# On the History of Material Theory – A Critical Review

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**Abstract.** Material theory in a strict sense is not older than just half a century and from the beginning characterized by fundamental disputes and changes of paradigms. A number of different suggestions have been made and - often - forgotten soon after their publication. In this article the main existing theories shall be briefly described and critically discussed. Some important demands for an adequate theory are raised and applied to these suggestions.

Originally, two totally different lines of approaches existed, namely that of *history functionals* and that of *inner variables* or *state theories*. Since both approaches suffer from fundamental deficiencies, neither of them really achieved global acceptance. And for a long time it remained unclear how the two approaches could be mutually related.

This was changed in 1972 by Noll´s *New Theory of Simple Materials* [19], in which a third approach was suggested that made it possible to compare the two preceding formats. The gain in generality was, however, accompanied by a loss of simplicity. Consequently, this theory has been used only by very few groups within the scientific community.

Since then the majority of the papers in the field of material modeling are pragmatic and do not claim for general validity. However, there remains a clear need for a general theory, as we will finally demonstrate within the context of thermodynamics.

**Keywords:** Material theory, Constitutive theory, Internal variables, State space.

## 1 Introduction

During the past several decades, material modeling has become a rich and blossoming branch of research activities. An overwhelming wave of papers,

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conferences, reports, etc. bear witness to this trend, the peak of which has surely not yet been reached. New materials, new applications, new loading conditions, new computational and experimental facilities, etc. create an almost unlimited demand for material models.

In the presence of this evolution of material models a need for a unifying theory can be stated. One wants to use a theoretical framework for the construction and comparison of particular models or model classes. Surprisingly enough, little research work has been invested in this interesting task during recent decades. This situation, however, has not always been like this. Clifford A. Truesdell (1919 - 2000) remarked in 1993[1]:

> "*It seems to me that in the late 1940s new kinds of continuum mechanics began to be envisioned and explored, different in spirit from the older kinds. (...) Rigorous mathematical analysis based upon consequences of fairly general principles (...) became appealing.*"

In fact, from the middle of the last century until the 1980's many attempts have been made to solve this problem. After this period, however, only a few papers have been published in this direction. A general theory was apparently not the focus of the scientific community. A more pragmatic way of extending particular models without placing them within a general framework became habitual thus leaving the situation rather unsatisfying.

With this paper, it is intended to raise the request for a general material theory again. And we will give some good reasons to substantiate this, not only under theoretical aspects, but also under rather practical ones. Further, it is intended to describe the propositions and paradigms which have been suggested in this field, to show their deficiencies, and, thus, to inspire other people to bring this problem closer to a solution.

## 2 Material Theory

First it should explained what is meant by *Material Theory* in order to prevent the reader from expecting something else. By *Material Theory* we do not have different theories of material models in mind like, e.g., viscoplasticity, micromorphy, or continuum damage theory. What is in fact meant is the theory behind all these examples, or a framework within which one can construct material models like those just mentioned. One may also call it a *(General) Constitutive Theory* or the like.

In this context, the topic of a *Material Theory* can be reduced to a simple question. If a material is elastic then we determine the current stresses by a constitutive function of the current deformation of the body or of a suitable neighborhood of the point under consideration. The question here is: which is the general form of the constitutive equation of a material which is *not* elastic?

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[1] See `http://www.math.cmu.edu/~wn0g/noll/TL.pdf`

At first glance this seems to be an easy question. However, we will see in the sequel that the answer is by no means trivial and has not been given in a satisfying way until today.

A theory which deserves the label *Material Theory* is expected to be

- conceptually sound, based on both mathematically and physically clear assumptions or axioms and well defined concepts,
- general in order to include essentially all branches of material modeling,
- practical and applicable.

And we will see when looking at the history of this subject that any theory which does not simultaneously meet all of these three requirements, will soon be a victim of Occam´s razor.

This article is organized as follows. First we want to explain the two original paradigms which exist in the field, namely (*i*) the theory of *history functionals* and (*ii*) the theory of *internal variables*. Then we refer to some attempts to unify them, and finally we describe the state of art and the remaining problems to be solved.

