Entropy and temperature gradients thermomechanics: Dissipation, heat conduction inequality and heat equation

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Abstract

An alternative and consistent approach, not appealing to the principle of virtual power and to Coleman-Noll procedure, is used to derive constitutive and governing equations involving temperature or entropy gradients, in thermomechanics of materials. Using the balance of energy, an analysis of the dissipation naturally leads to the definition of the temperature and the entropy as variational derivatives. The approach preserves the classical forms of the equations and yields to consistent form of the second law and heat conduction inequality. The framework of generalized standard materials is then suitable for deriving admissible constitutive laws. The methodology is applied, first using entropy and its gradient as state variables (with internal energy as thermodynamic potential), and second using

temperature and its gradient (starting from the free energy).

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Résumé

Thermomécanique avec gradients d'entropie et de température : dissipation, inégalité de la conduction et équation de la chaleur. Une approche alternative et cohérente, ne faisant pas appel au principe des puissances virtuelles et à la procédure de Coleman-Noll, est utilisée pour obtenir les lois de comportement avec gradients de température ou d'entropie, ainsi que les équations d'évolution en thermomécanique. En partant du bilan d'énergie, une analyse de la dissipation conduit naturellement à la définition de la température et de l'entropie par des dérivées variationnelles. Tout en préservant les formes classiques des équations, l'approche permet d'établir les formes cohérentes de l'inégalité de l'entropie (second principe) et de la conduction dont une nouvelle forme est proposée. Le formalisme standard généralisé offre ensuite un moyen commode d'établir des lois admissibles. La méthodologie est appliquée en prenant d'abord l'entropie et son gradient comme variables d'état (énergie interne comme potentiel), et ensuite la température et son gradient (énergie libre comme potentiel).

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Key words: Continuum mechanics ; continuum thermodynamics ; entropy gradient ; dissipation ; second law ; heat conduction inequality ; heat equation

Mots-clés : Milieux continus ; thermodynamique des milieux continus ; gradient d'entropie ; gradient de température ; second principe ; inégalité de la conduction de la chaleur, équation de la conduction

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1 Introduction

The approach proposed by Coleman and Noll [1] uses the Clausius-Duhem inequality as a tool to select constitutive laws by requiring that this inequality holds by all thermodynamic processes. Adopting the Truesdell and Toupin's principle of equipresence, Coleman and Mizel [2] used this inequality to show that all the response functions cannot depend on all the state variables; some of them must be independent of certain variables. More precisely, assuming that the heat flux, the specific internal energy and entropy are functions of the temperature and the first n spatial gradients of the temperature, they showed that the internal energy and the entropy are independent of the temperature gradients. This result is related to the forms chosen for thermal energy exchanges only through heat flux and radiation, as they mentioned. Within the same framework, Coleman and Gurtin [3] extended straightforward the result to obtain the independence of the free energy, the entropy and the stress on the temperature gradients in the case of nonlinear materials with internal state variables. However, this result is based on certain assumptions such as independence of stresses, or more generally of irreversible forces, on the rate of temperature gradient. One way to account for this dependence is to add an extra term of entropy flux [5,6,7,8,9] as constitutive quantity. Changes are also made in the energy balance by adding new contributions to the power of internal forces. Principle of virtual power on microscopic movements or micromorphic approaches (Frémond and Nedjar [10], Frémond and Nedjar [11], Frémond [12], Fried and Gurtin [13], Gurtin [14]) have been used by Forest and Amestoy [15], Forest and Aifantis [16] to account for entropy gradient. However, the physical meaning of the principle of virtual power involving virtual rates of variables as entropy (in [15]) is not obvious. An extra term of entropy production inside the volume has also been added by Ireman and Nguyen [17]. They showed that three different expressions of this quantities lead to different thermodynamical models. A variational-based field description coupled with the Generalized Standard Materials formalism for gradient temperature thermomechanics

is given by Nguyen and Andrieux [18] and Nguyen [19], followed by a justification through an homogenization process. It can be seen as a non-local generalized standard model as proposed by Lorentz and Andrieux [20,21]. The approach shows the way to derive the correct forms of intrinsic dissipation and to restore duality between internal and free energy. However, in all these works, the classical expression of the heat conduction inequality was maintained, while the introduction of the gradient of temperature or entropy is likely to affect its structure.

The objective of this work, is, while remaining strictly within the framework of the phenomenological theory of continuum thermodynamics, to derive the constitutive equations and inequations of the gradient thermomechanics, without appealing to to the principle of virtual power and to the Coleman-Noll procedure and the classical heat conduction inequality. The approach conducts to the adoption of variational based derivatives for the definition of the temperature and the entropy. These definitions lead to consistent forms of second law (generalized Clausius-Duhem inequality) and a new heat conduction inequality. Constitutive laws are postulated, based on the splitting of the dissipation in its intrinsic and thermal parts. They permit to recover the existing results on temperature and entropy gradients thermomechanics. The formal structure obtained is closely related to the one from the canonical thermomechanics with dual weakly non-local internal variables proposed by Berezovski et al. [22].

2 Entropy gradient: using internal energy

2.1 Energy balance

The basic principle is the energy balance (first law of thermodynamics) stating that energy cannot be generated. The variation of the energy of a system is solely due to exchange with the environment. The form of the energy exchanged with the outside defines therefore how to act on the system, that is to say its control variables. For the continuum medium, the external rate

of energy supply is generally composed of two terms:

