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Generalized thermomechanics with dual internal variables

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Abstract The formal structure of generalized continuum theories is recovered by means of the extension of canonical thermomechanics with dual weakly non-local internal variables. The canonical thermomechanics provides the best framework for such generalization. The Cosserat, micromorphic, and second gradient elasticity theory are considered as examples of the obtained formalization.

Keywords Generalized continua · Canonical thermomechanics · Internal variables · Microstructure · Cosserat medium · Micromorphic medium

1 Motivation

Generalized continuum theories extend conventional continuum mechanics by incorporating intrinsic microstructural effects in the mechanical behavior of materials [1; 2; 3; 4; 5]. Internal variable approach was always an alternative framework for the continuum modeling of such effects in materials [6; 7; 8; 9; 10; 11; 12]. However, the well established theory of internal variables of state [13; 14] cannot completely describe a generalized medium because an internal variable of state has no inertia, but it dissipates. If inertia is introduced, the internal variable must be treated as an actual degree of freedom [15]. Accordingly, the variable is not "internal" any more but can be controlled for instance at the boundary of a body.

A more general thermodynamic framework of the internal variable theory presented recently [16] is based on a duality between internal variables, which make possible to derive evolution equations both for internal variables of state and internal degrees of freedom. A natural question relates to the ability of this duality concept to comprise inertial effects. To answer this question, we show how the dual internal variables can be introduced into continuum mechanics and how certain generalized continuum theories can be interpreted in terms of the dual internal variables.

The most suitable framework for the generalization of continuum theory by weakly non-local dual internal variables enriched by an extra entropy flux is the material formulation of continuum thermomechanics [17; 18]. Therefore, basic definitions of the canonical thermomechanics [17] are recalled in the next section of the paper. Then dual variables are introduced and evolution equations for both

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dissipative and non-dissipative processes are derived. Linear Cosserat, micromorphic, and second gradient elasticity theories are reformulated in terms of internal variables to clarify the structure of the generalized continuum theories. At last, one-dimensional wave propagation problem in a medium with microstructure is considered and corresponding boundary conditions are discussed.

2 Canonical thermomechanics

In the framework of the material formulation of thermomechanics [17; 18], the motion of a body is represented as a time-parametrized mapping χ between position of a material point $\mathbf{X}$ in the reference configuration and its position $\mathbf{x}$ in the actual configuration:

$$\mathbf{x} = \chi(\mathbf{X}, t). \tag{1}$$

Accordingly, the deformation gradient is defined by

$$\mathbf{F} = \partial\chi/\partial\mathbf{X}|_t = \nabla_R \chi. \tag{2}$$

If the constitutive relation for free energy has the form $W = \overline{W}(\mathbf{F}, ..., \mathbf{X})$, then the first Piola-Kirchhoff stress tensor $\mathbf{T}$ is defined by

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}. \tag{3}$$

The canonical form of the energy conservation for sufficiently smooth fields at any regular material point $\mathbf{X}$ in the body has the following form [13; 14]

$$\left.\frac{\partial (S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{Q} = h^{int}, \quad h^{int} := \mathbf{T} : \dot{\mathbf{F}} - \left.\frac{\partial W}{\partial t}\right|_{\mathbf{X}}, \tag{4}$$

where $\mathbf{Q}$ is the material heat flux, S is the entropy density per unit reference volume, θ is the absolute temperature, $d/dt = \partial/\partial t|_X$ or a superimposed dot denotes the material time derivative. The right-hand side of Eq. $(4)_1$ is formally an internal heat source.

Correspondingly, the canonical (material) momentum conservation equation in the presence of a body force $\mathbf{f}_0$ per unit reference volume reads [13; 14]

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X}} - Div_R \mathbf{b} = \mathbf{f}^{int} + \mathbf{f}^{ext} + \mathbf{f}^{inh}, \tag{5}$$

where the *material momentum* $\mathbf{P}$, the material *Eshelby stress* $\mathbf{b}$, the material *inhomogeneity force* $\mathbf{f}^{inh}$, the material *external* (or body) force $\mathbf{f}^{ext}$, and the material *internal* force $\mathbf{f}^{int}$ are defined by

$$\mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{F}, \tag{6}$$

$$\mathbf{b} = -\left(L\mathbf{I}_R + \mathbf{T} \cdot \mathbf{F}\right), \quad L = K - W, \tag{7}$$

$$\mathbf{f}^{inh} := \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{expl} \equiv \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{fixed\ fields} = \left(\frac{1}{2}\mathbf{v}^2\right)\nabla_R \rho_0 - \left.\frac{\partial \overline{W}}{\partial \mathbf{X}}\right|_{expl}, \tag{8}$$

$$\mathbf{f}^{ext} := -\mathbf{f}_0 \cdot \mathbf{F}, \tag{9}$$

$$\mathbf{f}^{int} = \mathbf{T} : (\nabla_R \mathbf{F})^T - \nabla_R W|_{impl}. \tag{10}$$

Here ρ_0 is the mass density in the reference configuration, $\mathbf{v} = \partial\chi/\partial t|_X$ is the physical velocity, the subscript notations *expl* and *impl* mean, respectively, the material gradient keeping the fields fixed (and thus extracting the explicit dependence on $\mathbf{X}$), and taking the material gradient only through the fields present in the function.

The second law can be represented in the form

$$S\dot{\theta} + \mathbf{S} \cdot \nabla_R \theta \le h^{int} + \nabla_R \cdot (\theta \mathbf{K}), \tag{11}$$

where $\mathbf{S}$ is the entropy flux, and the "extra entropy flux" $\mathbf{K}$ vanishes in most cases, but this is not a basic requirement.

