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What is the General Constitutive Equation?

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Dedicated to Rudolf Trostel with appreciation and admiration on the occasion of his 65th birthday

While all other basic equations of mechanics have been well established and widely accepted for ages, the "missing link" in form of constitutive equations is still (and will probably always be) subject of intensive research work. This part of mechanics is the only one that cannot be completely solved, in principle, as the variety of material behaviour in nature is already unbounded, and man tries hard to even enlarge it by creating new materials. Moreover, more specific loading conditions and material requirements on the one hand, and rapidly developing computational facilities on the other, lead to an increasing need of new material models. This is surely one of the stimulating factors for all of us who earn our living and, at least some of us, our merits by suggesting new material laws or models. We do not run the risk of becoming workless, at least not all of us at the same time.

Of course, there are certain concepts within material theory, which are common to all materials, such as causality and determinism, objectivity, material symmetry, passivity, etc. Moreover, one wants to give general definitions of subclasses of material behaviour, such as isotropy, rate-(in-)dependence, aging, reversibility, and many more. For the formulation of these concepts a general framework is needed. So, despite of the infinite variety of material behaviour the following question arises: *What is the general form of the constitutive equation that covers all constitutive laws?*

Of course, one should be extremely careful when using the word "all". So let us be content, if we find a form general enough to cover all of the important and commonly used classes of reasonable material models, perhaps leaving out some very special ones that exist in literature but not in reality. Therefore, we will not use the word "general" in a strong and absolute sense but only in a rather weak one. We do not intend to frustrate immediately any attempt to answer our question by constructing counterexamples of any degree of sophistication that do not fit into such a general frame. Instead, we are modestly searching with a very weak and limited understanding of "general" in mind, freely obviating almost all stumbling blocks, such as follows.

- We will limit our consideration to pure mechanical behaviour. We will ignore all couplings with thermodynamics, electro- or magnetodynamics, and other non-mechanical influences on the materials.

- We will limit our considerations to classical materials by neglecting all relativistic effects.

- We will not try to include non-local effects or higher-gradient-dependencies, (see

TROSTEL [31, 32]), but will instead limit our considerations to non-polar simple materials (in the very classical sense of NOLL [20]) where a deterministic relation between local deformations and symmetric stresses is assumed to exist.

● Finally, for the sake of simplicity of our considerations, we will not include internal constraints. This may be done afterwards, if necessary.

If, further on, we use the notions of stresses and (local) deformations, we are thinking in terms of NOLL's [21] intrinsic concepts that seem to be the most natural ones for material theory. However, one may also use any other appropriate stress or strain measure. Of course, invariance under superimposed rigid body motions of these measures is advantageous, as material theory generally can be seen as just that part of mechanical interaction that fulfils such a requirement (see [4]). Eulerian stresses and deformation gradients may be appropriate for balancing forces/moments or deriving kinematic relations, respectively, but certainly not for material functions or relations.

However, all that which will be said further on equally holds if one thinks in terms of infinitesimal theory, i.e. in linear strains and small stresses. Moreover, 3-dimensionality is not important in this context. One may also think of uniaxial strains and stresses if one wants to.

When we previously used the expression "relation between stresses and strains", we intentionally left the decision open, how to distinguish between independent and dependent variables. Historically, stresses have often been taken as dependent variables, and the strains as independent ones, and not vice versa, although a civil engineer is probably more interested in the opposite direction: to determine the displacements caused by loads.

There are important classes of constitutive models, where the deformations do not fully determine the stresses (e.g. incompressible materials), but also for those, where the deformations are not fully determined by stresses (e.g. ideal gas). There are even prominent examples that simultaneously contradict both directions (e.g. rigid-perfectly plastic materials)(see [2, 3]). These problems, however, can be solved by different approaches and concepts:

● internal constraints (see [33] p. 69);
● multi- or set-valued-functions (see [3]);
● subdifferentiable functions in the context of convex analysis (see [29]);
● material *relations* instead of *functions*, which is probably the most general, but less customary form (see [26], [3] p. 119).

After so much confusion, let us take a decision, that leaves everything open. Let t be the time parameter, S our dependent variable, and G the independent one. S may stand for the (intrinsic) stress tensor, and G for the (intrinsic) configuration; or, likewise, vice versa. However, we should keep in mind during our discussion, that in nature there is no clear and certain distinction between dependent and independent variables.

