

## Chapter 2

# Introduction

**Abstract** Introduction of internal variables can be considered as a universal modelling tool for macroscopic field theories. It is based on minimal number of assumptions about the physical mechanism of the modelled phenomena. As long as evolution equations of internal variables are determined by basic macroscopic principles, we can expect that the validity of the evolution equations is independent of particular microscopic models.

### 2.1 Micro versus Macro

The purpose of thermomechanics is the prediction of the response of a body to an external mechanical or thermal loading. If the body is considered as an elastic one, then its isothermal response is governed by the Hooke law. The model of the elastic body is the simplest model of material behavior. On the other hand, the thermal response of a rigid body can be described by the Fourier law (again in the simplest case). It should be emphasized that these simple models have the distinct mathematical structure. The description of the dynamics of an elastic body includes a second-order time derivative in the equation of motion presented in terms of displacement [34]. Such an equation is a hyperbolic partial differential equation. The Fourier law, in its turn, provides the heat conduction equation with the first-order time derivative for temperature. Mathematically, the latter is a parabolic partial differential equation. Coupling of elastic and thermal effects results in the thermoeasticity theory for homogeneous bodies [65, e.g.].

In reality, all bodies are inhomogeneous, excluding perfect crystals and artificially refined materials. Usually materials possess a microstructure characterized by various size, distribution, and properties of inclusions or imperfections. Although the length scale of the microstructure is, as a rule, much smaller than the length scale of a body,

the impact of microstructure on overall response of the body may not be necessarily small. The demand of accounting of the influence of microstructure dictates the improvement of macroscopic material theories.

There exists several directions in the description of the microstructure influence. The first one is micromechanics, which serves for the determination of properties of “effective” media by homogenization methods [52, 60]. The homogenized “effective” medium is used then instead of the original microstructured material for the prediction of its thermomechanical response. The homogenization methods of micromechanics are well suited for static problems with periodic or statistically homogeneous distribution of inhomogeneities.

The second approach introduces memory and nonlocal effects in the model, either using memory functionals and nonlocal kernels (strong nonlocality) or higher order time and space derivatives (weak nonlocality) [8, 59]. Gradient models with nonlocality in space are typical examples of the latter method. Another theoretical method of this family is GENERIC [24, 63, 64]. The compatibility of gradient effects with the second law is considered in the framework of the rational thermodynamics by various techniques [13, 16, 74].

The third approach corresponds to generalized continuum theories. A number of advanced generalized continuum theories have been introduced over the past five decades to take into account the influence of the structural inhomogeneities on the macroscopic behavior of materials (see overview by Maugin [43]). In general terms, such theories include coarse grained morphological descriptors introduced to describe the morphology of the material element [9, 37]. The morphological descriptors represent certain additional independent kinematic fields. The most known example of the morphological descriptor is the microrotation vector in the Cosserat material. Another example is the second order symmetric tensor of microdeformation introduced by Mindlin [49], who considered the material element as a cell able to deform independently of the rest of the body. The relevant continuum theory is called micromorphic [21]. The micromorphic theory is the most successful top-down formulation of a two-level continuum model, in which the overall deformation is composed of the macroscopic continuous deformation and the internal microscopic deformation of the inner structure [22].

The distinction between homogenization methods, nonlocal and generalized continuum theories is not sharp. Generalized continua are probably the most flexible: morphological descriptors can be obtained by homogenization [21] and may have certain weak or strong nonlocality. The separation of the macro- and micromotion in generalized continuum theories needs to postulate separate balance laws at the macro- and the micro- levels, like in [49]. Then the suitable boundary conditions are required as well.

Some microstructural approaches extend the space-time representation of wanted fields by introducing additional mesoscopic characteristics of some material types. Those sometimes are variants of kinetic theory where the key is the characterization of interaction between mesoscopic actors, like crack or grains [7, 36, 71]. Another example is the mesoscopic theory of Muschik where the director concept is used at the mesoscopic level for liquid crystals [5, 56, 58].

Microstructure considered as material heterogeneity is best modelled by the material formulation of continuum mechanics [40] which provides the balance law of the macromotion including all the interaction forces within the solid accounting for microstructural effects, if they are described by internal variables. The evolution of internal variables is not governed by a balance law but determined by thermodynamic constraints.

It is clear that material elements in generalized continuum theories extend the classical thermodynamic state space beyond equilibrium one. This dictates to choose the method of the description of such non-equilibrium states, especially in the presence of dissipative processes. The classical theory of irreversible processes (TIP) [18] is not sufficient for such a description because its basic hypothesis is the local thermodynamic equilibrium. The choice of an appropriate thermodynamical description is essential.