The canonical equations for momentum and energy are consequences of local balance laws in the so-called Piola-Kirchhoff formulation (cf. Maugin [17]):

$$\left.\frac{\partial \rho_0}{\partial t}\right|_{\mathbf{X}} = 0, \tag{12}$$

$$\left.\frac{\partial (\rho_0 \mathbf{v})}{\partial t}\right|_{\mathbf{X}} - Div_R \mathbf{T} = \mathbf{f}_0, \tag{13}$$

$$\left.\frac{\partial (K+E)}{\partial t}\right|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T}\cdot\mathbf{v} - \mathbf{Q}) = \mathbf{f}_0 \cdot \mathbf{v}, \tag{14}$$

and the second law of thermodynamics

$$\left.\frac{\partial S}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = (\mathbf{Q}/\theta) + \mathbf{K}. \tag{15}$$

Here $K = \rho_0 \mathbf{v}^2/2$ is the kinetic energy, E is the internal energy per unit reference volume.

Our goal was to show how the dual internal variables can be introduced in the framework of canonical thermomechanics. The corresponding theory with a single internal variable is recently presented by Maugin [13, 14] and it is used as the pattern for the extension.

3 Dual internal variables

Usually, the introduction of internal variables is made without the specification of their tensorial nature. To be more precise, we will consider internal variables $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ as second-order tensors. Then the free energy per unit volume W is specified as the general sufficiently regular function

$$W = \overline{W}(\mathbf{F}, \theta, \boldsymbol{\alpha}, \nabla_R \boldsymbol{\alpha}, \boldsymbol{\beta}, \nabla_R \boldsymbol{\beta}). \tag{16}$$

The corresponding equations of state are given by

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad \mathbf{A} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}, \quad \mathcal{A} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}, \quad \mathbf{B} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\beta}}, \quad \mathcal{B} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\beta}}. \tag{17}$$

The accepted functional dependence (16) and the equations of state (17) lead to the representation of the internal force (10) in the form

$$\begin{aligned}\mathbf{f}^{int} &= \mathbf{T} : (\nabla_R \mathbf{F})^T - \nabla_R W|_{impl} = -\frac{\partial \overline{W}}{\partial \theta}\nabla_R \theta - \frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}\nabla_R \boldsymbol{\alpha} - \frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}\nabla_R(\nabla_R \boldsymbol{\alpha}) - \\ &- \frac{\partial \overline{W}}{\partial \boldsymbol{\beta}}\nabla_R \boldsymbol{\beta} - \frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\beta}}\nabla_R(\nabla_R \boldsymbol{\beta}) = S\nabla_R\theta + \mathbf{A} : (\nabla_R \boldsymbol{\alpha})^T + \mathcal{A} : \nabla_R(\nabla_R \boldsymbol{\alpha})^T + \\ &+ \mathbf{B} : (\nabla_R \boldsymbol{\beta})^T + \mathcal{B} : \nabla_R(\nabla_R \boldsymbol{\beta})^T = \mathbf{f}^{th} + \mathbf{f}^{intr}.\end{aligned} \tag{18}$$

Accordingly, the internal heat source h^{int} is calculated as follows:

$$\begin{aligned}h^{int} &= \mathbf{T} : \dot{\mathbf{F}} - \frac{\partial \overline{W}}{\partial t} = -\frac{\partial \overline{W}}{\partial \theta}\frac{\partial \theta}{\partial t} - \frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}\frac{\partial \boldsymbol{\alpha}}{\partial t} - \frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}\frac{\partial \nabla_R \boldsymbol{\alpha}}{\partial t} - \frac{\partial \overline{W}}{\partial \boldsymbol{\beta}}\frac{\partial \boldsymbol{\beta}}{\partial t} - \frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\beta}}\frac{\partial \nabla_R \boldsymbol{\beta}}{\partial t} = \\ &= S\dot{\theta} + \mathbf{A} : \dot{\boldsymbol{\alpha}} + \mathcal{A} : (\nabla_R \dot{\boldsymbol{\alpha}})^T + \mathbf{B} : \dot{\boldsymbol{\beta}} + \mathcal{B} : (\nabla_R \dot{\boldsymbol{\beta}})^T = h^{th} + h^{intr}.\end{aligned} \tag{19}$$

Here the introduced thermal source terms are defined in terms of temperature space and time derivatives

$$\mathbf{f}^{th} = S\nabla_R \theta, \quad h^{th} = S\dot{\theta}, \tag{20}$$

whereas "intrinsic" source terms are determined by the internal variables

$$\mathbf{f}^{intr} = \mathbf{A} : (\nabla_R \boldsymbol{\alpha})^T + \mathcal{A} : \nabla_R(\nabla_R \boldsymbol{\alpha})^T + \mathbf{B} : (\nabla_R \boldsymbol{\beta})^T + \mathcal{B} : \nabla_R(\nabla_R \boldsymbol{\beta})^T. \tag{21}$$

$$h^{intr} = \mathbf{A} : \dot{\boldsymbol{\alpha}} + \mathcal{A} : (\nabla_R \dot{\boldsymbol{\alpha}})^T + \mathbf{B} : \dot{\boldsymbol{\beta}} + \mathcal{B} : (\nabla_R \dot{\boldsymbol{\beta}})^T. \tag{22}$$