- the power of external forces $\mathcal{P}_{\text{e}}$, associated with the primal kinematic variables (displacement and another independent variable denoted $\boldsymbol{\alpha}$), given by:

$$\begin{aligned}\mathcal{P}_{\text{e}} = &\int_{\Omega(t)} \underline{f}_{\Omega u} \cdot \underline{v}\, d\Omega + \int_{\partial\Omega(t)} \underline{f}_{Su} \cdot \underline{v}\, da \\ &+ \int_{\Omega(t)} \mathbf{a}_{\Omega\alpha} \cdot \dot{\boldsymbol{\alpha}}\, d\Omega + \int_{\partial\Omega(t)} \mathbf{a}_{S\alpha} \cdot \dot{\boldsymbol{\alpha}}\, da\ ,\end{aligned} \tag{1}$$

  where $\underline{v}$ is the velocity, $\underline{f}_{\Omega u}$ (resp. $\mathbf{a}_{\Omega\alpha}$) and $\underline{f}_{Su}$ (resp. $\mathbf{a}_{S\alpha}$) are the external body and surface forces associated with the displacement (resp. with the variable $\boldsymbol{\alpha}$). Superimposed dot denotes time-derivative. $\boldsymbol{\alpha}$ is a state variable which typically represents microscopic motions as such damage associated to failure of bonds within the material particle [12]. This variable can be controlled by external forces (such as radiation in the case of damage). We assume that the external rate of energy supplies associated to $\boldsymbol{\alpha}$ are objective and the surface rate of energy related to $\boldsymbol{\alpha}$ depends only on the considered point, the surface normal vector and the time.
- The total heat supply per unit time $\mathcal{P}_{\text{cal}}$, associated with the thermal control variable, is given by:

$$\mathcal{P}_{\text{cal}} = \int_{\Omega(t)} r\, d\Omega + \int_{\partial\Omega(t)} Q\, da\ , \tag{2}$$

r is the external rate of heat supply per unit volume and Q is the external rate of heat supply per unit surface. For instance, one can have:

- as in Frémond 2002 [12],

$$r = R\,T \quad \text{et} \quad Q = Q_T T\ , \tag{3}$$

- or, consistent with the choice of entropy s as internal variable, the following form could be proposed

$$r = R_s\,\dot{s} \quad \text{and} \quad Q = Q_s\,\dot{s}\ . \tag{4}$$

The balance of energy is written as:

$$\begin{aligned}\dot{E} + \dot{e}\int_\Omega \rho\dot{\underline{v}}\cdot\underline{v}\,d\Omega + \int_\Omega \rho_a\gamma_a\cdot\dot{\boldsymbol{\alpha}}\,d\Omega = \int_\Omega \underline{f}_{\Omega u}\cdot\underline{v}\,d\Omega + \int_{\partial\Omega}\underline{f}_{Su}\cdot\underline{v}\,da \\ + \int_\Omega \mathbf{a}_{\Omega\alpha}\cdot\dot{\boldsymbol{\alpha}}\,d\Omega + \int_{\partial\Omega}\mathbf{a}_{S\alpha}\cdot\dot{\boldsymbol{\alpha}}\,da \\ + \int_\Omega r\,d\Omega + \int_{\partial\Omega} Q\,da\ .\end{aligned} \tag{5}$$

where the internal energy E is the objective and non kinetic part of the total energy of the system. The classical arguments (invariance under superposed rigid body motion and tetrahedron lemma applied on the energy balance) lead to the existence of a second order symmetric tensor $\underline{\underline{\sigma}}$, a vector $\underline{q}$ and also a tensor $\mathbf{A}$ ((order $\boldsymbol{\alpha}$) $+1$) such as:

$$\underline{f}_{Su} = \underline{\underline{\sigma}}\cdot\underline{n}\ , \quad Q = -\underline{q}\cdot\underline{n}\ , \quad \text{and} \quad \mathbf{a}_{S\alpha} = \mathbf{A}\cdot\underline{n}\ , \tag{6}$$

where $\underline{n}$ is the outward unit normal vector at the considered point. Some invariance requirements may allow to precise the form of $\mathbf{A}$ but are not considered in the paper as they have no direct influence on our purpose.

Using equation (6) in equation (5), one obtains:

$$\begin{aligned}\dot{E} = \int_\Omega \Big(\ (\operatorname{div}\underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \rho\dot{\underline{v}})\cdot\underline{v} \quad + \ \underline{\underline{\sigma}} : \underline{\underline{\nabla v}} \\ + \ (\operatorname{div}\mathbf{A} + \mathbf{a}_{\Omega\alpha} - \rho\underline{\gamma}_\alpha)\cdot\dot{\boldsymbol{\alpha}} \ + \mathbf{A} : \nabla\dot{\boldsymbol{\alpha}} \\ + \ (\operatorname{div}(-\underline{q}) + r)\ \Big)\, d\Omega\end{aligned} \tag{7}$$

We assume that the internal energy (extensive quantity) is regular ; e denotes the internal energy per unit volume. With suitable regularity (smoothness) assumptions for the different field quantities and assuming also the validity of equation (7) on Ω and any of its subdomains, we

obtain the local equation:

$$\begin{aligned}\dot{e} = \quad & (\text{div}\,\underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \rho\dot{\underline{v}}) \cdot \underline{v} \qquad + \underline{\underline{\sigma}} : \underline{\underline{\nabla v}} \\ & + (\text{div}\,\mathbf{A} + \mathbf{a}_{\Omega\alpha} - \rho_a \underline{\gamma}_\alpha) \cdot \dot{\boldsymbol{\alpha}} \;\; + \mathbf{A} : \nabla\dot{\boldsymbol{\alpha}} \\ & + (\text{div}\,(-\underline{q}) + r)\end{aligned} \tag{8}$$

Remark: If we use the assumption (4), the previous equation can be written as:

$$\begin{aligned}\dot{e} = \quad & (\text{div}\,\underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \rho\dot{\underline{v}}) \cdot \underline{v} \qquad + \underline{\underline{\sigma}} : \underline{\underline{\nabla v}} \\ & + (\text{div}\,\mathbf{A} + \mathbf{a}_{\Omega\alpha} - \rho\underline{\gamma}_\alpha) \cdot \dot{\boldsymbol{\alpha}} \;\; + \mathbf{A} : \nabla\dot{\boldsymbol{\alpha}} \\ & + (\text{div}\,\underline{Q}_s + R_s)\dot{s} \qquad\qquad + \underline{Q}_s \cdot \underline{\nabla\dot{s}}\end{aligned} \tag{9}$$