According to the classical formulation, in *local equilibrium* thermodynamic quantities and equations of state of equilibrium thermodynamics are valid locally, although the total system is not in equilibrium [18]. Therefore, local equilibrium suggests a localization, i.e., the transfer from the homogeneous thermostatics to a field theory. From the point of view of microscopic theories, local equilibrium is related to particularly (and thermodynamically) parameterized probability distribution functions of randomly moving particles. From the point of view of thermodynamic principles, normal material tends to equilibrium. Practically, only a small number of degrees of freedom will dominate this tendency. The slowest process survives. Therefore, few extra fields are enough to characterize a system near to equilibrium. The basic question is the meaning of near. The additional fields together with the complete thermodynamic framework ensure that distance from equilibrium is precise and the tendency toward it is meaningful.

Among several versions of non-equilibrium thermodynamics [57], the *thermodynamics with internal variables* (TIV) holds a specific place. This theory (TIV) is the direct extension of TIP beyond the local equilibrium [2]. This means that internal variables must be in the domain of a concave entropy function, and the entropy must increase in any insulated part of the material. We chose the thermodynamics with internal variables because it does not introduce any assumption about the physical mechanism of the modelled phenomenon in advance and, therefore, can be developed in an universal form. Moreover, it assumes the strict validity of thermodynamic concepts also for the internal variables. This way we insist the most conservative use of thermodynamics outside local equilibrium.

## 2.2 Internal Variables and Dynamic Degrees of Freedom

The starting point of the TIV is the introduction of an additional field variable of an arbitrary tensorial order. The tensorial order of the internal variable usually can be deduced from the properties of the modelled phenomenon. The use of an internal

variable suggests that the influence of an internal structure on the dynamic behavior of a material will be taken into account [67].

The unavoidable key question is the following: How to construct (or derive) the evolution equation for an internal variable? There are two answers on this question, i.e., there exist two basic methods to generate the evolution equations for internal variables. Both methods are based on fundamental principles.

The *first method* generates the evolution equations exploiting the entropy inequality. This approach uses exclusively thermodynamic laws, and the corresponding variables are called *internal variables of state* [42]. This framework has the advantage of operating with familiar thermodynamic concepts like thermodynamic force and entropy, however, no inertial effects are considered. Internal variables of state are usually introduced in the case of dissipative processes. They must satisfy only the second law of thermodynamics, and need not be balanced. The dissipation (or internal power) induced by an internal variable of state is equal to the product of its rate of change and the corresponding conjugated force [45, 54]. Accordingly, the evolution equation includes only first-order time derivative of the internal variable. In the internal variable theory, a concept of a local constrained non-equilibrium state is introduced. In other words, there always exists a local accompanying equilibrium (or quasi-equilibrium) state, onto which the local non-equilibrium state can be projected [28, 55]. Internal variables add extra dimensions to the thermodynamic state space.

The *second method* constructs the evolution equations through a Hamiltonian variational principle and therefore inertial effects are unavoidable. This approach has a mechanical flavor, and the corresponding variables are called *internal degrees of freedom*. Dissipation in this case is added by dissipation potentials. This theoretical frame has the advantage of operating with familiar mechanical concepts like force and energy. Internal degrees of freedom are endowed with both inertia and flux, where the latter is not necessarily purely dissipative (on the contrary, it could be purely non-dissipative) [42, 45]. The corresponding evolution equations contain the second-order time derivatives of the dynamic degrees of freedom.

Usually these two methods are considered as alternative and incompatible. Intuitively, however, it is natural to expect that the influence of microstructure should include both inertial and dissipative aspects. The distinction between the theoretical frames mentioned above affects the common application of variational principles and thermodynamics. That is well reflected by the appearance of dissipation potentials as separate theoretical entities in variational models of internal degrees of freedom dealing with dissipation. On the other hand, with pure thermodynamical methods—in the internal variables approach—inertial effects are not considered. Basic equations of thermodynamical origin do not have variational formulations, at least without any further ado [75].

Thus, one may have the impression that the doubling of the theoretical structure is a necessity, because the usage of both mechanical and thermodynamical laws cannot be avoided. This is the conceptual standpoint of the GENERIC approach (GENeral Non-equilibrium Equation of Reversible Irreversible Coupling) [24, 63, 64]. However, a doubled theoretical structure is not very convenient, because it doubles the number

of physical assumptions restricting predictive capabilities of the theory. We will examine the two concepts of internal variables in more detail.