3.1 Non-zero extra entropy flux

Accounting for the expression of the internal heat source (19), the dissipation inequality (11) can be rewritten as

$$\Phi = \mathbf{A} : \dot{\boldsymbol{\alpha}} + \mathcal{A} : (\nabla_R \dot{\boldsymbol{\alpha}})^T + \mathbf{B} : \dot{\boldsymbol{\beta}} + \mathcal{B} : (\nabla_R \dot{\boldsymbol{\beta}})^T - \mathbf{S} \cdot \nabla_R \theta + \nabla_R \cdot (\theta \mathbf{K}) \geq 0. \tag{23}$$

We rearrange the dissipation inequality by adding and subtracting the same terms

$$\begin{aligned} \Phi = \mathbf{A} : \dot{\boldsymbol{\alpha}} - (Div_R \mathcal{A}) : \dot{\boldsymbol{\alpha}} + (Div_R \mathcal{A}) : \dot{\boldsymbol{\alpha}} + \mathcal{A} : (\nabla_R \dot{\boldsymbol{\alpha}})^T + \mathbf{B} : \dot{\boldsymbol{\beta}} - \\ - (Div_R \mathcal{B}) : \dot{\boldsymbol{\beta}} + (Div_R \mathcal{B}) : \dot{\boldsymbol{\beta}} + \mathcal{B} : (\nabla_R \dot{\boldsymbol{\beta}})^T - \mathbf{S} \cdot \nabla_R \theta + \nabla_R \cdot (\theta \mathbf{K}) \geq 0, \end{aligned} \tag{24}$$

that leads to

$$\Phi = (\mathbf{A} - (Div_R \mathcal{A})) : \dot{\boldsymbol{\alpha}} + (\mathbf{B} - (Div_R \mathcal{B})) : \dot{\boldsymbol{\beta}} + \nabla_R \cdot \Big(\mathcal{A} : \dot{\boldsymbol{\alpha}} + \mathcal{B} : \dot{\boldsymbol{\beta}} + \theta \mathbf{K} \Big) - \mathbf{S} \cdot \nabla_R \theta \geq 0. \tag{25}$$

Following Maugin [19], we select the "extra" entropy flux as

$$\mathbf{K} = -\theta^{-1} \mathcal{A} : \dot{\boldsymbol{\alpha}} - \theta^{-1} \mathcal{B} : \dot{\boldsymbol{\beta}}. \tag{26}$$

Then one can check that the canonical equations of momentum and energy keep their form (cf. [13; 14])

$$\frac{\partial \mathbf{P}}{\partial t} - Div_R \widetilde{\mathbf{b}} = \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \tag{27}$$

$$\frac{\partial (S\theta)}{\partial t} + \nabla_R \cdot \widetilde{\mathbf{Q}} = h^{th} + \widetilde{h}^{intr}, \tag{28}$$

with the modified Eshelby stress tensor

$$\widetilde{\mathbf{b}} = -(L \mathbf{1}_R + \mathbf{T}.\mathbf{F} - \mathcal{A} : (\nabla_R \boldsymbol{\alpha})^T) - \mathcal{B} : (\nabla_R \boldsymbol{\beta})^T), \tag{29}$$

and intrinsic source terms

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathcal{A}} : \nabla_R \boldsymbol{\alpha} + \widetilde{\mathcal{B}} : \nabla_R \boldsymbol{\beta}, \quad \widetilde{h}^{intr} := \widetilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \widetilde{\mathcal{B}} : \dot{\boldsymbol{\beta}}. \tag{30}$$

In the above equations the following definitions are used (cf. [13; 14])

$$\widetilde{\mathcal{A}} \equiv -\frac{\delta \overline{W}}{\delta \boldsymbol{\alpha}} := -\left(\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}} - Div_R \frac{\partial \overline{W}}{\partial (\nabla_R \boldsymbol{\alpha})} \right) = \mathbf{A} - Div_R \mathcal{A}, \tag{31}$$

$$\widetilde{\mathcal{B}} \equiv -\frac{\delta \overline{W}}{\delta \boldsymbol{\beta}} := -\left(\frac{\partial \overline{W}}{\partial \boldsymbol{\beta}} - Div_R \frac{\partial \overline{W}}{\partial (\nabla_R \boldsymbol{\beta})} \right) = \mathbf{B} - Div_R \mathcal{B}, \tag{32}$$

$$\widetilde{\mathbf{S}} = \theta^{-1} \widetilde{\mathbf{Q}}, \quad \widetilde{\mathbf{Q}} = \mathbf{Q} - \mathcal{A} : \dot{\boldsymbol{\alpha}} - \mathcal{B} : \dot{\boldsymbol{\beta}}. \tag{33}$$

In this formulation the Eshelby stress complies with it role of grasping all effects presenting gradients since the material gradients of internal variables $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ play a role parallel to that of the deformation gradient $\mathbf{F}$.

3.2 Evolution equations

The corresponding dissipation inequality

$$\Phi = \widetilde{h}^{intr} - \widetilde{\mathbf{S}} \nabla_R \theta \geq 0, \tag{34}$$

is reduced in the isothermal case to

$$\widetilde{h}^{intr} := \widetilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \widetilde{\mathcal{B}} : \dot{\boldsymbol{\beta}} \geq 0. \tag{35}$$

In accordance with Eq. (35), the evolution equations for the internal variables $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are chosen as

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \mathbf{L} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & \mathbf{L}^{12} \\ \mathbf{L}^{21} & \mathbf{L}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}, \tag{36}$$

where components $\mathbf{L}^{11}, ..., \mathbf{L}^{22}$ of the linear operator $\mathbf{L}$ are dependent on state variables [20].