2.2 Intrinsic dissipation: definition of temperature and heat flux

Entropy is the extensive heat variable, naturally associated with the internal energy. We assume that the volumic internal energy depends on the kinematic variable $\underline{\underline{\nabla u}}_s, \boldsymbol{\alpha}, \nabla\boldsymbol{\alpha}$, the entropy per unit volume s and also on the entropy gradient $\underline{\nabla s}$ (as in [15,19]). $\underline{\underline{\nabla u}}_s$ is the symmetric part of $\underline{\underline{\nabla u}}$. The following quantities are defined:

$$T = e_{,s} \;\; , \quad \underline{T'} = e_{,\underline{\nabla s}} \;\; , \;\; \underline{\underline{\sigma}}^{nd} = e_{,\underline{\underline{\nabla u}}_s} \;\; , \;\; \mathbf{a}^{nd} = e_{,\boldsymbol{\alpha}} \;\; \text{and} \;\; \mathbf{A}^{nd} = e_{,\nabla\boldsymbol{\alpha}} \tag{10}$$

The non-local generalized standard approach (Nguyen and Andrieux [18]) has led to the appropriate expression of the intrinsic dissipation. Without recourse to the variational derivation, the intrinsic dissipation is defined as the part of heat rate which does not come from external sources and exchanges. It is therefore given by the difference between the rate of internal energy associated with the variation of entropic (or heat) variables (s and $\underline{\nabla s}$) and the rate of heat

supply from the environment,

$$\begin{aligned}\mathcal{D}_1 = \quad & \dot{e}|_{\{\underline{\underline{\nabla u}}_s, \boldsymbol{\alpha}, \nabla\boldsymbol{\alpha}\}} \quad -r + \operatorname{div}\underline{q} \\ = \quad & \overbrace{e_{,s}\,\dot{s} + e_{,\underline{\nabla s}} \cdot \underline{\nabla \dot{s}}} \; -r + \operatorname{div}\underline{q}\end{aligned} \tag{11}$$

By denoting:

$$\tilde{T} = T - \operatorname{div}\underline{\underline{T'}} \quad \text{and} \quad \underline{\tilde{q}}_s = \underline{q} + \underline{\underline{T'}}\dot{s}, \tag{12}$$

the following expression of the intrinsic dissipation is obtained:

$$\begin{aligned}\mathcal{D}_1 &= (T - \operatorname{div}\underline{\underline{T'}})\dot{s} - r + \operatorname{div}(\underline{q} + \underline{\underline{T'}}\dot{s}) \\ &= \tilde{T}\dot{s} - r + \operatorname{div}\underline{\tilde{q}}_s\end{aligned} \tag{13}$$

This form is similar to the one obtained in the classical approach (without entropy gradient), with the definitions of temperature as the variational derivative of the internal energy relative to the entropy ($\tilde{T} = e_{,s} - \operatorname{div} e_{,\underline{\nabla s}}$, as defined by Gouin, Gouin and Ruggeri [23,24]) and of the heat flux as ($\underline{\tilde{q}}_s = \underline{q} + \underline{\underline{T'}}\dot{s}$).

2.3 Second law and heat conduction inequality

To formulate the second law, we use the balance of entropy as proposed in Green and Naghdi [25] using the same assumptions while adopting the generalized temperature and heat flux. The external rate of supply of entropy per unit volume (resp. per unit surface) is given by the ratio of the external rate of volume heat supply r (resp. surface supply of heat $\underline{\tilde{q}}_s$) to the temperature $\tilde{T}$. Denoting the rate of internal production of volumic entropy by $\mathcal{S}_i$, the balance of entropy is:

$$\dot{s} = \mathcal{S}_i + \frac{r}{\tilde{T}} - \operatorname{div}\frac{\underline{\tilde{q}}_s}{\tilde{T}} \tag{14}$$

and the second law is thus written as:

$$\dot{s} - \frac{r}{\tilde{T}} + \text{div}\,\frac{\tilde{\underline{q}}_s}{\tilde{T}} \geq 0 \tag{15}$$

Let us notice that when there is no external volumic heat source ($r = 0$), the internal entropy production is reduced to:

$$\mathcal{S}_i = \dot{s} + \text{div}\left(\frac{\underline{T'}\dot{s}}{\tilde{T}}\right) + \text{div}\,\frac{\underline{q}}{\tilde{T}} \tag{16}$$

The proposed expression for the second law is different from that used as a starting point by Forest and Amestoy [15]. Indeed Forest and Amestoy [15] kept the classical form.

One notices that the entropy production can be written in the following form:

$$\mathcal{S}_i = \dot{s} - \frac{r}{\tilde{T}} + \text{div}\,\frac{\tilde{\underline{q}}_s}{\tilde{T}} = \frac{\mathcal{D}_1}{\tilde{T}} - \tilde{\underline{q}}_s \cdot \frac{\nabla\tilde{T}}{\tilde{T}^2} \tag{17}$$

Admitting the separation of the total dissipation in intrinsic and thermal parts, the thermal dissipation is therefore given by $-\tilde{\underline{q}}_s \cdot \frac{\nabla\tilde{T}}{\tilde{T}}$ and the conduction inequality is:

$$-\tilde{\underline{q}}_s \cdot \frac{\nabla\tilde{T}}{\tilde{T}} \geq 0 \quad \text{or} \quad -(\underline{q} + \underline{T'}\dot{s}) \cdot \frac{\nabla(T - \text{div}\,\underline{T'})}{T - \text{div}\,\underline{T'}} \geq 0 \tag{18}$$

which is again different from the classical heat conduction inequality ($-\underline{q} \cdot \frac{\nabla T}{T} \geq 0$).

