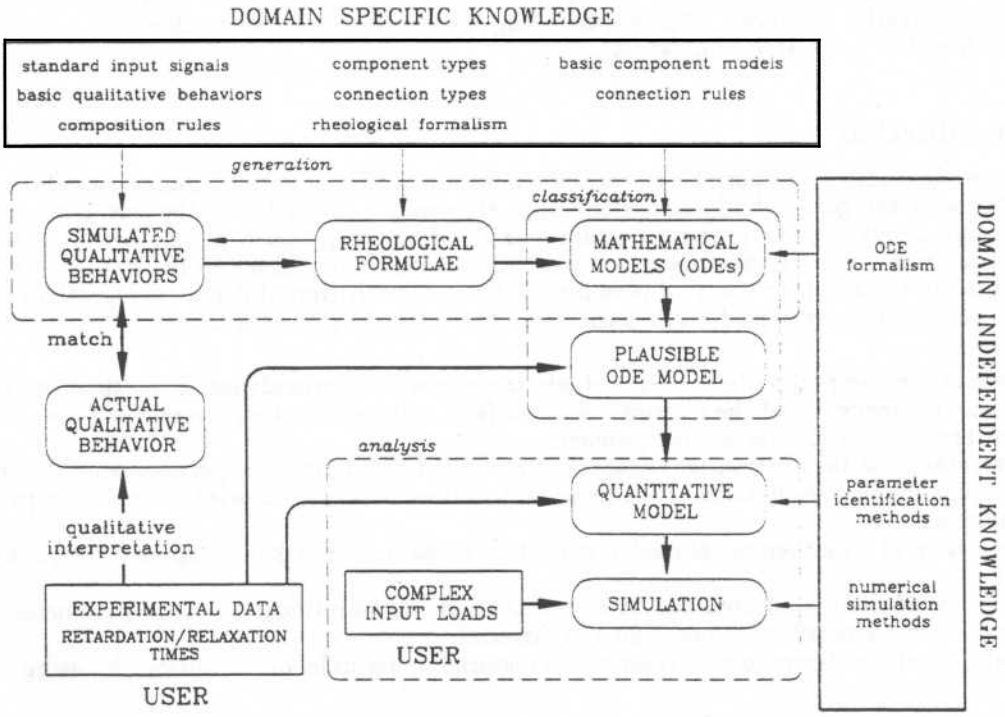


Figure 1 - Overview of the system. The main tasks of library generation, material classification and analysis are outlined by pointing out the basic steps they consist of. Arrows basically denote control flow: more precisely, thick arrows track data flows while marginal thin arrows denote system interactions with specific pieces of knowledge.

The designed system, whose structure is shown in Figure 1, integrates both domain specific and domain independent knowledge in order to classify and analyse the mechanical behaviours of materials. The analysis of a material, that is the precise study of the behaviour of the material under any complex signal load, is performed at a quantitative level and is grounded on numerical simulation. Performing the numerical simulations themselves is straightforward when a quantitative model of the material and numerical methods are given. The quantitative model is obtained by computing, through techniques of fitting of experimental data, the values of the parameters which appear in the ordinary differential equation which identifies the

material. Such an equation describes a class of ideal materials that best reproduce the response of the real material, and is selected within a library of models of ideal materials. Each model in the library is associated with its qualitative responses to standard experiments, and the result of the match of the experimental data, qualitatively interpreted, against the qualitative behaviours stored in the library allows to derive a set of candidate models for the material. Then, further pieces of information, e.g. the number of retardation or relaxation times, captured by the experimental data themselves, allow to identify within the set of candidates the most plausible mathematical model for the material.

The library of models and their qualitative responses is automatically generated, following an enumerative procedure and using a knowledge representation scheme based on rooted binary tree-like graphs.

The library generation process goes through the following three steps (Figure 1):

1. *Enumeration of the rheological formulae.* Symbolic descriptions of all non-equivalent analogical structures are generated by grouping structures with respect to equivalence relations and by selecting only one representative for each class.
2. *Generation of the mathematical models.* Given the set of rheological formulae built in step 1, its corresponding set of mathematical models is generated by exploiting, besides the basic component models and the connection rules, the ordinary differential equations formalism.
3. *Simulation of the qualitative responses of the generated models to standard input signals.* The behaviour of a material in response to the action of external forces is built starting from the rheological formula.

This paper details the methods and algorithms concerning the three above mentioned steps. The current implementation of the system is bounded to visco-elastic materials. Visco-elastic models describe the behaviour of a wide set of actual materials: for example, the mechanics of polymers, whose study is of great practical importance, is dominated by visco-elastic phenomena ([2], [16]). The extension to the plastic case, though conceptually compatible with the adopted approach, still poses some major problems in representing the discontinuity of the behaviour of the material.

This paper is organized as follows. First, the domain specific knowledge is described. This knowledge includes modelling assumptions, basic definitions, basic component models and connection laws. Next, three sections are devoted to the major algorithms of the library generation: enumeration of rheological formulae, generation of mathematical models and qualitative simulation. Then the overall process of selection of the most plausible model related to a given material is illustrated through an example. Finally the major contributions and limits of this work are discussed.