## 3 History Functionals

In the late 1950's Green, Rivlin (1915 - 2005), Noll, and others made suggestions to give continuum mechanics a rational or even an axiomatic form, like any other branch of mathematics, as they understood mechanics. The demanding aim was expressed under the challenging label *Rational Mechanics*. In the well-known journal *Archive of Rational Mechanics and Analysis*, many papers have been published with such an intention.

In 1965 the famous article *The Non-Linear Field Theories of Mechanics* [26] by Clifford A. Truesdell and Walter Noll appeared in the *Encyclopedia of Physics*. This book soon had an overwhelming impact on continuum mechanics. Here are some important dates of this work:

- January 2nd, 1965 first issue printed 4000 times
- 1971 identical reprint
- 1979 identical reprint
- for a long period unavailable
- 1992 reprint
- 2000 translated into Chinese
- 2004 reprint edited by S. Antman
- 2009 reprint as paperback

On page 56 of this book we find as a starting point of the theory the

**Principle of Determinism:** *The stress in a body is determined by the history of the motion of that body.*

This short axiom has some important implications like the following ones.

- In mechanics, certain variables are determined by mechanical events.

Perhaps a physicist working in quantum mechanics will not accept this statement. On the other hand, it is the philosophy of any engineer that practically everything in the mechanical world is determined and can be calculated, at least up to a certain degree of precision.

- It is the past that determines the present, whereas the future has no influence on the presence (causality).

This is perhaps the least questionable statement of this principle.

- The authors considered the kinematics (motion of the body) as the independent variables, and the stresses as the dependent ones.

Of course, this is not the only choice. One could also do it vice versa. For a civil engineer it is perhaps more natural to determine the deformations of a building by the given loads, so that the kinematical variables are determined by the dynamical ones. We will, however, see that the principle induces problems in any of these two directions[2]. In fact, the stresses do not determine the deformations, and the deformations not determine the stresses in all cases. This is why one introduces internal constraints.

There are also theories which avoid preferring stresses to strains or vice versa by using constitutive *relations* instead of functionals[3]. However, these concepts are rather complicated to handle and, hence, never really adopted by the community.

**Notations.** We will denote the dependent variables by $\sigma$ and the independent ones by $\varepsilon$ and call them *observable variables*. One may think of stresses and strains, respectively, but also vice versa, or in the thermodynamical context, by the vector of the caloro-dynamic state and the thermo-kinematic state, respectively. Both variables or sets of variables may be tensors of arbitrary order, i.e., elements of finite dimensional linear spaces with inner product. We will further-on distinguish between *histories* of semi-infinite duration notated as $\varepsilon(\tau)\Big|_{\tau=-\infty}^{t}$ for an $\varepsilon$-history with $\tau$ being the time parameter, and *processes* of finite duration notated as $\varepsilon(\tau)\Big|_{\tau=t_0}^{t}$ starting at some arbitrarily fixed starting time $t_0$ for an $\varepsilon$-process. Functions of such histories or processes are called *history functionals* and *process functionals*, respectively.

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[2] As an example one could consider a rigid - perfectly plastic model. This does not allow for a functional dependence of stresses and strains in any direction.

[3] See the method of preparation suggested by Perzyna/Kosiński [24] and Frischmuth/ Kosiński /Perzyna [11].

With the above *principle of determinism* and some other assumptions, Truesdell and Noll come to the conclusion that a history functional like

$$\sigma(t) = F\{\varepsilon(\tau)\Big|_{\tau=-\infty}^{t}\} \tag{1}$$

would be "*the most general constitutive equation*". We will examine this demanding title next.