Representing the linear operator $\mathbf{L}$ as the sum of symmetric and skew-symmetric components $\mathbf{L} = (\mathbf{L} + \mathbf{L}^T)/2 + (\mathbf{L} - \mathbf{L}^T)/2$, i.e.

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & (\mathbf{L}^{12} + \mathbf{L}^{21})/2 \\ (\mathbf{L}^{21} + \mathbf{L}^{12})/2 & \mathbf{L}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix} + \begin{pmatrix} 0 & (\mathbf{L}^{12} - \mathbf{L}^{21})/2 \\ (\mathbf{L}^{21} - \mathbf{L}^{12})/2 & 0 \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}, \tag{37}$$

we can see that the symmetry of the linear operator $\mathbf{L}$, which is equivalent to the Onsagerian reciprocity relations $\mathbf{L}^{12} = \mathbf{L}^{21}$, leads to the elimination of the antisymmetric part of the linear operator $\mathbf{L}$. However, we have no reasons to assume the symmetry of the linear operator $\mathbf{L}$ in the case of arbitrary internal variables.

A more general case corresponds to the Casimir reciprocity relations

$$\mathbf{L}^{12} = -\mathbf{L}^{21}, \tag{38}$$

which results in the decomposition of evolution equations into dissipative and non-dissipative parts

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & 0 \\ 0 & \mathbf{L}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix} + \begin{pmatrix} 0 & \mathbf{L}^{12} \\ -\mathbf{L}^{12} & 0 \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}. \tag{39}$$

It is instructive to consider two limiting cases, corresponding to pure symmetric and pure skew-symmetric linear operator $\mathbf{L}$.

3.3 A fully dissipative case

If we suppose that $\mathbf{L}^{12} = \mathbf{0}$, while $\mathbf{L}^{11}$ and $\mathbf{L}^{22}$ are positive definite, we return to the classical situation, where internal variables are fully independent

$$\dot{\boldsymbol{\alpha}} = \mathbf{L}^{11} . \widetilde{\mathcal{A}}, \tag{40}$$

$$\dot{\boldsymbol{\beta}} = \mathbf{L}^{22} . \widetilde{\mathcal{B}}, \tag{41}$$

and the dissipation inequality is satisfied

$$\widetilde{h}^{intr} = \widetilde{\mathcal{A}} : (\mathbf{L}^{11} . \widetilde{\mathcal{A}}) + \widetilde{\mathcal{B}} : (\mathbf{L}^{22} . \widetilde{\mathcal{B}}) \geq 0. \tag{42}$$

We use the "dot" notation for the product of two tensors and ":" for their inner product.

As one can see, the classical internal variable theory implicitly includes the Onsagerian reciprocity relations. In the fully dissipative case we are dealing with true internal variables of state. It is clear that in the fully dissipative case we do not need to introduce any dual internal variable: the conventional internal variable theory works well.

3.4 A non-dissipative case

In the skew-symmetric case ($\mathbf{L}^{11} = \mathbf{L}^{22} = \mathbf{0}$), the dissipation $\widetilde{h}^{intr}$ vanishes, while evolution equations for the two internal variables are fully coupled

$$\dot{\boldsymbol{\alpha}} = \mathbf{L}^{12}.\widetilde{\mathcal{B}}, \tag{43}$$

$$\dot{\boldsymbol{\beta}} = -\mathbf{L}^{12}.\widetilde{\mathcal{A}}. \tag{44}$$

In this case, the evolution of one internal variable is driven by another one that means the duality between the internal variables.

To be more specific, let us consider a simple case with $\mathcal{B} = \mathbf{0}$. In this case, the free energy function $\overline{W}$ is independent of $\nabla_R \boldsymbol{\beta}$, and the kinetic relations (43), (44) are reduced to

$$\dot{\boldsymbol{\alpha}} = \mathbf{L}^{12}.\mathbf{B}, \tag{45}$$

$$\dot{\boldsymbol{\beta}} = -\mathbf{L}^{12}.\widetilde{\mathcal{A}}. \tag{46}$$

Assuming further a quadratic dependence of the free energy function with respect to the internal variable $\boldsymbol{\beta}$

$$\mathbf{B} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\beta}} = -\boldsymbol{\beta}, \tag{47}$$

we reduce Eq. (45) to

$$\dot{\boldsymbol{\alpha}} = -\mathbf{L}^{12}.\boldsymbol{\beta}, \tag{48}$$

while Eq. (46) is not changed

$$\dot{\boldsymbol{\beta}} = -\mathbf{L}^{12}.\widetilde{\mathcal{A}}. \tag{49}$$

Substituting from Eq. (48) into Eq. (49), we obtain a hyperbolic evolution equation for the primary internal variable $\boldsymbol{\alpha}$:

$$\ddot{\boldsymbol{\alpha}} = (\mathbf{L}^{12}.\mathbf{L}^{12}).\widetilde{\mathcal{A}}. \tag{50}$$

This means that the introduced internal variable $\boldsymbol{\alpha}$ in the non-dissipative case is practically an internal degree of freedom, and the structure of Eqs. (48), (49) and (50) is similar to that in the case of elasticity.

Just this non-dissipative evolution equation is exploited in the representation of generalized continuum theories in terms of dual internal variables, as it will be shown in the next Sections.