## 2. Domain specific knowledge

When materials are studied from a mechanical point of view and at a macroscopic level, the usual classification which groups them into solids, liquids and gases according to their state of molecular aggregation is of scarce practical value. A more suitable classification should rather be based on the way materials respond to the action of external mechanical forces.

Beside *elastic*, *plastic* and *viscous* materials, whose behaviours are well defined ([5], [20]) and taken as fundamental, there are many other materials which can not be satisfactorily classified, not even approximately, into any of these archetypes, but whose behaviours are related at various degrees to the fundamental mechanical properties.

As a matter of fact, most actual materials feature complex behaviours which are a combination of the three basic ones. Goal of rheology is precisely to build models of materials explaining how the fundamental mechanical properties combine to yield complex behaviours ([22], [29]).

### *2.1. Modelling assumptions*

A material is assumed to be a continuous, homogeneous and isotropic medium. Only stable materials are considered and therefore the deformation of a body solely occurs when mechanical energy has been provided.

The classification of a material is based upon tests which are carried out in isothermal conditions by means of devices where material samples are subject to tensions and/or compressions, while either the external force or the deformation is kept constant. Since most experiments are carried out in one-dimension, the following further assumption is justified: only one-dimensional external forces and responses are considered.

The physical variables characterizing a rheological model are *strain* and *stress*. The strain $e(t)$ is a measure of the deformation produced by an external force acting along the longitudinal axis of a body, and is given by the relative elongation of the body, that is $e(t) = (l(t) - l_0)/l_0$ where $l(t)$ and $l_0$ are the length of the body at time $t$ and the original length of the body respectively. The stress $s(t)$ is a measure of the internal tension state, which is concomitantly created in the continuous medium, and is given by the ratio $s(t) = F(t)/A_0$, where $A_0$ is the area of the cross-section of the body at time $t_0$ when the external force is not yet acting and $F(t)$ is the modulus of the applied external force.

The way the deformation is carried out upon loading and the way it is recovered after unloading is called the *response* of the material, and can be mathematically described by an ordinary differential equation involving stress, strain and their time derivatives.

*2.2. Basic component models and connection laws*

The method we adopted for modelling the response of a material is based on a component- connection paradigm and on internal state variables. The purely elastic response is described by the Hooke's law:

$$s = Ee \tag{2.1}$$

while the purely viscous response is given by the Newton's law:

$$s = \eta \dot{e} \tag{2.2}$$

where $E$ and $\eta$ are constants (dot denotes the time derivative). The elastic response corresponds to an ideal material $H$ which can be analogically represented by a spring; similarly the viscous response is associated with a material $N$ analogically represented by a piston. Let us denote by $\mathcal{C} = \{H, N\}$ the set of the basic components of a visco-elastic structure.

In order to establish the constitutive equation of a complex material, an analogical mechanical device in which elements of $\mathcal{C}$ are suitably connected in series or in parallel is associated with it. Let us denote by $\mathcal{O} = \{-, |\}$ the set of the basic connection operators.

When components $C_1$ and $C_2$ (not necessarily basic components) are connected in series, each component takes the same load and the total elongation is the sum of the elongation of each component.

$$C_1 - C_2 \quad \Leftrightarrow \quad \begin{cases} s = s_1 = s_2 \\ e = e_1 + e_2 \end{cases} \tag{2.3}$$

If the components are connected in parallel, they undergo the same elongations while the total stress gets distributed among the components.

$$C_1 \mid C_2 \quad \Leftrightarrow \quad \begin{cases} s = s_1 + s_2 \\ \epsilon = e_1 = e_2 \end{cases} \tag{2.4}$$

The strain and stress $e_i, s_i$ $(i = 1, 2)$ associated with each component are not directly observable and are called *internal variables*.

At the lowest level, the behaviour of a material can be modeled by a *rheological formula*, which is a symbolic description of the analogical model in terms of connections between basic components. A description of a structure at such a level is enough to reason qualitatively on materials: the qualitative responses of $H$ and $N$ together with suitable composition rules are sufficient to assemble the qualitative response of the whole structure. This symbolic expression is strictly analog to an arithmetic one and can be graphically shown as a circuit-like configuration.

## 3. Rheological formulae: the generation algorithm

The construction of a library of models, wide enough to allow the classification of any given actual material, goes through a step of automatic generation of rheological formulae [6]. Since our aim is to build models of materials which exhibit different behaviours, the set of rheological formulae is filtered out with respect to mechanical equivalence.

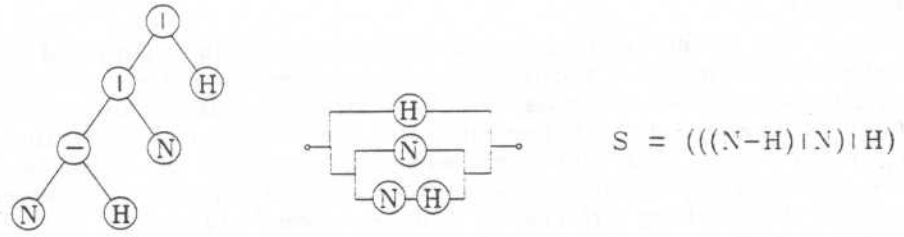


Figure 2 - Different representations of the same rheological structure: rooted binary tree, series-parallel circuit, rheological formula.