Such *history functionals* or *heredity functionals* were inspired by viscosity or viscoelasticity. Such laws typically consist of initial values weighted by an obliviator or influence function (like an exponential function with negative exponent) and a convolution integral of the deformation process or its rate and the obliviator function. If we consider a typical linear viscoelastic body like the well-known one-dimensional Maxwell model, we obtain for the stresses the integral form

$$\sigma(t) = \sigma(0)\ exp\left(-\frac{E}{D}t\right) + E\int_{0}^{t}\varepsilon(\tau)^{\bullet}\ exp\left(\frac{E}{D}(\tau-t)\right)d\tau \tag{2}$$

with material constants $E$ and $D$ and initial stress value $\sigma(0)$. Thus, the longer the process lasts, the smaller becomes the influence of the initial values. This effect is called *fading memory*. In the limit, the influence of the initial values has been completely forgotten, and we obtain the history functional

$$\sigma(t) = E\int_{-\infty}^{t}\varepsilon(\tau)^{\bullet}\ exp\left(\frac{E}{D}(\tau-t)\right)d\tau \tag{3}$$

which is formally simpler than the above integral since it is independent of initial values and initial time. The basic ingredient for this limit is in fact the fading memory property of the material. One has no chance to construct such a history functional for a classical elastoplastic material, since it does not forget the past and, thus, the limit does not exist, as it has been shown by Noll [19].

Such functionals have been extensively used by Green/Rivlin [13], Noll [18], Coleman [6], Wang [28], and many others to construct material theories. Astonishingly enough, the use of these functionals is often mathematically little exact. For example, one will hardly find any regularity conditions on the histories in Truesdell/Noll's book [26].

What are the advantages and disadvantages of the theory of history functionals?

Firstly, an important advantage of them is surely that no new primitive concepts are needed; only the observable variables stresses and strains are used. Secondly, the theory is well justified within viscoelasticity.

However, "*it is both philosophically unacceptable and practically questionable to use semi-infinite histories*" (Noll [19]). Moreover, this format is not general enough since it is essentially limited to fading memory materials and rules out plastic models. This fact, however, is not easy to see.

In *The Non-Linear Field Theories of Mechanics* [26] plasticity is not present at all. The authors claimed that at the time plasticity had not yet gained the state of a mathematical theory. Indeed, the first theories of finite plasticity did not appear before 1965 like, e.g., Green/Naghdi [12], Lee/Liu [16], and Mandel [17].

In 1971 Valanis[4] [27] suggested the *endochronic* theory, which can be considered as an attempt to enlarge the concept of history functionals to rate-independent materials by introducing an artificial time-like parameter. By this ansatz one can give rate-independent materials a form which is similar to that of finite linear viscoelasticity with fading memory. This creates a particular inelastic behavior, which shows effects that are in some ways similar to plasticity. Classical plasticity with elastic ranges, however, can not be brought into this form.

## 4 Internal Variables

The second format of material theory is concerned with *internal variables, hidden variables, state variables*, or whatever they are called, in contrast to the *observable* variables like $\sigma$ and $\varepsilon$. It is now difficult to find out who first introduced such variables. This branch was mainly inspired by thermodynamics[5]. We find internal variables already in the early thermodynamical works like those of Eckart [8], [9] who introduces "*certain other variables*" in a more intuitive way. We fully agree to Šilhavý [25]:

> "*Classical thermodynamics uses the concept of state in an informal way, which creates a good deal of confusion in its foundations*."

Percy Williams Bridgman (1882 - 1961) was probably one of the first to try to construct a general concept of state.

> "*Ordinarily the state of a body is characterized by all the measurable properties of the body.*" He assumes 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. (...) The "state" is determined by the instantaneous values of certain parameters and their history*."

Although Bridgman's state concept still remains rather vague and lacks of mathematical exactness, some of his ideas later led to concepts like the *method of preparation* and the *minimal state concept* as we will see in the sequel.

In internal variable theories one introduces a (finite) set of tensor-valued variables $z$ as a primitive concept, which enter the constitutive law $F$ (a function, not a functional) for the stresses as additional independent variables

[4] See also Haupt [14].

[5] For references to early thermodynamical works see Horstemeyer/Bammann [15] and Maugin/Muschik [20], for references to different state spaces see Muschik/Papenfuss/Ehrentraut [21].

$$\sigma(t) \;=\; F(\varepsilon(t),\, z(t)). \tag{4}$$

For the internal variables an evolution function is needed, which is assumed to be of the form of a process functional of the deformation process

$$z(t) \;=\; \mathcal{P}\{\varepsilon(\tau)\Big|_{\tau=t_0}^{t}\,,\, z(t_0)\} \tag{5}$$

or, simpler, by an evolution function of rate form (first order ODE)

$$z^{\bullet} \;=\; E(\varepsilon,\, z,\, \varepsilon^{\bullet}) \tag{6}$$

or even in an incrementally linear form

$$z^{\bullet} \;=\; e(\varepsilon,\, z)\,\varepsilon^{\bullet}. \tag{7}$$

The solution of the last two requires initial values at the starting time.

