

On General Frameworks for Material Modeling

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Abstract

During the last three decades various suggestions for a general theory of material behavior have been made. The early attempts were limited to materials with fading memory and turned out to be too restricted. In order to include plastic behavior, a state concept is needed. Theories with a derived state concept allow for general statements valid for a broad variety of materials including elasticity, viscoelasticity, plasticity, and viscoplasticity.

History

In the sixties and early seventies of our century, some effort was made to construct a framework for the description of general material behavior. This intention was probably initiated by Noll (1958) with a very early trial to approach continuum mechanics in a rather general axiomatic way. The work of this school, sometimes called *Rational Mechanics*, culminated in Truesdell and Noll's (1965) handbook article *The Non-Linear Field Theories of Mechanics*, which was at that time the most complete and compact exposition in material theory. It contained an exhaustive chapter on elasticity, some theories on viscoelasticity and another exhaustive chapter on viscous fluids. Surprisingly enough, plasticity was completely ignored in this context, although a technically relevant classical theory, always non-linear, and comparatively well-understood in material science.

On the other hand, *Non-Linear Field Theories* meant large deformation analysis, and in that sense a mathematical theory of plasticity did not exist before 1965. The first mathematical theories on finite plasticity appeared later: Green *et al.* (1965), Owen (1968), Lee (1969), Mandel (1971), to name just a few. It is one of the astonishing facts of the history of our science that, since finite elasticity had reached a certain mathematical level already in the middle of this century, finite plasticity – although with much broader fields of application – evidently does not so even half a century later.

In elasticity, the question after the most general form of a constitutive equation can easily be answered. A decision between dependent and independent variables has to be drawn. And since Hooke's times the deformations determine the stresses. Elasticity is then – simply – that a certain deformation tensor, or, more precisely, its current value, determines the current value of some stress tensor. In order to avoid conflicts with objectivity, one can choose material variables, such as the right Cauchy-Green tensor C and the 2. Piola-Kirchhoff stress-tensor S . More restrictions cannot be generally applied, and any further specification must be considered as a material specification or identification.

If we, however, leave the field of elasticity, things become much more complicated. If the present deformation is no more sufficient to determine the stresses, then what else could it be? The past deformations at discrete times, in some finite interval, or at all times prior to the present, i. e., the entire deformation history?

History Functionals

One straightforward generalization is motivated by the attempt to develop the recent history of deformation into a Taylor-series and to truncate after $q \geq 0$ terms, leading to the constitutive equations of a **material of the differential type of order q**

$$S = f_q(C, C', C'', \dots, C^{(q)})$$

with $C^{(q)}$ being the q -th material derivative with respect to time. For $q = 0$ this is again elasticity, for $q = 1$ we may obtain a Reiner-Rivlin fluid, which can be brought into the form

$$S = f_1(C, C').$$

If f_1 splits up into two function of the arguments

$$f_1(C, C') = f_{10}(C) + f_{11}(C')$$

then it describes a non-linear Kelvin-model.

This leads already into the field of viscoelasticity or rheology, which is at least in the linear case a well-known theory of material behavior (s. Tschoegl 1989, Giesekus 1994). The linear one-dimensional models of rheology lead to differential equations of p - q -type

$$P_0 \sigma + P_1 \sigma' + \dots + P_p \sigma^{(p)} = Q_0 \varepsilon + Q_1 \varepsilon' + \dots + Q_q \varepsilon^{(q)}$$

which can be uniquely solved for some given deformation process and sufficient initial data. A non-linear three-dimensional generalization is a **material of the rate type**

$$S^{(p)} = f_{pq}(S, S', S'', \dots, S^{(p-1)}, C, C', C'', \dots, C^{(q)}).$$

In order to define reasonable material behavior it must be assured that this non-linear differential equation has a unique solution, which maybe extremely difficult if not impossible in many cases. This is one of the reasons why Truesdell and Noll consider materials of this type „as artificial at best, and unworkable in general“ (Preface of the new edition 1992).

The second approach to viscoelasticity is based on the Boltzmann representation of heredity integrals given as a convolution of an obliviator function and the deformation process, giving raise to **materials of the integral type**. Such generalizations of the linear case are given in eqn. 37.2 of Truesdell *et al.* (1965), being too complicated to be reproduced here. The obliviator or influence functions tend to zero if the time parameter tends to minus infinity, such that the influence of events on the present response tends to zero, if enough time has passed away.