The generalized Clausius-Duhem inequality, in this case, reads:

$$\mathcal{D}_1 - \tilde{\underline{q}}_s \cdot \frac{\nabla\tilde{T}}{\tilde{T}} = \tilde{T}\dot{s} - r + \text{div}\,\tilde{\underline{q}}_s - \tilde{\underline{q}}_s \cdot \frac{\nabla\tilde{T}}{\tilde{T}} \geq 0 \tag{19}$$

Using equations (8), the intrinsic dissipation (11) is written as:

$$\begin{aligned} \mathcal{D}_1 = \quad & (\text{div}\,\underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \rho\dot{\underline{v}}) \cdot \underline{v} \qquad\qquad + \ (\underline{\underline{\sigma}} - e_{,\underline{\underline{\nabla u}}_s}) : \underline{\underline{\nabla v}} \\ & + (\text{div}\,\mathbf{A} + \mathbf{a}_{\Omega\alpha} - \rho\underline{\gamma}_\alpha - e_{,\boldsymbol{\alpha}}) \cdot \dot{\boldsymbol{\alpha}} \ + (\mathbf{A} - e_{,\nabla\boldsymbol{\alpha}}) : \nabla\dot{\boldsymbol{\alpha}} \end{aligned} \tag{20}$$

or:

$$\begin{aligned}\mathcal{D}_1 = \quad & (-\rho\dot{\underline{v}} + \underline{f}_{\Omega u} + \text{div}\,\underline{\underline{\sigma}}) \cdot \underline{v} \qquad\qquad + \ (\underline{\underline{\sigma}} - \underline{\underline{\sigma}}^{nd}) : \underline{\underline{\nabla v}}_s \\ & + (-\rho\underline{\gamma}_\alpha + \mathbf{a}_{va} - \mathbf{a}^{nd} + \text{div}\,\mathbf{A}) \cdot \dot{\boldsymbol{\alpha}} \ + (\mathbf{A} - \mathbf{A}^{nd}) : \nabla\dot{\boldsymbol{\alpha}}\end{aligned} \tag{21}$$

By denoting,

$$\begin{aligned}&\underline{f}^d = \text{div}\,\underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \rho\dot{\underline{v}} \ , \qquad\qquad \underline{\underline{\sigma}}^d = \underline{\underline{\sigma}} - \underline{\underline{\sigma}}^{nd} \ , \\ &\mathbf{a}^d = \text{div}\,\mathbf{A} - \mathbf{a}^{nd} + \mathbf{a}_{va} - \rho\underline{\gamma}_\alpha \quad \text{and} \quad \mathbf{A}^d = \mathbf{A} - \mathbf{A}^{nd}\end{aligned} \tag{22}$$

The term $\underline{f}^d$ is zero (this is the equilibrium equation, we notice that it can be obtained directly here by using the invariance of the energy balance (Eq. 5) relative to an observer in uniform translation). Then, one obtains:

$$\mathcal{D}_1 = \underline{\underline{\sigma}}^d : \underline{\underline{\nabla v}}_s + \mathbf{a}^d \cdot \dot{\boldsymbol{\alpha}} + \mathbf{A}^d : \nabla\dot{\boldsymbol{\alpha}} \ . \tag{23}$$

Finally, the dissipation inequality is written as:

$$\underline{\underline{\sigma}}^d : \underline{\underline{\nabla v}}_s + \mathbf{a}^d \cdot \dot{\boldsymbol{\alpha}} + \mathbf{A}^d : \nabla\dot{\boldsymbol{\alpha}} - \tilde{\underline{q}}_s \cdot \frac{\nabla\tilde{T}}{\tilde{T}} \geq 0 \ . \tag{24}$$

2.4 Constitutive and governing equations

The following quantities $T, \underline{T'}, \underline{\underline{\sigma}}^{nd}, \mathbf{a}^{nd}, \mathbf{A}^{nd}$ have already been defined constitutively by equations (10) using the internal energy.

Constitutive laws must be specified for the dissipative variables $\underline{\underline{\sigma}}^d, \mathbf{a}^d, \mathbf{A}^d$ and $\tilde{\underline{q}}_s$. They must allow to satisfy the second principle, or equivalently the dissipation inequality (24). Because, in the general case, the dissipative forces may depend on the rate on all state variables, Coleman and Noll procedure [1] is not adequate.

However, a stronger assumption we adopt here, is to require the positiveness of the intrinsic

and the thermal dissipations. In such a case, the constitutive model is completely determined by specifying, on the one hand the internal energy defining the non-dissipative forces and the temperature, and on the second hand the dissipative forces $\underline{\underline{\sigma}}^d, \mathbf{a}^{nd}$and $\mathbf{A}^d$ satisfying the following intrinsic dissipation inequality,

$$\underline{\underline{\sigma}}^d : \underline{\underline{\nabla v}}_s + \mathbf{a}^d \cdot \dot{\boldsymbol{\alpha}} + \mathbf{A}^d : \nabla\dot{\boldsymbol{\alpha}} \geq 0 \tag{25}$$

and the flux $\underline{\tilde{q}}_s$ fulfilling the heat conduction inequality.

Using the Standard Generalized Materials (SGM) formalism [26,27], a special class of material can be constructed if one postulates the existence of two pseudo-potentials with the suitable properties [18]: (i) an intrinsic dissipation potential which is function of the rates $\underline{\underline{\nabla v}}_s, \dot{\boldsymbol{\alpha}}$ and $\nabla\dot{\boldsymbol{\alpha}}$ with the state variables as parameters: $D(\underline{\underline{\nabla v}}_s, \dot{\boldsymbol{\alpha}}, \nabla\dot{\boldsymbol{\alpha}} \mid \underline{\underline{\nabla u}}_s, \boldsymbol{\alpha}, s)$, (ii) a heat potential which is function of the entropy gradient $\underline{\nabla s}$ and possibly of higher order gradients of s, with the state variable and possibly their time derivatives as parameters: $D_s(\underline{\nabla s}|\ s, \underline{\underline{\nabla u}}_s, \boldsymbol{\alpha}, \dot{s}, \dots)$, such as:

$$\underline{\underline{\sigma}}^d \in \partial D_{,\underline{\underline{\nabla v}}_s}\ , \quad \mathbf{a}^d \in \partial D_{,\dot{\boldsymbol{\alpha}}} \quad \text{and} \quad \mathbf{A}^d \in \partial D_{,\nabla\dot{\boldsymbol{\alpha}}}\ , \tag{26}$$

which is denoted:

$$\underline{\underline{\sigma}}^d = D_{,\underline{\underline{\nabla v}}_s}\ , \quad \mathbf{a}^d = D_{,\dot{\boldsymbol{\alpha}}} \quad \text{and} \quad \mathbf{A}^d = D_{,\nabla\dot{\boldsymbol{\alpha}}}\ , \tag{27}$$

and

$$-\underline{\tilde{q}}_s = \frac{\delta D_s}{\delta \underline{\nabla s}} \tag{28}$$