A unique knowledge representation scheme, based on rooted binary tree-like graphs [14] has been used. A structure consisting of $n$ elements can be represented by a rooted binary tree (Figure 2), whose internal node labels range in $\mathcal{O}$ (operator identifiers) and leaf labels in $\mathcal{C}$ (basic component identifiers).

A correct balance of operators and operands is guaranteed when internal nodes have exactly two children subtrees and amount to $n-1$, whereas the number of leaves is $n$; such trees are called *admissible*.

The enumeration of all the admissible structures is a combinatorial problem which can be approached by first generating all the unlabelled admissible trees and by subsequently labelling them.

Unlabelled admissible trees (briefly *u-trees*) are generated by recursively appending couples of new nodes to the leaves of previously generated trees. In order to limit the combinatorial explosion associated with the labelling step, the generated set of u-trees is filtered with respect to a kind of topological equivalence.

More precisely, let $\mathcal{T}_n$ be the set of all u-trees which underlie $n$-component structures. Let us denote by $\mathcal{T} = \bigcup_n \mathcal{T}_n$ and, $\forall t \in \mathcal{T}$, by $T_l(t)$ (respectively $T_r(t)$) the left (respectively right) subtree of the root of $t$ and define the following recursive relation $\chi$ in $\mathcal{T} \times \mathcal{T}$:

**Definition 1.** $t_1 \chi t_2 \Leftrightarrow$ both $t_1$ and $t_2$ have just one node
or $T_l(t_1) \chi T_l(t_2)$ and $T_r(t_1) \chi T_r(t_2)$
or $T_l(t_1) \chi T_r(t_2)$ and $T_r(t_1) \chi T_l(t_2)$.

It can be proved that $\chi$ is an equivalence relation in $\mathcal{T} \times \mathcal{T}$, which basically states the topological equivalence of u-trees that are equal apart from left/right subtree permutations. Therefore, the following recursive algorithm can be defined to generate a minimal set of u-trees $\mathcal{T}^* \subset \mathcal{T}$, by collecting only one representative for each $\chi$-equivalence class:

$(\mathcal{A}_1)$

$\mathcal{T}^* = \bigcup_n \mathcal{T}_n^*$, where $\mathcal{T}_n^*$ are recursively generated :

- $\mathcal{T}_1^* = \mathcal{T}_1$
- Given $\mathcal{T}_{n-1}^*$, $\mathcal{T}_n^*$ is generated as follows:

  $\forall t \in \mathcal{T}_{n-1}^*$ leaves are numbered by post-order traversal of $t$ :

  $\forall$ leaf $p$ of $t$ (following the above leaf ordering)

  Let $t'$ be the $n$-leaf tree obtained by appending the left and right direct descendents of $p$.

  If $t' \chi t^*$ is false $\forall t^* \in \mathcal{T}_n^*$ then $\mathcal{T}_n^* := \mathcal{T}_n^* \cup \{t'\}$:

After generating the sets $\mathcal{T}_n^*$, u-trees are given values in $\mathcal{O}^{n-1} \times \mathcal{C}^n$, i.e. $(2n-1)$-tuples of identifiers are provided to label the tree nodes. Consequently the elements of the sets $\mathcal{M}_n = \mathcal{T}_n^* \times \mathcal{O}^{n-1} \times \mathcal{C}^n$ and $\mathcal{M} = \bigcup_n \mathcal{M}_n$ are identified with rheological structures: the associated formulae are obtained by in-order traversing the labelled trees, placing the parentheses in order to keep all hierarchical information, as it is usually done for arithmetic expressions.

Then, adequate filter procedures, based on the algebraic properties of the connection operators, have been defined so that the set $\mathcal{M}$ is replaced by the smaller set of all algebraically distinct rheological structures.

For the sake of simplicity, let $\mathcal{M}_n$ and $\mathcal{M}$ still denote the resulting filtered sets. To catch the residual, least obvious, mechanical equivalences, the form of the differential equations associated with the generated formulae has to be investigated.

## 4. Automatic generation of the mathematical models.

The derivation of the set of mathematical models corresponding to the enumerated rheological formulae is performed through specifically tailored symbolic algebra procedures, by exploiting the hierarchical information captured by the labelled trees, the internal state variables, the mathematical models of the basic components (2.1), (2.2) and the connection laws (2.3), (2.4).

The general form of the equation associated with a rheological formula $M \in \mathcal{M}$ is a differential equation:

$$\sigma(D)s = \varepsilon(D)e \tag{4.1}$$

where $\sigma(D)$ and $\varepsilon(D)$ are polynomials in the time derivative operator $D$. $s$ is the stress and $e$ the strain.