### 2.2.1 Internal Variables of State

Let us consider a particular simple example, a heat conducting rigid material with the description of its microstructure by means of a scalar internal variable. The thermodynamic state of material points is characterized by the internal energy density  $E$  and an internal variable  $\alpha$ . The balance of internal energy in this simple case without internal heat sources reads

$$\dot{E} + \partial_i Q_i = 0, \quad (2.1)$$

where upper dot denotes material time derivative,  $Q_i$  is the heat flux, and  $\partial_i$  denote spatial derivatives. We use here a Cartesian coordinate system and the Einstein summation rule for the repeated indices. The entropy density  $S$  depends on the thermodynamic state, i.e., on the internal energy and on an internal variable,  $S = S(E, \alpha)$ . Its balance can be represented in the following form:

$$\dot{S} + \partial_i J_i = \Phi \geq 0, \quad (2.2)$$

where  $J_i$  is the entropy flux and  $\Phi$  is the entropy production.

According to standard thermodynamic rules, the partial derivative of the entropy with respect to the internal energy is the reciprocal temperature,

$$\frac{\partial S}{\partial E} = \frac{1}{\theta}. \quad (2.3)$$

The partial derivative of the entropy density with respect to internal variable  $\alpha$  is denoted as

$$A = \theta \frac{\partial S}{\partial \alpha}, \quad (2.4)$$

and called  $\alpha$ -affinity. These relations can be unified according to the usual thermodynamic terminology in the form of the Gibbs relation:

$$dE = \theta dS - A d\alpha. \quad (2.5)$$

Both the temperature and the  $\alpha$ -affinity depend on the internal energy and on the internal variable, i.e.,  $\theta = \theta(E, \alpha)$ ,  $A = A(E, \alpha)$ . This is clearly a point that deserves attention, because the temperature seems to loose its universality: having various microstructures one may measure different temperatures. While there is a lot of discussions on the non-equilibrium temperature, we accept the concept of a local

constrained non-equilibrium state [10, 12, 26]. This concept assumes that there always exists a local accompanying equilibrium state, onto which the local non-equilibrium state can be projected [28, 55].

The second law requires the non-negative entropy production. The entropy production can be calculated if the entropy flux is given. Applying the classical form the entropy flux  $J_i = Q_i/\theta$ , we arrive at the following expression of the entropy production:

$$\begin{aligned}\Phi &= \frac{\partial S}{\partial E} \dot{E} + \frac{\partial S}{\partial \alpha} \dot{\alpha} + \partial_i \left( \frac{Q_i}{\theta} \right) = \frac{\partial S}{\partial E} \dot{E} + \frac{\partial S}{\partial \alpha} \dot{\alpha} + \partial_i \left( \frac{Q_i}{\theta} \right) = \\ &= -\frac{1}{\theta} \partial_i Q_i - \frac{A}{\theta} \dot{\alpha} + \frac{1}{\theta} \partial_i Q_i + Q_i \partial_i \left( \frac{1}{\theta} \right) = Q_i \partial_i \left( \frac{1}{\theta} \right) - \frac{A}{\theta} \dot{\alpha} \geq 0.\end{aligned}\quad (2.6)$$

In the latter expression the constitutive, undetermined functions are the heat flux and the evolution equation of the internal variable. Since the internal variable is a scalar quantity and the heat flux is a vectorial one, both terms on the right hand side of Eq. (2.6) should be non-negative independently in isotropic materials. Therefore, looking for a linear solution of inequality (2.6), we arrive at the Fourier law of heat conduction

$$Q_i = \lambda \partial_i \left( \frac{1}{\theta} \right) = -\lambda_F \partial_i \theta, \quad (2.7)$$

and the evolution equation for the internal variable

$$\dot{\alpha} = k_1 \frac{A}{\theta}, \quad (2.8)$$

where  $\lambda$  is the thermodynamic parameter and  $\lambda_F = -\lambda/\theta^2$  is the Fourier heat conduction coefficient,  $k_1$  is an appropriate constant. Both  $\lambda$  and  $k_1$  must be non-negative due to the second law.

Introducing the internal variable we extend the thermodynamic state space. We keep the basic assumption of the thermodynamic stability, that is, entropy should be a concave function in all variables, including the internal ones. The simplest concave extension of the entropy function is

$$S = S_0(E) - k_2 \alpha^2/2. \quad (2.9)$$

Then  $A/\theta = k_2 \alpha$ ,  $k_2 > 0$  due to the concavity of entropy, and the internal variables evolves according to the simplest relaxation-type dynamics

$$\dot{\alpha} = -k_1 k_2 \alpha, \quad (2.10)$$

that results in an exponential decrease of any initial value of the internal variable to zero.