For instance, considering a potential D_s function of $\underline{\nabla s}$ and $\underline{\underline{\nabla\nabla s}}$ (and so, not adopting the principle of equipresence), one has:

$$-\underline{\tilde{q}}_s = D_{s,\underline{\nabla s}} - \text{div}\,(D_{s,\underline{\underline{\nabla\nabla s}}}) \tag{29}$$

To sum up, the following field equations are obtained:

$$\begin{cases} \text{div}\,\underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \rho\dot{\underline{v}} = 0 \\ \text{div}\,\mathbf{A} + \mathbf{a}_{va} - \mathbf{a} - \rho\underline{\gamma}_{\alpha} = 0 \\ \text{div}\,\underline{\tilde{q}}_s - r - (\underline{\underline{\sigma}}^d : \underline{\underline{\nabla v}}_s + \mathbf{a}^d \cdot \dot{\boldsymbol{\alpha}} + \mathbf{A}^d : \nabla\dot{\boldsymbol{\alpha}}) + \tilde{T}\dot{s} = 0 \end{cases} \tag{30}$$

$$\begin{cases} \underline{\underline{\sigma}}^{nd} = e_{,\underline{\underline{\nabla u}}_s} \\ \mathbf{a}^{nd} = e_{,\boldsymbol{\alpha}} \\ \mathbf{A}^{nd} = e_{,\nabla\boldsymbol{\alpha}} \\ \tilde{T} = \dfrac{\delta e}{\delta s} \end{cases} \quad \begin{cases} \underline{\underline{\sigma}}^{d} = D_{,\underline{\underline{\nabla v}}_s} \\ \mathbf{a}^{d} = D_{,\dot{\boldsymbol{\alpha}}} \\ \mathbf{A}^{d} = D_{,\nabla\dot{\boldsymbol{\alpha}}} \\ -\underline{\tilde{q}}_s = \dfrac{\delta D_s}{\delta \underline{\nabla s}} \end{cases} \quad \begin{cases} \underline{\underline{\sigma}} = \underline{\underline{\sigma}}^{nd} + \underline{\underline{\sigma}}^{d} \\ \mathbf{a} = \mathbf{a}^{nd} + \mathbf{a}^{d} \\ \mathbf{A} = \mathbf{A}^{nd} + \mathbf{A}^{d} \\ \underline{q} = -\underline{T'}\dot{s} + \underline{\tilde{q}}_s \end{cases} \tag{31}$$

with the following boundary conditions, on the surface $\partial\Omega$:

$$\begin{cases} \underline{\underline{\sigma}} \cdot \underline{n} = \underline{f}_{Su} \quad \text{or} \quad (\underline{\underline{\sigma}}^{nd} + \underline{\underline{\sigma}}^{d}) \cdot \underline{n} = \underline{f}_{Su} \\ \mathbf{A} \cdot \underline{n} = \mathbf{a}_{S\alpha} \quad \text{or} \quad (\mathbf{A}^{nd} + \mathbf{A}^{d}) \cdot \underline{n} = \mathbf{a}_{S\alpha} \\ (-\underline{q}) \cdot \underline{n} = Q \quad \text{or} \quad -(\underline{\tilde{q}}_s - \underline{T'}\dot{s}) \cdot \underline{n} = Q \end{cases} \tag{32}$$

The set of field equations obtained in this framework can be written in a compact manner as:

$$\begin{cases} \text{div}\,(e_{,\underline{\underline{\nabla u}}_s} + D_{,\underline{\underline{\nabla v}}_s}) + \underline{f}_{\Omega u} - \rho\ddot{\underline{u}} = 0 \\ \text{div}\,(e_{,\nabla\boldsymbol{\alpha}} + D_{,\nabla\dot{\boldsymbol{\alpha}}}) + \mathbf{a}_{va} - (e_{,\boldsymbol{\alpha}} + D_{,\dot{\boldsymbol{\alpha}}}) - \rho\underline{\gamma}_{\alpha} = 0 \\ \text{div}\,\dfrac{\delta D_s}{\delta \underline{\nabla s}} + r + (D_{,\underline{\underline{\nabla v}}_s} : \underline{\underline{\nabla v}}_s + D_{,\dot{\boldsymbol{\alpha}}} \cdot \dot{\boldsymbol{\alpha}} + D_{,\nabla\dot{\boldsymbol{\alpha}}} \cdot \nabla\dot{\boldsymbol{\alpha}}) - \dfrac{\delta e}{\delta s}\dot{s} = 0 \end{cases} \tag{33}$$

As established in subsection 2.3, the heat equation is

$$\tilde{T}\dot{s} + \text{div}\,\underline{\tilde{q}}_s - r - \mathcal{D}_1 = 0 \tag{34}$$

with

$$\tilde{T} = \frac{\delta e}{\delta s} = e_{,s} - \text{div}\, e_{,\underline{\nabla s}} \quad \text{and} \quad \underline{\tilde{q}}_s = \frac{\delta D_s}{\delta \underline{\nabla s}} \tag{35}$$

It is also written as:

$$T\dot{s} + \underline{T}' \cdot \underline{\nabla \dot{s}} + \text{div}\,\underline{q} - r - \mathcal{D}_1 = 0 \tag{36}$$