The following algorithm $\mathcal{A}_2$ recursively defines $\sigma(D)$ and $\varepsilon(D)$ from the polynomials $\sigma_i(D)$, $\varepsilon_i(D)$ $(i = 1, 2)$ associated with the binary components $M_i$ of $M$:

$$(\mathcal{A}_2)\ \begin{cases} \bullet \text{ if } M \text{ is a basic component :} \\ \quad M = H \ \Rightarrow\ \sigma(D) = 1,\ \varepsilon(D) = E \quad \text{according to (2.1).} \\ \quad M = N \ \Rightarrow\ \sigma(D) = 1,\ \varepsilon(D) = \eta D \quad \text{according to (2.2):} \\ \bullet \text{ if } M \text{ is a complex component :} \\ \quad M = M_1 - M_2 \ \Rightarrow\ \begin{cases} \sigma(D) = \sigma_1(D)\cdot\varepsilon_2(D) + \sigma_2(D)\cdot\varepsilon_1(D) \\ \varepsilon(D) = \varepsilon_1(D)\cdot\varepsilon_2(D) \end{cases} \qquad (4.2) \\ \quad M = M_1 \mid M_2 \ \Rightarrow\ \begin{cases} \sigma(D) = \sigma_1(D)\cdot\sigma_2(D) \\ \varepsilon(D) = \sigma_1(D)\cdot\varepsilon_2(D) + \sigma_2(D)\cdot\varepsilon_1(D) \end{cases} \qquad (4.3) \end{cases}$$

The equations (4.2)-(4.3) are the formal result of the elimination of the internal variables by exploiting (2.3)-(2.4). The final form of the polynomials $\sigma(D)$ and $\varepsilon(D)$ is then obtained by dividing both $\sigma(D)$ and $\varepsilon(D)$, either in (4.2) or in (4.3), by their greatest common divisor and by the coefficient of the term of $\sigma(D)$ with the lowest degree.

For example, the mathematical model of the material $K = H|N$ is straightforward obtained from (4.3): $\sigma_1(D) = 1$ , $\varepsilon_1(D) = E$ , $\sigma_2(D) = 1$ , $\varepsilon_2(D) = \eta D$ hence $\sigma(D) = 1$ , $\varepsilon(D) = \eta D + E$ . that is $s = Ee + \eta\dot{e}$ holds.

**Definition 2.** Let us call *formal equation* associated with $M \in \mathcal{M}$. the differential equation obtained from its corresponding equation by giving all of its non-zero coefficients the value 1.

The mechanical equivalence of two formulae can now be established by comparing the associated formal equations. The following equivalence relation $\rho$ can be defined in $\mathcal{M}$:

**Definition 3.** $M_1\ \rho\ M_2 \Leftrightarrow M_1$, $M_2$ share the same formal equation.

By filtering with respect to $\rho$, the goal of building solely mechanically distinct rheological formulae is fully achieved.

**Theorem.** The admissible formal equations have one of the following forms:

$$(I) \qquad \sum_{i=0}^{m} D^i s \ = \ \sum_{i=0}^{m} D^i e \qquad\qquad (II) \qquad \sum_{i=0}^{m} D^i s \ = \ \sum_{i=1}^{m+1} D^i e$$

$$(III) \qquad \sum_{i=0}^{m} D^i s \ = \ \sum_{i=0}^{m+1} D^i e \qquad\qquad (IV) \qquad \sum_{i=0}^{m} D^i s \ = \ \sum_{i=1}^{m} D^i e$$

where $m \geq 0$ in the first three equations, and $m \geq 1$ in $(IV)$.

*Proof*: From (4.2)-(4.3) it follows that:

*i)* if $\sigma_1(D) = 1 + D + \phi_1(D)$, $\sigma_2(D) = 1 + D + \phi_2(D)$ then $\sigma(D) = 1 + D + \phi_3(D)$ ($\phi_1$, $\phi_2$, $\phi_3$ are polynomials in $D$ with degree $> 1$);

*ii)* if $\varepsilon_1(D) = 1 + D + \phi_1(D)$, $\varepsilon_2(D) = 1 + D + \phi_2(D)$ then $\varepsilon(D) = 1 + D + \phi_3(D)$;

*iii)* if $\varepsilon_1(D) = D + \phi_1(D)$, $\varepsilon_2(D) = D + \phi_2(D)$ then $\varepsilon(D) = D + \phi_3(D)$;

*iv)* if $\varepsilon_1(D) = 1 + D + \phi_1(D)$, $\varepsilon_2(D) = D + \phi_2(D)$ (or vice versa) then $\varepsilon(D) = D + \phi_3(D)$;

*v)* if the intermediate terms of the polynomials $\sigma_1(D)$, $\sigma_2(D)$, $\varepsilon_1(D)$, $\varepsilon_2(D)$ are non-zero then the intermediate terms of $\sigma(D)$ and $\varepsilon(D)$ are non-zero;

*vi)* either $degree[\varepsilon(D)] = degree[\sigma(D)]$ or $degree[\varepsilon(D)] = degree[\sigma(D)] + 1$. where $degree[\cdot]$ denotes the degree of the polynomial.

Let us remark that for $m = 0$ the equations $(I)$, $(II)$, $(III)$ respectively correspond to the formulae $H$, $N$, and $K$; for $m = 1$, the equation $(IV)$ corresponds to the formula $H - N$. It can be proved by induction that the number of the formal equations associated with formulae made up of at most $n$ components is $2n$.

Moreover, through arguments based on the Laplace transform, the number of retardation times associated with each type of the above equations can be determined (see e.g. [16], [29] for a precise definition of retardation and relaxation times, which is theoretically based on the form of the solution of the differential equation, but can often be related to experimentally observable phenomena). More precisely, $m$ retardation times correspond to equation-types $(I)$ and $(II)$, $m+1$ to $(III)$, and $m-1$ to $(IV)$. For example, in the simple case of the material $K$, whose equation is $s = Ee + \eta\dot{e}$, there is only one retardation time ($\tau_r = \eta/E$) which is a measure of the time needed to attain a significant fraction of the extension of the spring to its equilibrium length while retarded by the piston.