### 2.2.2 Internal Dynamic Degrees of Freedom

A completely different approach to the evolution of an internal variable supposes that its reversible non-dissipative part can be derived by variational principles, and the dissipative part is added by a dissipation potential. One assumes that there exists a Lagrangian  $\mathcal{L}(\alpha, \dot{\alpha})$ , and the corresponding equation of motion can be calculated with the help of the variational derivative and by a dissipation potential  $\mathcal{D}(\dot{\alpha})$  [23, 39, 41]:

$$\frac{\delta \mathcal{L}}{\delta \alpha} = \frac{\partial \mathcal{L}}{\partial \alpha} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\alpha}} = \frac{\partial \mathcal{D}}{\partial \dot{\alpha}}. \quad (2.11)$$

Here  $\delta \mathcal{L} / \delta \alpha$  denotes the functional derivative of the Lagrangian with respect to  $\alpha$ .

In the case of the heat conducting rigid material, the Lagrangian can be assumed in the following special form for a single dynamic degree of freedom

$$\mathcal{L}(E, \alpha, \dot{\alpha}) = \mathcal{K}(\dot{\alpha}) - W(E, \alpha). \quad (2.12)$$

where  $W(E, \alpha) = E - \theta S$  is the Helmholtz free energy. Keeping the form of entropy dependence (2.9) and supposing the quadratic function for the kinetic part of the Lagrangian

$$\mathcal{K}(\dot{\alpha}) = \frac{m}{2} \dot{\alpha}^2, \quad (2.13)$$

we have the field equation for the internal degree of freedom  $\alpha$

$$\frac{\delta \mathcal{L}}{\delta \alpha} = -\frac{\partial \mathcal{L}}{\partial \alpha} - \frac{d}{dt} (m\dot{\alpha}) = \frac{\partial \mathcal{D}}{\partial \dot{\alpha}}. \quad (2.14)$$

This equation contains the second-order time derivative of the internal degree of freedom for any choice of the dissipation potential

$$m\ddot{\alpha} = k_2\theta\alpha - \frac{\partial \mathcal{D}}{\partial \dot{\alpha}}. \quad (2.15)$$

because

$$\frac{\partial \mathcal{L}}{\partial \alpha} = -\frac{\partial W}{\partial \alpha} = \theta \frac{\partial S}{\partial \alpha} = -k_2\theta\alpha$$

according to Eq. (2.9). The corresponding dissipation is calculated by the entropy production accounting the contribution from the dissipation potential [45]:

$$\theta Q_i \partial_i \left( \frac{1}{\theta} \right) + \frac{\partial \mathcal{D}}{\partial \dot{\alpha}} \dot{\alpha} \geq 0, \quad (2.16)$$

and the dissipation potential have to be chosen to fulfill the dissipation inequality.

### 2.2.3 Similarity and Differences

Both internal variables of state and internal degrees of freedom are used to take into account the influence of internal processes on the global behavior of materials. Both of them are introduced in addition to classical field quantities. However, the differences in the approaches are much larger. Internal variable of state is characterized by:

- the extension of the thermodynamic state space; the extended entropy function should be concave,
- the calculation of the entropy production accounting the internal energy balance and the evolution equation of the internal variable,
- the solution of the dissipation inequality providing properly introduced constitutive functions; usually a linear solution is good enough.

In its turn, the main features for the dynamic degree of freedom are:

- the thermodynamic state space is not extended,
- evolution equation for a dynamic degree of freedom is determined by the choice of a Lagrangian and the independent choice of a dissipation potential.

Both theories can have a weakly nonlocal extension. In that case natural boundary conditions can be calculated by variational means in the case of dynamics degrees of freedom and by the zero entropy flux prescription at boundaries in the case of internal variables. The most important difference between the two approaches consists in the parabolicity of evolution equations for internal variables of state and hyperbolicity of balance laws for the dynamic degrees of freedom. It is also important to observe that internal degrees of freedom need the variational method and thermodynamic relations simultaneously, whereas for internal variables of state there is no need anything beyond thermodynamics.