When Fourier law is adopted one recovers the form proposed by Nguyen [19]. This form is different the one obtained by the micromorphic approach of Forest and Amestoy [15] in the absence of intrinsic dissipation. Indeed, Forest and Amestoy [15] adopt the classical forms of the heat equation and the Fourier law

$$T\dot{s} + \text{div}\,\underline{q} - r = 0 \quad \text{and} \quad \underline{q} = -\kappa \underline{\nabla T} \tag{37}$$

but define the temperature with a state law

$$T = e_{,s} - \frac{a_s}{\rho} \quad \text{and} \quad \underline{b}_s = e_{,\underline{\nabla s}} \tag{38}$$

Using a principle of virtual work on entropy, the justification of which is not obvious, they find the equilibrium equation associated with the variable s, readily:

$$\text{div}\,\underline{b}_s - a_s = 0 \tag{39}$$

Thus, we have:

$$T = e_{,s} - \frac{1}{\rho}\text{div}\,\underline{b}_s = e_{,s} - \text{div}\,(e_{,\underline{\nabla s}}) \tag{40}$$

which is exactly the variable denoted $\tilde{T}$ here, and therefore, with our notations,

$$\underline{q} = -\kappa \underline{\nabla \tilde{T}} \tag{41}$$

which is a particular form of the law (28). More specifically, in our case, by taking:

$$e = T_0 s + \frac{1}{2} a_1 s^2 + \frac{1}{2} a_2 \underline{\nabla s} \cdot \underline{\nabla s} \tag{42}$$

one obtains: $\tilde{T} = T_0 + a_1 s - a_2 \Delta s$. The potential

$$D_s = \kappa(a_1 \underline{\nabla s} \cdot \underline{\nabla s} - a_2 \underline{\underline{\nabla \nabla s}} : \underline{\underline{\nabla \nabla s}}) \tag{43}$$

leads to the generalized Fourier law (41). And finally the heat equation (34) is:

$$(T_0 + a_1 s - a_2 \Delta s)\dot{s} + r + \kappa(a_1 \Delta s - \kappa a_2 \Delta^2 s) = 0 \; . \tag{44}$$

The linearization of this equation gives the equation obtained in [15].

3 Temperature gradient: using the Helmholtz free energy

In this section, the temperature and its gradient as adopted as internal variables instead of the entropy and its gradient. A complementary description to the previous one, in term of Helmholtz free energy, is established. It leads to the same results as the variational formulation of Nguyen and Andrieux [18], except for the heat conduction inequality given here by a new inequality.

The point of departure is still the balance of energy in its global and then local form (equations (7) and (8)). As s and $\underline{\nabla s}$ are no longer state variables and replaced by T and $\underline{\nabla T}$, the more convenient thermodynamic function is no longer the internal energy but its conjugate function obtained by a Legendre transformation on the entropic variables (dual variables of T and ∇T). These variables, denoted respectively s and $\underline{s}'$, are related to T and ∇T by:

$$T = \frac{\partial e}{\partial s} \quad \text{and} \quad \underline{\nabla T} = \frac{\partial e}{\partial \underline{s}'} \tag{45}$$

The thermodynamic function w keeping the duality, as established by Nguyen and Andrieux [18], is defined as:

$$w = e - Ts - \underline{\nabla T} \cdot \underline{s}' \tag{46}$$

Thus:

$$s = -w_{,T} \quad \text{and} \quad \underline{s}' = -w_{,\nabla T} \tag{47}$$

w is the Helmholtz free energy per unit volume defined in a non classical way. In this context, it is a function of $\underline{\underline{\nabla u}}_s, \boldsymbol{\alpha}, \nabla\boldsymbol{\alpha}, T$ and $\underline{\nabla T}$.

As $\dot{e}|_{s,\underline{s}'} = \dot{w}|_{T,\underline{\nabla T}}$, the intrinsic dissipation $\mathcal{D}_1$ given by (13) becomes:

$$\begin{aligned} \mathcal{D}_1 &= T\dot{s} + \dot{\underline{s}}' \cdot \underline{\nabla T} - r + \text{div}\,(\underline{q}) \\ &= (\dot{s} - \text{div}\,\dot{\underline{s}}')T - r + \text{div}\,(\underline{q} + T\dot{\underline{s}}') \end{aligned} \tag{48}$$

If we set $\dot{\tilde{s}} = \dot{s} - \text{div}\,(\dot{\underline{s}}')$ and $\underline{\tilde{q}}_T = \underline{q} + T\underline{\dot{s}}'$, we obtain

$$\mathcal{D}_1 = T\dot{\tilde{s}} - r + \text{div}\,\underline{\tilde{q}}_T \tag{49}$$

This form is similar to the one obtained in the classical approach (without temperature gradient), with the definitions of entropy as the variational derivative of the Helmholtz free energy relative to the temperature ($\tilde{s} = w_{,T} - \text{div}\, w_{,\underline{\nabla T}}$) and of the heat flux as ($\underline{\tilde{q}}_T = \underline{q} + T\dot{\underline{s}}'$).

3.1 Second law and heat conduction inequality

Given the entropy $\tilde{s}$ and the total heat flux $\underline{\tilde{q}}_T$, the internal production of entropy $\mathcal{S}_i$ is, as previously in section 3.1, given by:

$$\mathcal{S}_i = \dot{\tilde{s}} - \frac{r}{T} + \text{div}\,\frac{\underline{\tilde{q}}_T}{T} \tag{50}$$

and the second law is defined as:

$$\dot{\tilde{s}} - \frac{r}{T} + \text{div}\,\frac{\underline{\tilde{q}}_T}{T} \geq 0 \tag{51}$$

Let us notice that when there is no external volumic heat source ($r = 0$), the internal entropy

production is reduced to:

$$\mathcal{S}_i = \dot{s} + \underline{\dot{s}}' \cdot \frac{\nabla T}{T} + \text{div}\,\frac{\underline{q}}{T} \tag{52}$$

which is exactly the expression proposed by Nguyen and Andrieux and Nguyen [19] while Cardona et al. [15] keep the classical form.