Let us remark that if non-linear models of the basic components are considered, $\sigma(D)$ and $\varepsilon(D)$ generally are not polynomials any more; consequently, the elimination of the internal variables is not formally performed as in (4.2)-(4.3) but can be achieved by symbolic manipulation according to the kind of non-linearity.

## 5. The qualitative simulation algorithm.

In this section an algorithm for the qualitative simulation of the response of visco-elastic materials to rheological experiments [7] is considered. The mathematical models of visco-elastic materials are ordinary differential equations of type $(I)-(IV)$ whose order $m$ can be high when the structure is complex. Therefore QSIM-like algorithms [18] are not adequate due to the large number of auxiliary variables that need to be introduced in order to write the corresponding qualitative equations.

The rheological experiments, ideal or actual, to be simulated consist in applying an external force and in observing the caused deformation (creep-like experiments) or vice versa in imposing a deformation and in measuring the corresponding force (relaxation tests), i.e. the time course of a state variable is given as input and the evolution over time of the other one has to be determined. The algorithm operates at the lowest level of description, that is on the rheological formula, and currently considers only creep-like experiments. More precisely, given as input a formula and a qualitative description of a stress signal $s(t)$ in terms of its significant time-points, the qualitative time course of the strain $e(t)$ is provided in output. The time evolution of the produced deformation is recursively built from the qualitative behaviour of the basic components at the deepest level of the representing tree by combining them in agreement with the compositional rules stated by the connection operator. At this level of study only positive signals, i.e. traction forces are considered.

The algorithm is based on the strain response to a standard signal:

$$s(t) = s_0[H(t-t_0) - H(t-t_1)],$$

where $s_0$ is a positive constant, $t_0$, $t_1$ are the significant time-points, and $H(t)$ is the Heaviside function, i.e. $H(t) = 0$ if $t < 0$, and $H(t) = 1$ if $t \geq 0$.

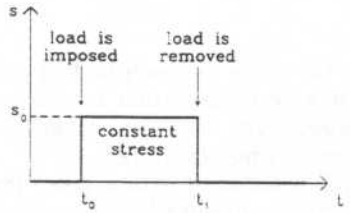


Figure 3 - Creep test: a constant stress state is imposed for a time $\Delta t = t_1 - t_0$.

In a standard creep test, a cylindrical specimen of the material to be analysed is subjected for a time $\Delta t = t_1 - t_0$ to a state of constant stress $s_0 > 0$ (Figure 3) and the resulting strain variation $e(t)$ is observed.

Though it is based on the response to a basic creep test, the algorithm can actually handle more complex signals. In fact – thanks to the Boltzmann principle of superposition – the strain response $e(t)$ to successive step loadings $s_i$ is straightforward:

$$s(t) = \sum_{i=1,n} s_i\, H(t-t_i) \quad \Rightarrow \quad e(t) = \sum_{i=1,n} e_i(t)$$

where $e_i(t)$ is the individual strain response to $s_i H(t-t_i)$. More generally, an input signal $s(t)$ can be approximated by a step function $\sum_i s_i H(t-t_i)$ and, consequently, the response is obtained by approximating $e(t)$ with $\mathcal{S}(\sum_i e_i(t))$ where $\mathcal{S}$ is a suitable operator.

### *5.1. Qualitative properties of the strain response*

The time course of the strain of visco-elastic materials in response to creep tests in simple tension can be seen as resulting from the superposition of an elastic (instantaneous $e_{ins}$ and delayed $e_{del}$) deformation and

a viscous, irrecoverable deformation $e_{irr}$:

$$e = \underbrace{e_{ins} + e_{del}}_{\text{elastic strain}} + \underbrace{e_{irr}}_{\text{viscous strain}} \tag{5.1}$$

The absence in (5.1) of one or more strain properties strictly depends on the structure of the material, that is on the modality the basic components are combined, and allows a classification of the material according to its prevailing characteristics of deformation. If, for example, $e_{irr} = 0$, the deformation is completely recovered after unloading and elasticity is the dominant property of the material; such a material can be classified as solid-like. Let us remark that, in a purely visco-elastic frame, a deformation is always observed if $s_0 \neq 0$ (see also equations (2.1)-(2.4)); this implies that $e_{ins} = e_{del} = e_{irr} = 0$ is physically impossible.

A strain response resulting from all three of the strain contributions is shown in Figure 4 and discussed.

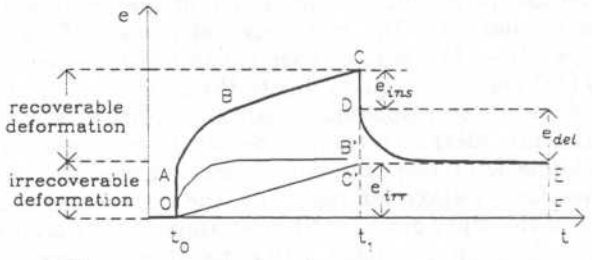


Figure 4 - A typical strain response to a creep test.