Here all variables are taken at the same time and the same point so that we may suppress the temporal and spatial arguments.

This format is simple and practical, and many specific material models can be brought into it. The important disadvantage of internal variable theories is, however, that the internal variables are not defined but introduced in an ad hoc manner as primitive concepts.[6] In doing so there is hardly any way to assure uniqueness. In fact, in almost all examples one can show that the choice of these variables is rather arbitrary, and so is the structure of the state space.

Apart from non-uniqueness, one can state that not all material models allow for a state space with a finite dimensional linear structure. As a counterexample we could mention history functionals where the histories belong to a functional space of infinite dimension.

In order to give a more concrete example we consider plastic bending of beams[7]. For this purpose, a beam element is modeled by a one-dimensional linear elastic-perfectly plastic law. If we assume Bernoulli's hypothesis, then we can determine the elongation of each fiber by the local curvature of the beam as a linear function of the transversal coordinate $x$. The stresses in each fiber depend on the deformation process, as usual in plasticity. The resulting moment is the integral over the cross section

$$M \;=\; \int_A \sigma(x)\, x\, dA. \tag{8}$$

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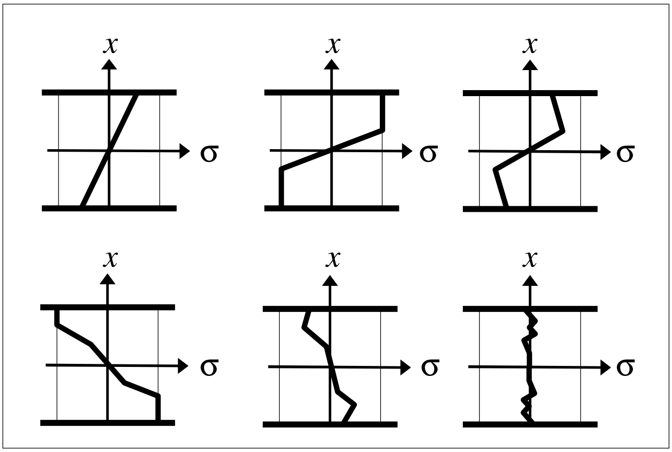
[6] Casey/Naghdi [4] state that "*for a constitutive theory of plasticity it is not enough to assume a constitutive equation for plastic strain (or for its rate). It is necessary, in addition, to provide a prescription for how plastic strain (or even its rate) can be determined from stress and strain measurements, at least in principle.*" This statement can also be applied in the same way to any theory of inelasticity other than plasticity.

[7] This example was given by S. Govindjee (2010) in a private communication.




The stress distribution σ(*x*) is a function of the curvature process and will always be piecewise linear in *x*. In the Figure a series of cross sections initially, after the first yielding, after reverse yielding, etc. is sketched. The number of possible turning points is countable infinite. Therefore, the bending moment resulting from the past curvature process can not be described by a finite number of variables, in principle.

## 5 Noll´s New Theory of Simple Materials

For some decades these two paradigms of history functionals and internal variables coexisted, but the relationship between them remained unclear for a long time. This unsatisfying situation ended in 1972, when Noll published his *New Theory of Simple Materials* [19]. As a motivation, Noll claimed that the theory of history functionals

> "*has failed to give an adequate conceptual frame for the mathematical description of such phenomena as plasticity, yield, and hysteresis.*"

Hysteresis could surely be described by such functionals as long as it is not rate-independent, but plasticity (and yield, which is included in plasticity) could in fact not be described in the format of history functionals. So there was good reason to leave the history functionals behind and to create a new theory.