4 Example: Cosserat media

4.1 Linear micropolar media

In a Cosserat (or micropolar) medium, material points possess properties similar to rigid particles, which can translate and independently rotate. Accordingly, each material point is endowed with translation and rotation degrees of freedom, that describe its displacement and rotation. The following infinitesimal measures of deformation are used for a linear micropolar elastic solid [21]: the associated Cosserat deformation e_{ij}

$$e_{ij} = \frac{\partial u_j}{\partial x_i} - \varepsilon_{ijk}\phi_k, \tag{51}$$

and the torsion-curvature (or wryness) tensor γ_{ij}

$$\gamma_{ij} = \frac{\partial \phi_i}{\partial x_j}, \tag{52}$$

where ϕ_i is the rotation vector and ε_{ijk} is the signature of the permutation (i, j, k).

The nonsymmetric stress tensor t_{ij} and couple-stress tensor m_{ij} are then represented with constitutive equations [21]

$$t_{ij} = \frac{\partial \overline{W}}{\partial e_{ij}}, \quad m_{ij} = \frac{\partial \overline{W}}{\partial \gamma_{ij}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \tag{53}$$

where, for a materially inhomogeneous thermoelastic polar solid, we have a free energy density given by

$$W = \overline{W}(e_{ij}, \gamma_{ij}, \theta; x). \tag{54}$$

The stress and couple-stress tensors satisfy the equations of balance of momentum and of balance of moment of momentum [22]:

$$\rho_0 \ddot{u}_i - \partial_j t_{ji} = f_i, \tag{55}$$

$$\rho_0 j_{ij}\, \ddot{\phi}_j - \partial_j\, m_{j\,i} - \varepsilon_{ipq} t_{pq} = c_i, \tag{56}$$

where volume forces f_i, volume couples c_i, and the rotational inertia j_{ij} have been introduced. It is often assumed that this microinertia is isotropic, i.e. $j_{ij} = I\delta_{ij}$.

4.2 Microrotation as an internal variable

Let us consider a deformable medium with two dual internal variables, one of which is an axial vector noted ϕ_i (microrotation) with gradient noted γ_{ij} and another vectorial "internal" variable noted ψ_i.

Suppose that there exists a motion equation similar to Eq. (55) with a non necessarily symmetric stress t_{ij}

$$t_{ij} = \frac{\partial \overline{W}}{\partial u_{ij}}, \quad u_{ij} = u_{j,i}, \tag{57}$$

where the latter quantity is the full displacement gradient.

In the case with internal variables, the only energy density we can start with reads thus

$$W = \overline{W}(u_{ij}, \phi_i, \gamma_{ij}, \psi_i, \theta; x). \tag{58}$$

Repeating all the considerations of Section 3, we arrive at the evolution equation (50) where $\boldsymbol{\alpha}$ is replaced by ϕ_i

$$\ddot{\phi}_j = (\mathbf{L}^{12}.\mathbf{L}^{12})_{ij} \left(-\frac{\partial \overline{W}}{\partial \phi_i} + \partial_j \frac{\partial \overline{W}}{\partial (\gamma_{j\,i})} \right). \tag{59}$$

Assume that $\overline{W}$ in the last expression can depend on the internal variable ϕ_i only through the new objective variable e_{ij} defined by Eq. (51). This mean that the free energy function (58) can be represented as

$$W = \overline{W}(u_{ij}, \phi_i, \gamma_{ij}, \psi_i, \theta; x) \equiv \overline{W}(e_{ij}, \gamma_{ij}, \psi_i, \theta; x). \tag{60}$$

It follows from (60) that the non-symmetric stress t_{ij} is determined now similarly to micropolar theory

$$t_{ij} = \frac{\partial \overline{W}}{\partial e_{ij}}, \tag{61}$$

and we can calculate the derivative of free energy with respect to the internal variable ϕ_k

$$\frac{\partial \overline{W}}{\partial \phi_k} = \frac{\partial \overline{W}}{\partial e_{ij}} \frac{\partial e_{ij}}{\partial \phi_k} = -t_{ij}\, \varepsilon_{ijk}, \tag{62}$$

Now we can rewrite the evolution equation (59) as follows:

$$(\mathbf{L}^{12}.\mathbf{L}^{12})^{-1}_{ij} \ddot{\phi}_j = \varepsilon_{ipq} t_{pq} + \partial_j m_{ji}. \tag{63}$$

The latter equation almost coincides with the equation of motion (56) in the linear micropolar medium under the identification of the inverse of the square of linear operator $\mathbf{L}^{12}$ with the rotational inertia tensor, i.e. $(\mathbf{L}^{12}.\mathbf{L}^{12})^{-1}_{ij} \equiv \rho_0 j_{ij}$. But even by identifying the inertia, we will never be able to obtain the full of Eq. (56) above because the reasoning yielding Eq. (59) is purely thermodynamical and will never allow us to introduce the external couple c_i. Thus the identification is only partial due to the initial nature of internal variables.

5 Example: micromorphic linear elasticity

5.1 Mindlin theory

In the framework of the Mindlin micromorphic theory [3], each material point is endowed with three translational degrees of freedom u_i and a full microdeformation tensor ψ_{ij} with nine independent components. Three strain tensors are deduced: the classical strain tensor ε_{ij}

$$\varepsilon_{ij} \equiv \frac{1}{2}\left(\partial_i u_j + \partial_j u_i\right), \tag{64}$$

the relative deformation tensor γ_{ij}

$$\gamma_{ij} \equiv \partial_i u_j - \psi_{ij}, \tag{65}$$

and the microdeformation gradient $\varkappa_{ijk}$ defined by

$$\varkappa_{ijk} \equiv \partial_i \psi_{jk}. \tag{66}$$

The free energy density W is supposed to be a homogeneous, quadratic function of forty-two variables $\varepsilon_{ij}, \gamma_{ij}, \varkappa_{ijk}$ [3]

$$W = \frac{1}{2}c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2}b_{ijkl}\gamma_{ij}\gamma_{kl} + \frac{1}{2}a_{ijklmn}\varkappa_{ijk}\varkappa_{lmn} + d_{ijklm}\gamma_{ij}\varkappa_{klm} + f_{ijklm}\varkappa_{ijk}\varepsilon_{lm} + g_{ijkl}\gamma_{ij}\varepsilon_{kl}. \tag{67}$$