For *elastic* materials the case is rather simple: the value for S at any instant t depends exclusively on the value of G at the same instant

$$S(t) = f[G(t)] \ . \tag{1}$$

Thus, any mapping, that relates an *S* to any *G* constitutes an elastic material, and any elastic material determines such a mapping.

The problem arises, if the response is inelastic. We expect, generally, that the current value of *S* depends on the current *and* past values of *G*. This statement is still too vague to deserve the label *Principle of Determinism*, but there are two clear assumptions in it, which are widely accepted and seem not to exclude physically relevant material models.

First, it claims determination of such a dependence. The philosophical background is, that we understand the (mechanical) reality as reproducible; identical experiments will lead to identical results.

Second, the future does not influence the past (causality).

We will have to focus our attention on the following question: *How does the past enter the general constitutive equation?* The literature gives us basically three answers to this question.

The Answer by the Internal Variable Concept

The first suggestion stems from very practical experience with material laws. If the stresses do not only depend on the deformations, but on other mechanical quantities, that may be quite different in nature for different materials, then these quantities are not directly measurable by a general method for someone who is able to measure only forces, geometry and time. These dummies are therefore called *hidden* or *internal* or *state variables*. It is customary to put them into an n-dimensional vector-notation $\underline{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_n)$ with linear and differentiable structure. The general constitutive equation is now

$$S(t) = g[G(t), \underline{\alpha}(t)] \,, \tag{2}$$

a direct generalization of the elastic one. For the internal variables an evolution function is needed that enables us to determine the present value of them as a function of its initial value and the deformation process since then. Usually this is done by integrating a first-order differential equation in time

$$\underline{\alpha}^{\cdot} = h[G(t), \underline{\alpha}(t), G^{\cdot}(t)] \tag{3}$$

that is assumed to have a unique solution along any *G(t)*-process with certain initial conditions.

There are countless examples for such constitutive structures in the literature, but only very few general theories on them, even if we include thermodynamics where internal variables perhaps are even more popular than in pure mechanics. COLEMAN/ GURTIN [7] and NOLL [21] are just two prominent examples for the latter.

The lack of a general and widely accepted theory makes it difficult to appreciate or to criticize the internal-variable-concept. But the general dilemma is the following: if one assumes properties of the space of internal variables and the evolution equation, then the concept becomes more practical and more restrictive at the same time. On the other hand, the less we assume, the less we gain by the whole concept.

If, for example, one assumes that the internal variables form a finite-dimensional vector space, then its topological, linear, differentiable structure allows us to work comfortably in this space. However, this structure is induced by mere assumption and not by nature, so we are left without any idea whether the results have anything to do with physics or not.

If, on the contrary, one does not specify the structure of the internal variables at all, then no further conclusion can be drawn. It is just like substituting some unknown quantity by another.

Consequently, whatever we do, the theory is either restrictive and artificial, or vacuous, or even both.

There is fortunately a way out of this dilemma, carefully demonstrated by NOLL [21] (see also FABRIZIO/ LAZZARI [14]). The solution is not to *assume* an a priori structure of the state space, but to *derive* it in terms of stresses, strains, and time in a *natural way*. NOLL's *natural topology/ uniformity* are constructed in such a way. I wonder whether it is possible to construct a differentiable structure on the state space in an analogous way. We will again refer to such a procedure in the last section. However, such approaches are extremely rare, if not singular in works of internal variables.

As a conclusion, we may state that internal variables, as they are commonly understood, are not useful for general considerations within material theory, although they are extremely practical and popular in special applications.

The Answer of "Rational Mechanics"

The second answer to our question comes from another school within continuum mechanics, which tries to treat mechanics in an axiomatic or mathematical way and became well-known under the label "Rational Mechanics". Its development has been documented in detail in the issues of the "Archive of Rational Mechanics and Analysis" for more than three decades. Clear assumptions or axioms are stated at the beginning, followed by propositions and theorems, all strictly derived or proven. The most important compendium of this school is surely the "Non-Linear Field Theories in Mechanics" [33] in Handbuch der Physik, which has good chances of becoming the most important and influential book in continuum mechanics of this century. Although not written in an axiomatic way, it was clear and precise enough to define concepts and quantities that are now used worldwide in this sense and notation. In the preface to its second edition of 1992 the authors even claimed that it had been complete at the time of its first publication. We will see, that completeness is a rather relative expression, as the treatise omits almost half the material world.

