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A non-commutative diagram in the theory of materials

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THE NOTE examines the order of two procedures commonly used in the theory of materials: the procedure of finding the thermodynamical restrictions on constitutive functionals and the procedure of simplifying the constitutive functionals by approximations or restrictions. It is pointed out that these two procedures are not interchangeable. This has consequences on interpretations of various results of thermodynamical analysis. In particular, it is explained that the Clausius–Duhem inequality does not exclude the presence of higher gradients of deformation in the static response functions.

1. Introduction

IN THE CONTEMPORARY phenomenological theory of materials the Clausius–Duhem inequality (CDI) plays a central role. The assumption that the CDI is satisfied in every thermodynamical process compatible with the balance equations and the constitutive equations places restrictions on the constitutive functionals. A systematic procedure was developed by COLEMAN and NOLL [1] to find these restrictions in 1963. Since then the Coleman–Noll procedure (CNP) has been applied by many authors to analyse various constitutive assumptions. In this note I give examples which demonstrate that the CNP is not interchangeable with the simplifications of the constitutive functionals such as approximations in slow processes or restrictions to static situations. That is, the application of the CNP to the simplified constitutive functionals does not always lead to the same result as the simplification of the already thermodynamically restricted constitutive functionals. Although, in general, the lack of such interchangeability is rather obvious, in concrete situations this fact seems to be neglected when interpreting the results obtained within specific constitutive classes. Moreover, so far the *interchangeability* has been considered as a desirable feature and conditions have been sought to guarantee it. I shall indicate a class of phenomena for which the *noninterchangeability* is crucial for their description within the framework of traditional thermodynamics based on the CDI.

2. Two procedures in the theory of materials

In order to understand and describe certain phenomena from the phenomenological point of view, one usually starts by making assumptions concerning the smoothness of the constitutive functionals which reflect the basic qualitative features of the behaviour of the body. Such assumptions are, for example, the elasticity, fading memory, or viscosity of the body. On selecting the proper constitutive class, one employs the CNP to obtain the information the CDI provides about the constitutive functionals. These, in turn, help in the further analysis of the behaviour of the body.

In specific situations such as slow motions, small deformations, or static circumstances, the general constitutuive functionals can be replaced by simpler ones. The simplification procedure (SP) may consist in approximations or just in restricting the functionals to a subset of the original set of arguments. For example, in slow processes the constitutive functionals of materials with fading memory can be approximated by constitutive functions of an appropriate viscous material (the Coleman–Noll retardation theorem, [2]). A more universal example is that in static situations the response functionals of many materials can be reduced to the constitutive functions formally similar to the constitutive functions of a thermoelastic body.

The restrictions the CDI places on the general constitutive functionals imply certain restrictions on the simplified constitutive functionals. In order to find these restrictions, one might be tempted to reverse the order of the operations: first to replace the general unrestricted functionals by the simpler ones and only then to apply the CNP. It turns out that this reverse order of operations leads to different (and obviously incorrect) results.

The following diagram describes schematically the two possible orderings of the operations:

$$\begin{array}{ccc} \text{General constitutive class} & \xrightarrow{\text{CNP}} & \text{Constitutive class compatible with the CDI} \\ \downarrow \text{SP} & & \downarrow \text{SP} \\ \text{Simplified constitutive class} & \xrightarrow{\text{CNP}} & \text{Simplified constitutive class compatible with the CDI} \end{array}$$

The diagram is not commutative.

Consider, for example, a material with fading memory compatible with the CDI, and the viscous material which approximates it via the Coleman–Noll retardation theorem. The CDI places restrictions on the viscous material indirectly through the restrictions on the original material with fading memory. These restrictions on the viscous material can be made explicit (Šilhavý [3]) and surprisingly they do not entirely coincide with the usual thermodynamic restrictions on viscous materials. The details will be given elsewhere [3].

Generally one cannot even say which of the two orderings CNP → SP and SP → CNP will result in stronger restrictions. Examples can be given where CNP → SP leads to stronger restrictions and other examples can be given where SP → CNP leads to stronger restrictions (Šilhavý [3], [4]).

3. The static response of inelastic materials

In one case the noninterchangeability seems to be of immediate interest. As it has already been pointed out, in static situations the response of many materials is governed by the constitutive functions resembling the thermoelastic materials. This means that the equilibrium values of the stress, entropy, and free energy are completely determined by the corresponding fields of the temperature and by the deformation of the body. The simplification procedure — the restriction to static situations — leads to the equations of thermoelasticity here. The static response may be nonlocal if the general response functionals are nonlocal. On the other hand, a result of GURTIN [5] says that for (possibly nonlocal) thermoelastic bodies the CNP implies that actually the response of the stress, entropy, and free energy at the given point is completely determined by the values of temperature and deformation gradient at that point, and that the stress and the entropy response functions are expressed through the derivatives of the free energy in the usual way. Applying this result to the equations governing the equilibrium response of inelastic bodies would thus exclude not only all nonlocal dependences, but also the dependence of the response on the higher gradients of deformation. Howerver, this conclusion, obtained via SP $\rightarrow$ CNP, is incorrect. The correct sequence, CNP $\rightarrow$ SP, leads to completely different results. Namely, it can be shown (ŠILHAVÝ [4]) that the only restriction which is implied on the static response functions by CNP $\rightarrow$ SP is the static heat conduction inequality; the static response functions for stress, entropy, and free energy are completely arbitrary unless additional assumptions about the material are made. In particular, the static response functions can depend on the higher gradients of deformations and need not satisfy the usual relations.

Apparently, these possibilities are realized in nature. There are many phenomena whose existence requires that the static stress depends on the higher gradients of deformation. The capillarity phenomena and phase transitions are two examples among many others. Usually modifications of the thermodynamical structure are proposed in order to escape from the above mentioned result of Gurtin. That this is not necessary is shown in [6] where I analyse the phase transitions and capillarity phenomena within the framework of the traditional thermodynamics with internal variables based on the CDI.

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