As it was emphasized, only 903 of the 1764 coefficients in the former equation are independent. In the case of centrosymmetric, isotropic materials the number of independent coefficients is greatly reduced [3]

$$\begin{aligned} W = {} & \frac{1}{2}\lambda\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}\varepsilon_{ij} + \frac{1}{2}b_1\gamma_{ii}\gamma_{jj} + \frac{1}{2}b_2\gamma_{ij}\gamma_{ij} + \\ & + \frac{1}{2}b_3\gamma_{ij}\gamma_{ji} + g_1\gamma_{ii}\varepsilon_{jj} + g_2\left(\gamma_{ij}+\gamma_{ji}\right)\varepsilon_{ij} + \\ & + a_1\varkappa_{iik}\varkappa_{kjj} + a_2\varkappa_{iik}\varkappa_{jkj} + \frac{1}{2}a_3\varkappa_{iik}\varkappa_{jjk} + \frac{1}{2}a_4\varkappa_{ijj}\varkappa_{ikk} + \\ & + a_5\varkappa_{ijj}\varkappa_{kik} + \frac{1}{2}a_8\varkappa_{iji}\varkappa_{kjk} + \frac{1}{2}a_{10}\varkappa_{ijk}\varkappa_{ijk} + a_{11}\varkappa_{ijk}\varkappa_{jki} + \\ & + \frac{1}{2}a_{13}\varkappa_{ijk}\varkappa_{ikj} + \frac{1}{2}a_{14}\varkappa_{ijk}\varkappa_{jik} + \frac{1}{2}a_{15}\varkappa_{ijk}\varkappa_{kij}. \end{aligned} \tag{68}$$

The corresponding stress tensors are the following ones [3]:

Cauchy stress

$$\sigma_{ij} \equiv \frac{\partial W}{\partial \varepsilon_{ij}} = \sigma_{ji} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} + g_1\delta_{ij}\gamma_{kk} + g_2(\gamma_{ij}+\gamma_{ji}), \tag{69}$$

relative stress

$$\tau_{ij} \equiv \frac{\partial W}{\partial \gamma_{ij}} = g_1\delta_{ij}\varepsilon_{kk} + 2g_2\varepsilon_{ij} + b_1\delta_{ij}\gamma_{kk} + b_2\gamma_{ij} + b_3\gamma_{ji}, \tag{70}$$

and double stress

$$\mu_{ijk} \equiv \frac{\partial W}{\partial \varkappa_{ijk}}. \tag{71}$$

The equations of motion in terms of stresses have the form [3]

$$\rho\ddot{u}_j = \partial_i\left(\sigma_{ij} + \tau_{ij}\right) + f_j, \tag{72}$$

$$\frac{1}{3}\rho' d^2_{ji}\ddot{\psi}_{ik} = \partial_i\mu_{ijk} + \tau_{jk} + \Phi_{jk}, \tag{73}$$

where $\rho' d^2_{ji}$ is a microinertia tensor, f_j is the body force, and Φ_{jk} is the double force per unit volume.

It should be noted that the balances of linear momentum both at micro and at macrolevel (Eqs. (72) and (73), respectively) are introduced independently.

5.2 Rearrangement

In order to apply the internal variable theory, it is more convenient to represent the constitutive relations in the Mindlin theory in terms of distortion $\partial_j u_i$ and microdeformation tensor ψ_{ji}. For the free energy we will have then

$$\begin{aligned} W = &\frac{1}{2}\lambda\partial_i u_i \partial_j u_j + \frac{1}{4}\mu(\partial_i u_j + \partial_j u_i)(\partial_i u_j + \partial_j u_i)+ \\ &+ \frac{1}{2}b_1(\partial_i u_i - \psi_{ii})(\partial_j u_j - \psi_{jj})+ \\ &+ \frac{1}{2}b_2(\partial_i u_j - \psi_{ij})(\partial_i u_j - \psi_{ij}) + \frac{1}{2}b_3(\partial_i u_j - \psi_{ij})(\partial_j u_i - \psi_{ji})+ \\ &+ g_1(\partial_i u_i - \psi_{ii})\partial_j u_j + \frac{1}{2}g_2\left(\partial_i u_j - \psi_{ij} + \partial_j u_i - \psi_{ji}\right)(\partial_i u_j + \partial_j u_i)+ \\ &+ a_1\varkappa_{iik}\varkappa_{kjj} + a_2\varkappa_{iik}\varkappa_{jkj} + \frac{1}{2}a_3\varkappa_{iik}\varkappa_{jjk} + \frac{1}{2}a_4\varkappa_{ijj}\varkappa_{ikk}+ \\ &+ a_5\varkappa_{ijj}\varkappa_{kik} + \frac{1}{2}a_8\varkappa_{iji}\varkappa_{kjk} + \frac{1}{2}a_{10}\varkappa_{ijk}\varkappa_{ijk} + a_{11}\varkappa_{ijk}\varkappa_{jki}+ \\ &+ \frac{1}{2}a_{13}\varkappa_{ijk}\varkappa_{ikj} + \frac{1}{2}a_{14}\varkappa_{ijk}\varkappa_{jik} + \frac{1}{2}a_{15}\varkappa_{ijk}\varkappa_{kij}. \end{aligned} \tag{74}$$