## 2.3 Generalization: Dual Internal Variables

Let us fix the state of the art. There exist two clearly distinctive types of internal variables: internal degrees of freedom and internal variables of state [42, 45]. By definition, internal variables of state must have no inertia, and they produce no external work. The internal variables of state are not governed by a field equation, i.e., by their own balance law; the power expended by internal variables will be only of the dissipative type. On the contrary, the internal degrees of freedom obey their own balance law. Both internal degrees of freedom and internal variables of state are introduced to capture microstructural properties in a macroscopic description. The thorough thermomechanical theory with weakly nonlocal internal variables of state is presented recently by Maugin [42]. It can be called as a *single internal variable* theory. In the case of internal degrees of freedom the complete description is not finished yet [38]. This is why “a unified continuum mechanical description of materials with inherent microstructure is to date not available” [30].

The introduction of any kind of internal variables should be in the correspondence with the second law of thermodynamics. The latter indicates the direction for an unified continual description of materials with microstructure. The main idea is that one can obtain the form of the evolution equation and also the connection to other processes, considering only basic principles, first of all, the second law of thermodynamics. Evolution equations derived from any structural, mesoscopic, or microscopic realization of the extra field variable must belong to this general form, as long as they are restricted by the same basic principles.

We propose an uniform approach based exclusively on thermodynamic laws. Our suggestion requires dual internal variables and a generalization of the usual postulates of non-equilibrium thermodynamics: we do not require the satisfaction of the Onsagerian reciprocity relations [61, 62]. With dual internal variables we are able to include inertial effects and to reproduce the evolution of dynamic degrees of freedom. In other words, instead of the doubling of the theoretical structure we suggest the doubling of the number of internal variables. This is the price we pay for the generalization.

We will follow the terminology of Maugin and Muschik [45] with some important extensions. We call internal variables of state those physical field quantities—beyond the classical ones—whose evolution is determined by thermodynamical laws. We call internal degrees of freedom those physical quantities—beyond the classical ones—whose dynamics is determined by mechanical laws.

In spite of the fine details where these notions are different for various authors (controllability, boundary conditions, weak nonlocality, etc.), we can find a sufficiently general framework where these concepts are combined. This framework appears to be a powerful modelling tool of modern continuum physics [72, 73]. In what follows, we will demonstrate the constructive modelling power of this conceptual framework.

As long as evolution equations of internal variables are determined by basic macroscopic principles, we can expect that the validity of the evolution equations is independent of particular microscopic models. The method of internal variables can be considered as a universal modelling tool for macroscopic field theories. It is based on minimal number of assumptions about the physical mechanism of the modelled phenomena.

## 2.4 Historical Remarks

The concept of internal variables has a long history [44]. As it is pointed out [69], Duhem was the first who introduced what are now called internal state variables. In 1940s, Bridgman proposed an introduction of a large scale thermodynamic parameter of state [6]. The first application of thermodynamical ideas for continua is due to Eckart, who investigated deviations from ideal elastic behaviour, in other words, anelasticity [19, 20]. In solid mechanics, internal variables are introduced by Meixner and Reik [48]. A thermodynamical framework for anelasticity with internal

variables was also treated by Biot [4] and developed by Kluitenberg as a state variable theory [31, 32]. The terminology of *internal degrees of freedom* were introduced in thermodynamics as an extension of the configurational space with statistical and probabilistic aspects [18, 66]. The thermodynamic theory of *internal variables of state* presented by Coleman and Gurtin [17] had presupposed first-order evolution equations for the internal variables and did not include their gradients. In 1970s the internal variable theory was well formalized [29, 33, 35, 67, 70]. The interest to internal variables was enlarged with the introduction of the local accompanying state concept [1, 2, 23, 50]. This concept was elaborated by Muschik [53], Maugin [39], Muschik [54, 55] and Kestin [27, 28] in 1990s. It is worth to mention the theory of *dynamic degrees of freedom* by Verhás [77], which is actually an internal variable theory with zero values of the internal variables at the thermodynamic equilibrium according to the maximum entropy principle. This approach extends the Kluitenberg theory to fluids [11] and also gives a weakly nonlocal extension with a generalized entropy flux introducing the transport of dynamic degrees of freedom [76].

The state of the art of the theory of internal variables with a number of applications was exposed by Maugin and Muschik [45, 46], where the clear distinction between internal variables of state and dynamic degrees of freedom was shown. Attempts to improve and enlarge the applications of the internal variables theory were continued in [77, 78], [68], [14], [79], [47], [15]. The most general weakly nonlocal thermomechanical theory with single internal variable enriched by the extra entropy flux is presented recently by Maugin [42]. Less systematic applications are popular for various phenomena in solids, sometimes without any thermodynamical background [25]. Contemporary view on the internal variable theory can be found in [51], [3], [44].

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