When the load is applied, the material deforms: a part of the deformation occurs instantaneously at time $t = t_0$, as soon as the load is imposed, and a part occurs more slowly during the loading time $]t_0, t_1[$ . The instantaneous part of the deformation (*instantaneous elastic strain*) is recovered as soon as the load is removed at time $t = t_1$: in Figure 4, OA and CD are expression of the *instantaneous elasticity*. More attention has to be paid to the analysis of what happens at $]t_0, t_1[$ and, correspondingly, at $]t_1, \infty[$: as the time increases, the strain usually increases non linearly (AB), but eventually a rectilinear line may appear (BC); on recovery, a curved line (DE) may lead asymptotically to a constant residual strain, the *irrecoverable (or viscous) strain* (EF), which is proportional to the total loading time and to the strain rate observed at BC, while the recovered part of the deformation (DC') is still expression of a sort of elasticity, usually referred to as *delayed elasticity*. Graphically, the curve AC is the sum of a straight line OC'//BC and a nonlinear curve OB', which is specular to DE.

*5.2. The algorithm*

The qualitative strain response can therefore be described in terms of just three properties: instantaneous elasticity, delayed elasticity, irrecoverable deformation (viscosity). Let us associate these properties with three logical parameters $\alpha, \beta, \gamma$ respectively. So, for instance, $\alpha$ is TRUE when there is instantaneous elasticity, FALSE when such a property is not exhibited.

The *qualitative behaviour* $QB[M]$ associated with a given formula $M$ and defined by the logical triplet $(\alpha, \beta, \gamma)$ is recursively determined from the qualitative behaviour of its parts as follows:

$$(\mathcal{A}_3) \begin{cases} \bullet \text{ if } M \text{ is a basic component :} \\ \qquad QB[H] = (T, F, F) \text{ according to (2.1),} & (5.2) \\ \qquad QB[N] = (F, F, T) \text{ according to (2.2);} & (5.3) \\ \bullet \text{ if } M = M_1 o M_2 \ (o \in \mathcal{O}), \text{ and } QB[M_i] = (\alpha_i, \beta_i, \gamma_i) \ (i = 1, 2) : \\ \qquad QB[M_1 - M_2] = (\alpha_1 \vee \alpha_2,\ \beta_1 \vee \beta_2,\ \gamma_1 \vee \gamma_2) & (5.4) \\ \qquad QB[M_1 \mid M_2] = (\alpha_1 \wedge \alpha_2,\ (\alpha_1 \wedge \gamma_2) \vee (\alpha_2 \wedge \gamma_1) \vee \beta_1 \vee \beta_2,\ \gamma_1 \wedge \gamma_2) & (5.5) \end{cases}$$

where the symbols $\vee$, $\wedge$ denote the logical OR, AND operators respectively.

It can be easily verified that, starting from (5.2)-(5.3), the impossible qualitative behaviour $(F, F, F)$ is never obtained; on the other hand, the remaining seven behaviours are all generated and physically

meaningful. The composition rules (5.4), (5.5) have been obtained having the analogical model in mind, and have a straightforward mechanical interpretation. However, it is possible to give a more formal justification of the algorithm by exploiting the correspondence between analogical models and differential equations which, for their special structure, can be grouped into classes which are in one-to-one correspondence with the qualitative behaviours (see Theorem in the previous section).

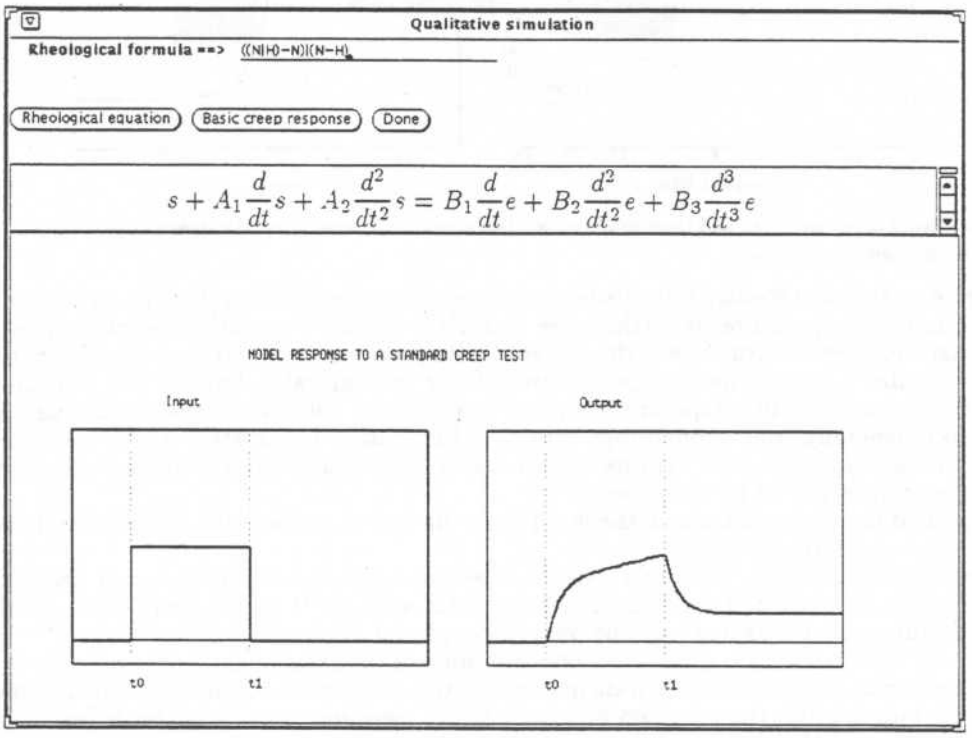


Figure 5 - Outcome of the computer simulation of the behaviour of the material modelled by the formula $((N|H)-N)|(N-H)$ in response to a creep test in simple tension.