Accordingly, the stresses are represented as follows:

$$\begin{aligned} \sigma'_{ij} \equiv \frac{\partial W}{\partial(\partial_i u_j)} &= \lambda\delta_{ij}\partial_k u_k + \mu(\partial_i u_j + \partial_j u_i)+ \\ &+ g_1\delta_{ij}(\partial_k u_k - \psi_{kk}) + g_2\left(\partial_i u_j - \psi_{ij} + \partial_j u_i - \psi_{ji}\right)+ \\ &+ b_1\delta_{ij}(\partial_k u_k - \psi_{kk}) + b_2(\partial_i u_j - \psi_{ij}) + b_3(\partial_j u_i - \psi_{ji}), \end{aligned} \tag{75}$$

and

$$\tau'_{ij} \equiv \frac{\partial W}{\partial \psi_{ij}} = -g_1\delta_{ij}\partial_k u_k - g_2(\partial_i u_j + \partial_j u_i) - b_1\delta_{ij}(\partial_k u_k - \psi_{kk}) - b_2(\partial_i u_j - \psi_{ij}) - b_3(\partial_j u_i - \psi_{ji}). \tag{76}$$

The double stress remains unchanged. At last, equations of motion (72) and (73) take on the form

$$\rho\ddot{u}_j = \partial_i\sigma'_{ij} + f_j, \tag{77}$$

$$\frac{1}{3}\rho' d_{ij}^2\ddot{\psi}_{ik} = \partial_i\mu_{ijk} - \tau'_{jk} + \Phi_{jk}. \tag{78}$$

5.3 Microdeformation tensor as an internal variable

Now we consider the microdeformation tensor ψ_{ij} as an internal variable $\boldsymbol{\alpha}$ and apply the formalism developed in Section 3. The microdeformation gradient $\varkappa_{ijk}$ plays the role of the gradient of the internal variable $\boldsymbol{\alpha}$, and we introduce a dual internal variable $\boldsymbol{\beta}$ in the same way as in Section 3.4. In the non-dissipative case, the dual internal variable $\boldsymbol{\beta}$ is auxiliary and does not affect the calculation of derivatives of free energy with respect to microdeformation and double stress. Therefore, the evolution equation for the internal variable $\boldsymbol{\alpha}$ can be symbolically written as

$$\ddot{\boldsymbol{\alpha}} = (\mathbf{L}^{12}.\mathbf{L}^{12}).\left(-\frac{\partial W}{\partial\boldsymbol{\alpha}} + Div\,\frac{\partial W}{\partial(\nabla\boldsymbol{\alpha})}\right). \tag{79}$$

In terms of components of the microdeformation tensor ψ_{ij} the latter evolution equation takes on the form

$$\left(\mathbf{L}^{12}.\mathbf{L}^{12}\right)^{-1}_{ji}\ddot{\psi}_{ik} = \left(-\frac{\partial W}{\partial\psi_{jk}} + Div\,\frac{\partial W}{\partial(\nabla\psi_{jk})}\right) = \partial_i\mu_{ijk} - \tau'_{jk}. \tag{80}$$

As one can see, the evolution equation for the microdeformation (80) is practically the same as the equation of motion at microlevel (78) in the rearranged Mindlin theory. As in the case of the micropolar medium, the external double force cannot appear in the internal variable theory. It should be noted that the equation of motion (80) is not postulated, but it follows from the dissipation inequality for the chosen functional dependence of the free energy in the considered non-dissipative case.

5.4 Remark on second gradient elasticity

It is well known that the gradient elasticity theory corresponds to the vanishing relative deformation tensor in the micromorphic theory, i.e. $\psi_{ij} = \partial_i u_j$ and $\varkappa_{ijk} = \partial_k \varepsilon_{ij}$ [23; 22].

Similarly, for the second gradient elasticity in the spirit of Aifantis [24], we can assume $\psi_{ij} = l^2 \nabla^2 \varepsilon_{ij}$, where l is a length scale. The corresponding stress tensor follows from Eq. (75) for $b_1 = b_2 = b_3 = 0$:

$$\sigma'_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2\mu \varepsilon_{ij} + g_1 \delta_{ij} (\varepsilon_{kk} - l^2 \nabla^2 \varepsilon_{kk}) + 2 g_2 \left(\varepsilon_{ij} - l^2 \nabla^2 \varepsilon_{ij} \right). \tag{81}$$

Comparing the latter equation with the constitutive equation proposed by Aifantis [24]

$$\sigma_{ij} - c_1 l^2 \nabla^2 \sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2\mu \varepsilon_{ij} - c_2 l^2 \nabla^2 (\lambda \delta_{ij} \varepsilon_{kk} + 2\mu \varepsilon_{ij}), \tag{82}$$

one can see additional non-gradient terms in the right hand side of Eq. (81).

A simpler expression for the stress tensor can be obtained under the assumption of the gradient nature of the relative deformation tensor $\gamma_{ij} = l^2 \nabla^2 \partial_i u_j$. In this case we have following Eq. (69)

$$\sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2\mu \varepsilon_{ij} + g_1 l^2 \nabla^2 \delta_{ij} \varepsilon_{kk} + 2 g_2 l^2 \nabla^2 \varepsilon_{ij}. \tag{83}$$

The latter two equations can be converted one into the other by a proper choice of coefficients in each case.