All these three classes of materials (differential type, rate type, integral type) have in common that they describe materials with **fading memory**. The independent variables are deformation histories of semi-infinite length submitted to certain regularity restrictions seldom really mentioned. These classes are non-linear generalizations of materials being well known in the context of viscosity and viscoelasticity. Principally, only three concepts, i. e., *time*, *deformation*, and *stress* are sufficient.

Other concepts like internal variables or states are not needed so far. And they indeed span a large variety of material behavior.

This was the state of art of 1965, when the history functionals like

$$S(t) = \mathcal{H}^t(C(\tau))$$

were considered world-wide as the most general form of constitutive equations. They have, however, some severe defects. Firstly, it is in principal questionable if any material existed already since infinity. But even if this were the case, we would surely not know its entire deformation history. Practically we will always have to consider deformation processes of finite duration instead of (semi-infinite) histories. And this is not compatible with the above form.

Another severe shortcoming of the concept of a history functional is that there are certain classes of paramount technological importance that generally cannot be described in such a way. These are, among others, all plastic materials and all viscoplastic ones. The reason for this fact is simply that such materials do not possess the fading memory property, but instead have a permanent memory. If we bend a nail and then leave it, it will never forget this event and will remain bent as long as we want.

State Concepts

For materials with permanent memory, if not for all materials, it is both natural and practical, to define the finite deformation process out of some initial state as the independent variables for a constitutive model that determines the stresses at the end of this process. As initial state of a material class one might choose the moment of its generation, formation, or solidification. But one may also choose any further moment, e. g., the time of delivery of the test-samples.

The difficulty of this approach is that a new concept appears, namely the *state* of a material. For specific material models it might be easy to define state-variables. For a plastic material, these could be the accumulated deformation as well as a set of hardening variables. In general, however, this is by no means a trivial task. And if we intent to formulate a general constitutive theory, all fundamental concepts should be precisely introduced. Of course, many authors do not submit themselves to such rigor. They introduce *ad hoc* state variables or internal variables without generally specifying them. And, for the evolution of them, an evolution equation is given by some ansatz function, usually in the form of a 1st order differential equation in time, depending on the current value of all state variables and the increment of the deformation tensor. One requirement should be satisfied by such an approach. The choice of the state variables must be such that they uniquely determine the further response of the material in combination with the evolution equation if submitted to any deformation process starting from this state. If this cannot be assured, the concept could clash with the principle of determinism, the basis of all constitutive theory. In most cases, however, this requirement is not assured, not even claimed to do so.

If we further suppose that this requirement is fulfilled, then the choice of the state variables does not need to be unique, i. e., there are other choices of variables that would also satisfy the principle of determinism. But this remaining ambiguity is not an objection against the state variable approach, as one should be content if he had found one appropriate choice for them.

Another difficulty turns out to be more serious. As the choice of the state variables depends on the specific material class under consideration, it is extremely difficult, if not impossible, to fix general properties, e. g. , their transformation behavior under symmetry transformations, changes of observer, etc., which is needed for the elaboration of a general theory (see Bertram 1993).

All these difficulties allow the conclusion that *ad hoc* state-variable concepts, although extremely practical in specific cases, are of little use for deriving a general theory of material behavior.

An alternative approach, which avoids these problems, is that of a **derived state concept** (Noll 1972, Bertram 1982, Bertram 1989). The leading idea of such an approach is to not introduce state variables *ad hoc* as primitive concepts, but instead to define them in terms of stresses and strains. The basic idea of this definition is, roughly speaking, that two deformation processes bring the material into the same state, if the response of the material to any continuing deformation process is identical. In this sense, a state is just an equivalence class of deformation processes.

This approach essentially stems from systems theory. It was suggested by Onat (1966) to continuum mechanics, although already roughly anticipated by Bridgman (1959). It can be made mathematically precise and turns out to be both general enough and natural. With this concept, we are able to derive all information needed for a general material theory. As an example, the relation between material symmetry and this state-concept has been exhaustively examined in Bertram (1989).

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