If the stresses do not only depend on the present deformation, but also on the past ones, this can be formalized by using the deformation-process as independent variable rather than discrete deformations. And, as one cannot expect that the memory of materials in terms of time-intervals is limited in general, one took into account the semi-infinite deformation *history*. The general constitutive equation of simple materials is given in [33] p. 60 as

$$S(t) = \mathscr{F}(G^{(t)}) , \tag{4}$$

if translated into our notation. Here $\mathscr{F}$ indicates a *history functional* of the entire past history of G, where the time parameter ranges on the semi-infinite interval from $-\infty$ up to the present time t. Such a history functional is nothing more than a function on an appropriate function space that has not been specified in [33], but in many articles on materials of the fading memory type (see COLEMAN/ NOLL [8 - 11], WANG [34, 35]).

At first glance this form of constitutive equation looks rather general and convincing. First of all, there are no further variables involved such as mysterious hidden variables or state-vectors, just stresses, strains, and time that are altogether assumed to be well-known and measurable. Consequently, there are no more constitutive functions or evolution equations needed apart from this functional. Moreover, no limitation seems to be imposed on the dependence on past events. The current stresses may depend on remote deformation events that happened any time in the past, regardless of how long ago.

Accordingly, these theories with history functionals became rather popular. For a long time and worldwide there were books and papers published suggesting to the reader that almost any material can be described by functionals. In fact, the applications of such constitutive functionals in viscoelasticity and viscosity were convincing.

There was, however, a broad field of material theory, where history functionals never had any influence, and that was *plasticity*. In the opinion of the authors of [33] plasticity simply did not yet exist as a non-linear field theory (see remarks on p. 8 and 11 in [33]). In fact, little development of classical infinitesimal plasticity theory towards finite (= non-linear) deformation plasticity had taken place at that time. And, moreover, the few early suggestions on finite plasticity were far from meriting the title "rational". On the other hand, the majority of our "rational mechanics" totally ignored plasticity (early works by OWEN [24, 25] and TROSTEL [30] are just the exceptions from the rule), although there was indeed a great need for non-linear theory, as there are uncountable examples for large plastic deformations in metal forming, soil and rock mechanics, granular and porous media, etc.

The reason for this disjointedness of the rational and the plasticity club was bilateral. The rationalists were not able to help the plasticity fellows, and the latter were excluded from the former by a very firm lock, namely the *history functional*. It took quite a long time until this fact was fully recognized and publicly declared. In 1972 NOLL [21] wrote: "The original theory has failed to give an adequate conceptual framework for the mathematical description of such phenomena as *plasticity, yield* and *hysteresis*." He did not give a proof of this statement, and, indeed, it is not trivial to do so. The problem arises from fundamental logic: to demonstrate, that something does not fit into a system, cannot be done inherently, i.e. in terms of this system. First it was necessary to generate a more general framework, into which both could be imbedded, the history functionals *and* the plastic materials. And exactly this was done by NOLL's paper [21], as we will discuss in the next section.

In the same paper [21], NOLL refers to another more fundamental shortcoming of the history functionals. We may doubt whether there exists any material point in the whole universe that has existed since infinite past. But even if this were the case, we would not be able to know the entire history. And clearly, it is rather difficult, if not impossible, to construct or to identify a history functional in general, as we must know its response to just *all* histories. In principle and in praxis, we will never be able to identify such a functional, if it really depends on the infinite past. So there is good reason to presume that history functionals describe only those materials where the infinite past does *not* influence the present stresses, which is commonly known as *fading memory*. The very surprising and almost paradox looking conclusion is, that history functionals are appropriate to describe materials with fading memory, but not those with permanent memory, as in plasticity. And this must be considered, of course, as a serious and unacceptable shortcoming for a general theory.

There have been attempts to modify this theory in order to remove this shortcoming. One attempt is to restrict the domain of the functional, i.e. the deformation-histories, in such a way that they are constant (rest-histories) before a certain time. By this trick the semi-infinite history is essentially reduced to a finite one plus a constant initial value. This procedure, however, involves some fundamental restrictions and problems, as can be read in [21].