As an example, Figure 5 shows a computer output corresponding to the structure $((N|H) - N)|(N - H)$: both the qualitative behaviour in graphical form and the differential equation are automatically and independently produced.

Let us denote by *qualitative behaviour class* the set $QB^{-1}(\alpha, \beta, \gamma)$ of formulae which exhibit the same qualitative behaviour $(\alpha, \beta, \gamma)$. For example, the formula $((N|H) - N)|(N - H)$ belongs to the qualitative behaviour class $QB^{-1}(F, T, T)$ which includes also $((N|H) - N)$, $((((((N - H)|N) - H)|N) - H)|N)$, etc.

The algorithm predicts the only and all actual physical behaviours. The simulation of the enumerated formulae has pointed out that all the different qualitative behaviours could be obtained by simulating structures made up of not more than four elements. Nevertheless there is the need to consider structures with a greater number of elements since the mathematical models corresponding to structures made up of not more than four elements do not exceed the second order and, therefore, do not adequately describe the behaviour of complex materials. However, if there were no possibility of discriminating a model from another in the same qualitative behaviour class, the generation of a library of models with a greater number of elements would not be justified. As a matter of fact, important pieces of information captured by the experimental data, for example the number of retardation times, make it possible to map any actual material to a mathematical model representing the mechanical properties of the material with good accuracy.

## 6. An example of application of the system.

To illustrate the process of mapping an actual material to a plausible mathematical model, we use some results of experiments carried out by B.W. Barry and A.J. Grace [3] in order to investigate the rheological properties of white soft paraffins. Such semisolid materials, which result from refining crude petroleum and blending processes, have been widely used in pharmacy. The results of the creep experiments carried out at constant temperature levels $T = 5°C$, $T = 25°C$ are reported in Figure 6a; the stresses applied were less than 900 dyne $cm^{-2}$.

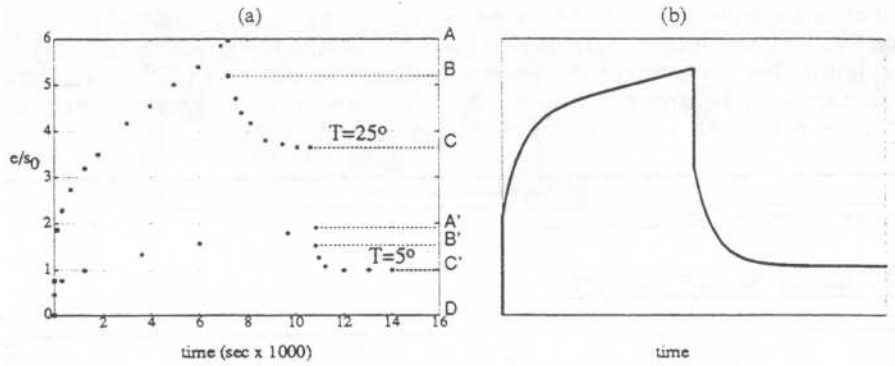


Figure 6 - Experimental creep plots (a) and their qualitative abstraction (b): experimental values of $\epsilon(t)/s_0$ are plotted against time at two different temperature levels.

The discrete retardation spectra were also determined and are reported in [3]. The number of retardation times depends on the temperature level (there are 5 at $5°C$, 4 at $25°C$): this was explained by the authors by assuming that the internal structure of the material changes when temperature reaches a transition point.

In this particular case, the qualitative features of the mechanical behaviour are not affected by the temperature change and the two experimental plots in Figure 6a collapse to the single qualitative plot of Figure 6b. More generally, the temperature acts as a bifurcation parameter, which might influence the featured qualitative behaviour. To capture such aspects, more sophisticated models accounting for the influence of temperature should be considered.

With respect to the designed system, the input from the user consists of the experimental data of Figure 6a and the *number* of retardation times.

Both experimental plots in Figure 6a clearly reveal an only partial capability of recovery ($CD$ and $C'D > 0$), which is attained in part instantaneously ($AB$ and $A'B'$) and in part more slowly ($BC$ and $B'C'$). These features are abstracted into the qualitative plot of Figure 6b.

Let us remark that making the qualitative interpretation of the experimental data automatic is a difficult task [9]. In order to map sets of numerical data into qualitative properties, suitable domain-specific conversion rules, which take into account the precision and accuracy of measurements, must be defined.