To do this, Noll introduced the following concepts:

- a *process class* as a collection of all possible deformation processes the material could be submitted to starting from some initial state
- a *state space* as a primitive concept
- an *evolution function* for the state in the form of a process functional
- an *output function* for the stresses
- an *output function* for the strains

One can call this theory also a *state variable theory*. Noll´s state space is a primitive concept but with a precise mathematical meaning. In a mathematical sense it is uniquely defined, although it may have different representations.

Within this setting, Noll was able to establish an embedding of the theory of *history functionals* within the new theory. According to this, two facts can be stated. Firstly, a representation of a material as a history functional is only possible if it has a fading memory property. And, secondly, the theory of history functionals is a subclass of the internal variable theory if properly constructed ("*semi-elastic*").

Although this theory is rather general and unifies all other ones, its acceptance within the scientific community remained rather limited. This has surely to do with two of its properties. Firstly, it is a rather complicated and demanding construction and, thus, by no means simple. Secondly, the concept of the state space remains rather abstract and difficult to construct. It has hardly any structure. Only a uniform structure on subsets of the state space is introduced in a natural way[8]. It does not possess a linear structure, so nothing can be said about its dimension, neither does a differentiable structure exist a priori which could be used for evolution equations in the form of ODFs like Eq. (6).

It was C. A. Truesdell who wrote us in a personal letter in 1980:

> "*Although Noll's paper presenting his "new theory" was dedicated to me, I cannot understand it. It took me ten years to master his "old theory", and now I am much older.*"

In fact, the paper was conceptually overloaded[9] and difficult to understand by a non-mathematician.

## 6 Minimal State Space

In the following decades, the community became rather pragmatic with respect to general frameworks. Only few papers or books have been published with the claim of presenting a general constitutive theory. The key problem for this seems to be the construction of the state space. In 1966 and 1968, Emin Turan Onat (1925 - 2000) [22], [23] suggested a construction of the state space in a way which is used in systems theory known there as the *minimal state space*. This concept has been later worked out by Bertram in detail for materials with internal constraints [1] and without constraints [2].

The construction of this state space is rather simple. We assume that we have infinitely many replicas of the material in the same initial situation[10] like

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[8] See Fabrizio/ Lazzari [10] for the topology of the state space.

[9] In the same paper [20] Noll introduced the intrinsic description which does not make use of any reference placement but instead of concepts of differential geometry, another rather demanding concept for non-mathematicians which has also gained little acceptance in the scientific community.

[10] Which precisely means that all replicas respond to the same $\varepsilon$-process with the identical $\sigma$-value.

Bridgman [3] did. Then we can perform certain deformation processes out of this initial situation, the collection of which is called *process class* (in the strain space). And finally it is assumed that at the end of any of these processes we can measure the stresses.

We now define an equivalence relation on the process class. Two processes are considered as equivalent if

(*i*) both can be continued by the same set of deformation processes.

(*ii*) the responses (stresses) to all of them are pairwise identical.

Or in other words, two processes are equivalent if no difference in the future behavior can be detected. The equivalence classes according to this equivalence relation define the *state space*.

This state space is unique, although it may allow for different representations. Moreover, it has exactly the right size. If we would drop one bit from it, it would be insufficient and violate determinism. This is why it is named *minimal state space*. And if we would add one bit, it would lead to a redundancy.[11] So it would also deserve the name *maximal state space*.

In the quoted works, the *minimal state space* concept has been related to Noll's new simple materials. There is no principle contradiction with Noll´s *new simple materials*, although the construction of the *minimal state space* is now much simpler. Accordingly, we can at least partly adopt Noll´s concepts. For example, Noll gives a way to construct a topology and a uniformity on state space sections. By the same procedure such a topological structure can also be given to the minimal state space. However, to the best of our knowledge nobody has ever introduced a differentiable structure on this state space in a natural way. This is needed for many purposes like the application of the second law of thermodynamics as it is demonstrated in the next section.

As a résumé, the advantages of this theory are manifold:

- It is very general. In fact there is no class of deterministic models known that does not fit into this format. Moreover, it can also be directly applied to thermodynamics, electrodynamics, and other branches of deterministic sciences.
- No new primitive concepts are needed other than the observable quantities which we called stresses and strains.
- It is based on a derived state concept which is unique and constructed in a physically clear, mathematically exact, and practical way. This state space has precisely the right size.
- Also the evolution equation for the states can be derived.