One notices that the entropy production can be written in the following form:

$$\mathcal{S}_i = \tilde{s} - \frac{r}{T} + \text{div}\,\frac{\tilde{\underline{q}}_T}{T} = \frac{\mathcal{D}_1}{T} - \tilde{\underline{q}}_T \cdot \frac{\nabla T}{T^2} \tag{53}$$

Admitting the separation of the total dissipation in intrinsic and thermal parts, the thermal dissipation is therefore given by $-\tilde{\underline{q}}_T \cdot \frac{\nabla T}{T}$ and the conduction inequality is:

$$-\tilde{\underline{q}}_T \cdot \frac{\nabla \tilde{T}}{\tilde{T}} \geq 0 \quad \text{or} \quad -(\underline{q} + T\underline{\dot{s}}') \cdot \frac{\nabla T}{T} \geq 0 \tag{54}$$

which is again different from the classical heat conduction inequality ($-\underline{q} \cdot \frac{\nabla T}{T} \geq 0$).

The Clausius-Duhem inequality, in this case, reads:

$$\mathcal{D}_1 - \tilde{\underline{q}}_T \cdot \frac{\nabla T}{T} = T\dot{\tilde{s}} - r + \text{div}\,\tilde{\underline{q}}_T - \tilde{\underline{q}}_s \cdot \frac{\nabla \tilde{T}}{\tilde{T}} \geq 0 \tag{55}$$

The free energy w depends on $\underline{\underline{\nabla u}}_s$, $\boldsymbol{\alpha}$, $\nabla\boldsymbol{\alpha}$, T, $\underline{\nabla T}$, we thus define:

$$\underline{\underline{\sigma}}^{nd} = w_{,\underline{\underline{\varepsilon}}} \ , \quad \mathbf{a}^{nd} = w_{,\boldsymbol{\alpha}} \ , \quad \mathbf{A}^{nd} = w_{,\nabla\boldsymbol{\alpha}} \ , \quad s = -w_{,T} \quad \text{and} \quad \underline{s}' = -w_{,\nabla T} \tag{56}$$

The intrinsic dissipation is given by equation (23) and the dissipative forces $\underline{\underline{\sigma}}^d, \mathbf{a}^d, \mathbf{A}^d$ and $\tilde{\underline{q}}_s$ are defined by equation (22).

3.2 Constitutive and governing equations

The same approach as previously is used. The following quantities $T, \underline{T'}, \underline{\underline{\sigma}}^{nd}, \mathbf{A}^{nd}$ are defined constitutively by equation (56) using the free energy. Constitutive laws are specified for the dissipative variables $\underline{\underline{\sigma}}^d, \mathbf{a}^d, \mathbf{A}^d$ and $\tilde{\underline{q}}_s$. They must satisfy the second principle, or equivalently the

dissipation inequality (24). Because, in the general case, the dissipative forces may depend on the rate on all state variables, Coleman and Noll procedure [1] is not adequate. The constitutive model is completely determined by specifying, on the one hand the internal energy defining the non-dissipative forces and the temperature, and on the second hand the dissipative forces $\underline{\underline{\sigma}}^d, \mathbf{a}^d$ and $\mathbf{A}^d$ satisfying the positiveness of $\mathcal{D}_1$, and the flux $\underline{\tilde{q}}_s$ fulfilling the heat conduction inequality.

Using the SGM formalism [26,27], a class of constitutive models can be constructed using two pseudo-potentials with the suitable properties [18]: (i) an intrinsic dissipation potential which is function of the rates $\underline{\underline{\nabla v}}_s, \dot{\boldsymbol{\alpha}}$ and $\nabla\dot{\boldsymbol{\alpha}}$ with the state variables as parameters: $D(\underline{\underline{\nabla v}}_s, \dot{\boldsymbol{\alpha}}, \nabla\dot{\boldsymbol{\alpha}} \mid \underline{\underline{\nabla u}}_s, \boldsymbol{\alpha}, T)$, (ii) a thermal dissipation potential which is function of the temperature gradient $\underline{\nabla T}$ and possibly of higher order gradients of T, with the state variable and possibly their time derivatives as parameters: $D_T(\underline{\nabla T} \mid\ T, \underline{\nabla u}_s, \boldsymbol{\alpha}, \dot{T}, \dots)$, such as:

$$\underline{\underline{\sigma}}^d \in \partial D_{,\underline{\underline{\nabla v}}_s}\ , \quad \mathbf{a}^d \in \partial D_{,\dot{\boldsymbol{\alpha}}} \quad \text{and} \quad \mathbf{A}^d \in \partial D_{,\nabla\dot{\boldsymbol{\alpha}}}\ , \tag{57}$$

that we denote:

$$\underline{\underline{\sigma}}^d = D_{,\underline{\underline{\nabla v}}_s}\ , \quad \mathbf{a}^d = D_{,\dot{\boldsymbol{\alpha}}} \quad \text{and} \quad \mathbf{A}^d = D_{,\nabla\dot{\boldsymbol{\alpha}}}\ , \tag{58}$$

and

$$-\underline{\tilde{q}}_T = \frac{\delta D_T}{\delta \underline{\nabla T}} \tag{59}$$

For instance, considering a potential D_T function of $\underline{\nabla T}$ and $\underline{\underline{\nabla\nabla T}}$ (and so, not adopting the principle of equipresence), one has:

$$-\underline{\tilde{q}}_T = D_{T,\underline{\nabla T}} - \text{div}\,(D_{T,\underline{\underline{\nabla\nabla T}}}) \tag{60}$$