6 Microstructure in one-dimension: boundary conditions

In the one-dimensional case, the governing equation is the balance of linear momentum

$$\frac{\partial}{\partial t}(\rho_0 v) = \frac{\partial \sigma}{\partial x}. \tag{84}$$

We suppose that the free energy depends on the internal variables α, β and their space derivatives

$$W = \overline{W}(u_x, \alpha, \alpha_x, \beta, \beta_x), \tag{85}$$

where u is the displacement. Then the constitutive equations follow

$$\sigma := \frac{\partial \overline{W}}{\partial u_x}, \quad \tau := -\frac{\partial \overline{W}}{\partial \alpha}, \quad \eta := -\frac{\partial \overline{W}}{\partial \alpha_x}, \quad \xi := -\frac{\partial \overline{W}}{\partial \beta}, \quad \zeta := -\frac{\partial \overline{W}}{\partial \beta_x}. \tag{86}$$

Suppose that the internal variables are coupled as in the non-dissipative case (cf. Eqs. (43), (44))

$$\dot{\alpha} = L_{12}(\xi - \zeta_x), \tag{87}$$

$$\dot{\beta} = -L_{12}(\tau - \eta_x). \tag{88}$$

The simplest free energy dependence is a quadratic function (cf. [25])

$$\overline{W} = \frac{1}{2}(\lambda + 2\mu) u_x^2 + A \alpha u_x + \frac{1}{2} B \alpha^2 + \frac{1}{2} C \alpha_x^2 + \frac{1}{2} D \beta^2, \tag{89}$$

where essential terms (to our understanding) are kept.

The first two terms in the right hand side of Eq. (89) correspond to the macroscopic part of the free energy function

$$\widetilde{W} = \frac{1}{2}(\lambda + 2\mu) u_x^2 + A \alpha u_x, \tag{90}$$

while the rest represents its "internal" part

$$W' = \frac{1}{2}B\alpha^2 + \frac{1}{2}C\alpha_x^2 + \frac{1}{2}D\beta^2. \tag{91}$$

This means that the stress components are determined as follows:

$$\sigma = \frac{\partial \overline{W}}{\partial u_x} = (\lambda + 2\mu)u_x + A\alpha, \quad \eta = -\frac{\partial \overline{W}}{\partial \alpha_x} = -C\alpha_x, \quad \zeta = -\frac{\partial \overline{W}}{\partial \beta_x} = 0. \tag{92}$$

Accordingly, τ coincides with the interactive internal force

$$\tau = -\frac{\partial \overline{W}}{\partial \alpha} = -Au_x - B\alpha, \tag{93}$$

and

$$\xi = -\frac{\partial \overline{W}}{\partial \beta} = -D\beta. \tag{94}$$

It follows from Eqs. (87) and (94) that

$$\dot{\alpha} = -L_{12}D\beta, \tag{95}$$

and Eq. (88) can be represented as a hyperbolic equation

$$\ddot{\alpha} = L_{12}^2 D(\tau - \eta_x). \tag{96}$$

As a result, we arrive at the equations of motion (84), (96) in the form

$$\begin{aligned} \rho_0 u_{tt} &= (\lambda + 2\mu)u_{xx} + A\alpha_x, \\ I\alpha_{tt} &= C\alpha_{xx} - Au_x - B\alpha, \end{aligned} \tag{97}$$

where $I = 1/(L_{12}^2 D)$ plays the role of an internal inertia measure.

In terms of stresses introduced by equations of state (86), the same system of equations is represented as

$$\rho_0 \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x}, \quad I\frac{\partial^2 \alpha}{\partial t^2} = -\frac{\partial \eta}{\partial x} + \tau. \tag{98}$$

It is worth to note that the same equations are derived from another consideration by Engelbrecht, Cermelli and Pastrone [26].

The equations of motion (97) or (98) can also be rewritten in the form of systems of first order partial differential equations

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_0 v) &= (\lambda + 2\mu)\frac{\partial \varepsilon}{\partial x} + A\frac{\partial \alpha}{\partial x}, \\ \frac{\partial \varepsilon}{\partial t} &= \frac{\partial v}{\partial x}, \end{aligned} \tag{99}$$

and

$$\begin{aligned} I\frac{\partial w}{\partial t} &= C\frac{\partial \alpha}{\partial x} - \int (A\varepsilon + B\alpha)dx, \\ \frac{\partial \alpha}{\partial t} &= \frac{\partial w}{\partial x}, \end{aligned} \tag{100}$$

where the variable w is introduced as follows

$$\frac{\partial w}{\partial x} = L_{12}D\beta. \tag{101}$$

It is easy to see that the systems of equations (99) and (100) are fully coupled. As it is mentioned in [16], "natural" boundary conditions for microstructure should provide zero extra entropy flux at boundaries. According to the definition of the extra entropy flux (26), the latter condition is equivalent to $\dot{\alpha} = 0$ and $\dot{\beta} = 0$ at boundaries, which provides zero boundary conditions for the microstructure with zero initial conditions. A non-trivial solution for microstructure will appear due to the coupling even if initial and boundary conditions for the microstructure are equal to zero.

7 Conclusions

In the paper, dual weakly non-local internal variables and extra entropy fluxes are introduced in the canonical thermomechanics on the material manifold. This allows one to recover a hyperbolic evolution equation in the non-dissipative case.

It is demonstrated that the structure of Cosserat, micromorphic, and second gradient elasticity theories can be recovered in terms of dual internal variables in a natural way. However, the external couples cannot be deduced in the fully thermodynamical approach. It should be emphasized, however, that any new balance laws has not been introduced; only the Clausius-Duhem inequality was exploited for the derivation of evolution equations for the dual internal variables.

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