The main lack of this state concept is that this state space has little mathematical structure. In particular, it does not have a natural linear structure nor

[11] This state space coincides with the large state space of Muschik/Papenfuss/Ehrentraut [21]. While within most theories the state space results from the material class under consideration, Muschik/Papenfuss/Ehrentraut start with the state space and work out the material class compatible with it.

a differentiable structure. In examples, this all can be introduced and then it can be of finite or infinite dimension. What we have in mind, however, is a natural way to generally define such structures. And this is still the main open problem.

## 7 Thermodynamic Consistency

In the sequel we will give an argument for the need of additional mathematical structure of the state space like a differentiable one.

In order to exploit the second law of thermodynamics in the form of the Clausius-Duhem inequality with the entropy $\eta$, the mass density $\rho$, and the heat flux $\mathbf{q}$

$$\varphi^\bullet + \eta\,\theta^\bullet - \frac{1}{\rho}\sigma \cdot \varepsilon^\bullet + \frac{\mathbf{q} \cdot \mathbf{g}}{\rho\ \theta} \leq 0 \tag{9}$$

we have to introduce the free energy as a function of state $z$ and the current independent variables like strain $\varepsilon$, temperature $\theta$, and temperature gradient $\mathbf{g}$

$$\varphi(\varepsilon, \theta, \mathbf{g}, z) \tag{10}$$

so that its time derivative is composed by the partial derivatives

$$\varphi(\varepsilon, \theta, \mathbf{g}, z)^\bullet = \partial_\varepsilon \varphi\, \varepsilon^\bullet + \partial_\theta \varphi\, \theta^\bullet + \partial_{\mathbf{g}} \varphi\, \mathbf{g}^\bullet + \partial_z \varphi\, z^\bullet. \tag{11}$$

Then $z^\bullet$ must be substituted by the evolution law for the states. Only after that we are able to draw necessary and sufficient conditions for the Clausius-Duhem inequality. However, the last term requires a differentiable structure in the state space.

In Coleman/Gurtin [5] a way to exploit the Clausius-Duhem inequality in this way is given. Since these authors use an evolution equation for the internal variables of the form

$$z^\bullet = E(\varepsilon, \theta, grad\,\theta, z) \tag{12}$$

which is less general than Eq. (6), only few material classes like the ideal gases are included, for which they specialize their theory. In particular, plasticity, viscoplasticity, damage, phase changes, etc. are not included since the rates of the independent variables are not included in the list of arguments of the evolution function.

Only for history-functionals with fading memory are the consequences of the Clausius-Duhem inequality given by Coleman [6] in a rather general way[12]. Here, the free energy is derived with respect to thermo-kinematical histories as Frechet-differentials in Hilbert spaces. Besides the usual potentials, a residual dissipation inequality remains, which has to be satisfied.

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[12] See also Coleman/Owen [7].

It would be desirable to apply this procedure to exploit the CDI for essentially all materials and to establish necessary and sufficient conditions like the potentials and the residual inequality. However, this is only feasible if the state space has a differentiable structure.

## 8 Résumé

During the last 50 to 60 years many new branches of material theory have been introduced like, e.g., viscoplasticity, continuum damage mechanics, finite plasticity, micromorphic and gradient materials, polar theories, etc. Most authors worked with ad hoc introduced internal variables, a both pragmatic and practical procedure. Nevertheless, a globally accepted general theory or framework for all of these particular material classes is still lacking. Metaphorically speaking, the tree of material theory has gained an overwhelming variety of blossoming branches, while its trunk still remains (conceptually) weak.

If we enlarge our frame and include thermodynamics into our considerations, then we have to state that also here the lack of a general theory leads to undesirable effects like, e.g., that for each and every new constitutive model the thermodynamical consistency has to be proven anew without being able to just refer to a general representation.

We are still far from being able to consider *Material Theory* as a finalized, conceptually sound, and practical theory. Instead, although some progress has been made during its 50 year history, there is still a sizeable piece of work to be done. This article is meant to focus the discussion and stimulate investigations on this important issue.

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