From the qualitative abstraction of the creep plots (Figure 6b), the $QB$ of the investigated material is therefore assessed as being $(T, T, T)$, and is matched against the simulated $QB$s in the library of models (in the current implementation, 20 is the maximum number of basic components the models consist of). The qualitative behaviour class is then obtained:

$$QB^{-1}(T,T,T) = \{M_1, M_2, .... M_9\} \subset \mathcal{M}$$

where

$$M_1 = (((N - H)|N) - H) \qquad \text{(4 basic elements)}$$
$$M_2 = (((((N - H)|N) - H)|N) - H) = ((M_1|N) - H) \qquad \text{(6 basic elements)}$$
$$\ldots$$
$$M_9 = ((M_8|N) - H) \qquad \text{(20 basic elements),}$$

whose respective formal rheological equations with their associated number of retardation times are automatically derived:

$$s + Ds + D^2s = De + D^2e \qquad \text{(1 retardation time)}$$
$$s + Ds + D^2s + D^3s = De + D^2e + D^3e \qquad \text{(2 retardation times)}$$
$$\ldots$$
$$s + Ds + ... + D^{10}s = De + D^2e + ... + D^{10}e \qquad \text{(9 retardation times)}$$

The availability of the number of retardation times helps at further reducing the plausible models subset. As a matter of fact, in both cases only one model is left: for $T = 5°$ there are 5 retardation times, and therefore the mathematical model for the material is given by the formal equation:

$$s + Ds + ... + D^6s = De + D^2e + ... + D^6e$$

while for $T = 25°$ (4 retardation times) the selected equation is:

$$s + Ds + ... + D^5s = De + D^2e + ... + D^5\epsilon.$$

Therefore, the quantitative model of the material, for example in the latter case, can be obtained from

$$s + a_1 Ds + ... + a_5 D^5 s = b_1 De + b_2 D^2 e + ... + b_5 D^5 e$$

by identifying the parameters $a_i, b_i$ through the fitting of the experimental data.

## 7. Discussion

This paper has presented a system whose goal is to map, automatically, each actual material to a "good" model of its mechanical behaviour so that its response to any load can be quantitatively simulated. The system works in the following way: given a set of observed data obtained from experiments on a specific material, it automatically provides a mathematical model, that is the constitutive law, and then a quantitative model for the material itself. The mathematical model is selected within a library of models automatically derived from a set of rheological formulae, which are descriptions at a symbolic qualitative level of the materials and are automatically generated by connecting variously in series or in parallel $n$ basic components. Let us remark that there is a practical limit to the complexity of the structure ($n \leq 20$ is advisable). This limit is suggested not by computational complexity reasons but because, when the quantitative model is derived, the sensitivity of the numeric values of parameters decreases if there is a great number of parameters to be identified. However the restriction of $n$ to 20 is not an actual limit for the system since structures made up of 20 elements are associated with rather complex materials.

The selection of the model is grounded on the qualitative comparison of the observed behaviours against the simulated behaviours of the set of pre-enumerated solutions. This approach is derived from model-based diagnosis ([8], [11], [25], [26]), although our goal is not to detect faults but to find a model explaining the observed behaviour of a material. Since the current system deals with only visco-elastic materials, whose behaviours are qualitatively characterized by three properties (instantaneous and delayed elasticity, and viscosity), the selection process is simple.

The number of the possible different responses in correspondence to the same signal amounts to seven, three of which describe the behaviour of $H$, $N$ and $H|N$. The other ones characterize four subsets of models as behaving qualitatively in the same way. The qualitative interpretation of experimental data in terms of the three above mentioned properties allows an easy selection of the candidate subset. The knowledge of the number of retardation times, which is derived from the experimental data, makes it possible to select within the set of candidates the most plausible model for the material.

Besides the capability of automating the model formulation, another important feature of the system lies in the incorporation of qualitative and quantitative knowledge. Both kinds of knowledge are used in an engineering context and therefore their integration is essential in order to build systems capable of emulating the engineer's way of reasoning. The importance of integrating qualitative and quantitative information is evidenced in [10], [17], [19], [23], [24], [30], [31].

This work is a first step towards the construction of a model-based system for reasoning about materials. At the current stage some strong simplifications have been made: materials are studied only from the mechanical perspective, and only visco-elastic materials are considered. As soon as the plastic element is introduced, elasto-plastic, visco-plastic, elasto-visco-plastic materials will be considered as well. In such a case, the generation, qualitative simulation and selection algorithms will need significant modifications. The modifications of the first two algorithms will be suggested by domain specific knowledge, while, as far as the model selection is concerned, techniques for organizing the set of models, so that the search of the most appropriate model is efficient (e.g. [1], [15], [27]) will have to be considered. Such techniques should also take a multi-perspective view into account.

However, the current simplified version of the system is of practical value as it provides the user with a rich set of methods, ranging from the qualitative to the numerical ones, for the automated classification and analysis of visco-elastic materials, which are a wide set of actual materials. But some work has still to be done in order to make the system really utilizable. First, the qualitative simulation algorithm needs some extensions: complex input signals, including also compression forces, and relaxation-like experiments will be considered. Another important problem to be solved is the automatic analysis of quantitative experimental data in order to extract information about the qualitative strain (stress) properties of the material and about the number of retardation (relaxation) times. Finally the system will have to be integrated with standard numerical procedures for parameter identification and simulation.

The whole system is planned to be experimented by exploiting data related to polymeric materials used in pharmacological research.

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