To sum up, the following field equations are obtained:

$$\begin{cases} \operatorname{div} \underline{\underline{\sigma}} + \underline{f}_{\Omega u} - \dot{\underline{v}} = 0 \\ \operatorname{div} \mathbf{A} + \mathbf{a}_{va} - \mathbf{a} - \underline{\gamma}_{\alpha} = 0 \\ \operatorname{div} \tilde{\underline{q}}_T - r - (\underline{\underline{\sigma}}^d : \underline{\underline{\nabla v}}_s + \mathbf{a}^d \cdot \dot{\boldsymbol{\alpha}} + \mathbf{A}^d : \nabla \dot{\boldsymbol{\alpha}}) + T\dot{\tilde{s}} = 0 \end{cases} \tag{61}$$

$$\begin{cases} \underline{\underline{\sigma}}^{nd} = w_{,\underline{\underline{\nabla u}}_s} \\ \mathbf{a}^{nd} = w_{,\boldsymbol{\alpha}} \\ \mathbf{A}^{nd} = w_{,\nabla\boldsymbol{\alpha}} \\ \tilde{s} = -\dfrac{\delta w}{\delta T} \end{cases} \quad \begin{cases} \underline{\underline{\sigma}}^{d} = D_{,\underline{\underline{\nabla v}}_s} \\ \mathbf{a}^{d} = D_{,\dot{\boldsymbol{\alpha}}} \\ \mathbf{A}^{d} = D_{,\nabla\dot{\boldsymbol{\alpha}}} \\ -\tilde{\underline{q}}_T = \dfrac{\delta D_T}{\delta \underline{\nabla T}} \end{cases} \quad \begin{cases} \underline{\underline{\sigma}} = \underline{\underline{\sigma}}^{nd} + \underline{\underline{\sigma}}^{d} \\ \mathbf{a} = \mathbf{a}^{nd} + \mathbf{a}^{d} \\ \mathbf{A} = \mathbf{A}^{nd} + \mathbf{A}^{d} \\ \underline{q} = -T\underline{\dot{s}}' + \tilde{\underline{q}}_T \end{cases} \tag{62}$$

with the following boundary conditions, on the surface $\partial\Omega$:

$$\begin{cases} \underline{\underline{\sigma}} \cdot \underline{n} = \underline{f}_{Su} \quad \text{or} \quad (\underline{\underline{\sigma}}^{nd} + \underline{\underline{\sigma}}^{d}) \cdot \underline{n} = \underline{f}_{Su} \\ \mathbf{A} \cdot \underline{n} = \mathbf{a}_{S\alpha} \quad \text{or} \quad (\mathbf{A}^{nd} + \mathbf{A}^{d}) \cdot \underline{n} = \mathbf{a}_{S\alpha} \\ -\underline{q} \cdot \underline{n} = Q \quad \text{or} \quad -(\tilde{\underline{q}}_T - T\underline{\dot{s}}') \cdot \underline{n} = Q \end{cases} \tag{63}$$

The set of field equations obtained in this framework, consistent with the results of [19], can be written in a compact manner as in [19]:

$$\begin{cases} \operatorname{div}(w_{,\underline{\underline{\nabla u}}_s} + D_{,\underline{\underline{\nabla v}}_s}) + \underline{f}_{\Omega u} - \rho\ddot{\underline{u}} = 0 \\ \operatorname{div}(w_{,\nabla\boldsymbol{\alpha}} + D_{,\nabla\dot{\boldsymbol{\alpha}}}) + \mathbf{a}_{va} - (w_{,\boldsymbol{\alpha}} + D_{,\dot{\boldsymbol{\alpha}}}) - \rho\underline{\gamma}_{\alpha} = 0 \\ \operatorname{div}\dfrac{\delta D_T}{\delta \underline{\nabla T}} + r + (D_{,\underline{\underline{\nabla v}}_s} \cdot \underline{\underline{\nabla v}}_s + D_{,\dot{\boldsymbol{\alpha}}} \cdot \dot{\boldsymbol{\alpha}} + D_{,\nabla\dot{\boldsymbol{\alpha}}} \cdot \nabla\dot{\boldsymbol{\alpha}}) + \dfrac{\delta w}{\delta T}\dot{T} = 0 \end{cases} \tag{64}$$

with the boundary conditions:

$$\begin{cases} (w_{,\underline{\underline{\nabla u}}_s} + D_{,\underline{\underline{\nabla v}}_s}) \cdot \underline{n} = \underline{f}_{Su} \\ (w_{,\boldsymbol{\alpha}} + D_{,\dot{\boldsymbol{\alpha}}}) \cdot \underline{n} = \mathbf{a}_{S\alpha} \\ \left(\dfrac{\delta D_T}{\delta \underline{\nabla T}} + T \overbrace{\dot{w}_{,\nabla T}} \right) \cdot \underline{n} = Q \end{cases} \tag{65}$$

3.2.1 Heat equation and comparisons

As established in subsection 3.1, the heat equation is

$$T\dot{\tilde{s}} + \text{div}\, \underline{\tilde{q}}_T - r - \mathcal{D}_1 = 0 \tag{66}$$

with

$$\dot{\tilde{s}} = \dot{s} - \text{div}\,(\underline{\dot{s}}') = -\overbrace{(\dot{w}_{,T} - \text{div}\, w_{,\underline{\nabla T}})} \quad \text{and} \quad -\underline{\tilde{q}}_T = \frac{\delta D_T}{\delta \underline{\nabla T}} \tag{67}$$

It is the equation obtained from the variational formulation of Nguyen and Andrieux [18]. Suitable choices of the potentials permit also to recover results obtained in [28,29].

4 Conclusion

This work is intended to give some physical insights into the entropy and temperature gradients thermomechanics, without using variational approach or virtual work principle. Departing from the expression of the intrinsic dissipation, it is shown that, when using the variational derivation to define temperature and entropy, the (temperature or entropy) gradient thermodynamics preserves the classical forms of equations and leads to consistent formulations of the second law and the heat conduction inequality. More particularly, the obtained heat conduction inequality is different from the classical one. Its expression is clearly related to the form and the nature of the entropy fluxes. Finally, the GSM formalism can be used as systematic tool for proposing ther-

modynamic admissible constitutive laws. Note that, as suggested by Nguyen and Andrieux [18], the extension to higher order gradient is straightforward adopting the variational derivatives.

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