First of all, it can hardly be expected that there exists a universal time or age such that all materials have forgotten what has happened to them before that time. Such a limit cannot even be expected for each individual material. A counterexample is again plasticity.

Moreover, the assumption of a remote rest history is artificial, awkward, unnatural, and thus unacceptable. It is just the helpless attempt to rescue a theory that is not general enough in principle. However, there is something in this attempt that points in the right direction, namely, to use finite processes and initial conditions instead of infinite histories, which takes us towards the third answer to our question.

The Answer by a Derived State Concept

The solution of our problem was given by ONAT [22] in 1966 (see also [23, 16]), although it had already been roughly anticipated by BRIDGMAN [6] in 1950 as "Method of Preparation" (see [17, 26, 15]). The important new conceptual issue of this suggestion was to introduce a state concept in a natural way and not by mere assumption.

Two material points (or one point at different times) are defined to be in the same *state*, if their responses to every admissible (finite) deformation-process is pairwise identical for the two points. Or, in other words, two states of a material are identical, if and only if no difference in all future behaviour can be detected.

Thus the basic assumption is "[...] the possibility of an indefinite number of replicas of the original system, all in the same state. Any desired property which determines the state may then be found [...] by making the appropriate measurement on a fresh replica. Identical replicas may be prepared by starting each replica from the same initial condition [...] and subjecting it to the identical history" (BRIDGMAN [6]). Once the *initial state* has been introduced, one can define all further states by introducing an equivalence relation on the process-class of the independent variables: two processes are equivalent, if (i) both can be continued by the same set of processes, and (ii) the responses to all of them are again pairwise identical. The equivalence classes of this relation establish the state space of the material.

NOLL's [21] axiomatic structure, although at first glance quite different from ONAT's suggestion, gives rise to more or less the same state-concept (see [3] p. 127). This is, by the way, essentially the well-known concept of the *minimal state space* from systems theory (see [1, 19, 27] for further hints).

There are some important advantages of this procedure:

- the definition holds in precisely the same way, whatever the independent and the dependent variables are; it can be applied to thermodynamics or any other science where deterministic input/ output relations of "black boxes" are considered;
- the states are defined exclusively in terms of independent and dependent variables, i.e. physical quantities, that are considered as fundamental and measurable, as in our case in stress, strain, and time; in this sense it is *natural;*
- the state space is in fact minimal, as it includes exactly the amount of information, that is needed, and nothing more;
- this state-concept is definable in a clear mathematical manner avoiding any ambiguity or need for intuition;
- only processes of finite duration are needed; the life-time of the individual material may be bounded or unbounded; one can freely define the birthdate of a specific material.

By using this state-concept, we are able to formulate the general constitutive equation as

$$S(t) = k[z(t_o), G^{(t)}] \qquad (5)$$

where $z(t_o)$ is an initial state and $G^{(t)}$ is the configuration process in the (finite) time-interval $[t_o, t]$ that starts from the initial state. The initial state need not be uniquely determined; it is sufficient to just find a state from which all others can be reached. The existence of such a state is generally stated within this theory.

Based on this state-concept, all general concepts of material theory can be introduced in a natural way: objectivity, material isomorphy and symmetry, the evolution function of states, the topological structure of the state space, passivity, and so on (see [3, 4, 18]). The resulting theory is not far from NOLL's "New Theory of Simple Materials" [21], that covers the old history functionals as a subclass. It may be, and in fact has been shown, that this theory essentially includes all materials that can be described by internal variables and/or by history functionals, and may therefore be considered as the most general one. SILHAVY/ KRATOCHVIL [28], DEL PIERO [12, 13], KRAWIETZ [18], and others have shown in detail that materials with permanent memory fit into this framework without conceptual problems.

In contrast to internal variable theories, all primitive concepts of this theory are formulated in terms of stresses, configurations, and time. This gives it a conceptual and methodological clearness, that is not only desirable, but also necessary for a scientific theory.

There have been generalizations of this framework in order to include classical and non-classical internal constraints as well as thermodynamical and other physical variables (see [3]). And it has been shown in [5] five years ago on a similar occasion, that the same framework can be used to formulate a general constitutive law for friction between continuous bodies.

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