Gradient thermodynamics and heat equations

Modèle thermodynamique à gradients et l'équation thermique

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ABSTRACT

In this Note, a thermodynamic description is proposed to include the gradient of the temperature in the set of state variables. It is based upon an original expression of the entropy and of the internal energy taking account of the presence of the temperature gradient by Legendre transform with respect to the variable $(T, \nabla T)$. The proposed description can be justified in a homogenization process. In particular, the associated heat equation is derived and discussed in comparison with the existing results of the literature. It is shown that this equation removes the paradox of instantaneous propagation.

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RÉSUMÉ

On propose dans cette Note un cadre thermodynamique incluant le gradient de la température comme une variable d'état supplémentaire. Cette théorie est construite à partir d'une relation originale reliant les expresssions de l'énergie interne et l'énergie libre par transformation de Legendre étendue aux variables $(T, \nabla T)$. La description proposée peut être justifiée par un passage micro–macro. En particulier, l'équation thermique résultante est discutée et comparée avec les résultats antérieurs de la littérature. On montre que cette équation enlève le paradoxe de propagation instantanée.

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1. Introduction

The internal variable theory of Continuum Thermodynamics is based upon the axiom of the local state which is the assumption that an element of matter is in thermodynamic equilibrium, cf. [1]. The local state is thus described by the set of state variables which are the temperature and other physical variables (deformation,...). For example, the common theories of thermo-elasticity and thermo-plasticity are given in this framework.

However, in many applications in thermo-mechanics, the temperature fields present very high gradients and it is natural to wonder if the temperature gradient might be introduced in the constitutive equation [2], in particular to wonder if the temperature gradient might be introduced as a state variable. When the temperature gradient is included in the expression of the free energy, the assumption of the equilibrium local state of Continuum Thermodynamics is clearly not respected. Such a situation deviates from the classical framework of Continuum Thermodynamics but still makes sense when the local state is in a steady state. It is then necessary to define a non-classical relationship between the internal energy and the free energy. This subject has been discussed in the literature by Forest et al. [3,4] and by Nguyen and Andrieux [5]. The ideas developed in [6–8], concerning the gradients of internal parameters are followed by Forest et al. while Nguyen and

Andrieux proposed an extended expression of the internal energy in terms of the free energy respecting the duality by Legendre transform with respect to the temperature and temperature gradient. The present discussion is devoted to the last description and explores in more details its consequences. In particular, it is shown that the proposed framework can be understood by an academic example of micro–macro modeling and gives an original possibility to solve the paradox of instantaneous conduction.

2. Continuum thermodynamics

In classical thermodynamics and in a Lagrangian description, it is well known that the free energy w per unit volume of a solid is related to the internal energy e and the entropy s per unit volume by

$$e = Ts + w(T, \nabla u, \psi), \quad s = -w,_T \tag{1}$$

where T denotes the temperature, u is the displacement and ψ is a set of internal parameter, $(T, \nabla u, \psi)$ is a system of state variable of the material. For any material volume V, the first and second principles when taking account of the dynamical equation, can be written as

$$\begin{cases} \dot{E} = P_i + P_{cal} \\ P_{entr} = \dot{S} + \int_V \frac{q}{T} \cdot n \, da \geqslant 0 \\ E = \int_V e \, dV, \quad P_i = \int_V \sigma : \nabla \dot{u} \, dV, \quad P_{cal} = -\int_{\partial V} q \cdot n \, da, \quad S = \int_V s \, dV \end{cases} \tag{2}$$

where E is the internal energy of V, P_i is the internal mechanical work, P_{cal} is the heat supply, S is the entropy of V, σ is the unsymmetric Lagrangian stress. These equations also equivalent to the local equation of energy and the positivity of the total dissipation:

$$\begin{cases} \dot{e} + \nabla \cdot q = \sigma : \nabla \dot{u} \\ d_{total} = d_i + d_T \geqslant 0, \quad d_i = T\dot{s} + \nabla \cdot q, \quad d_T = -\nabla T \cdot \frac{q}{T} \geqslant 0 \end{cases} \tag{3}$$

where d_i is the intrinsic dissipation, d_T is the thermal dissipation and d_{total} is the dissipation per unit volume. In terms of the free energy, it has been shown that

$$d_i = \sigma_{IR} : \nabla \dot{u} - w,_\psi : \dot{\psi}, \qquad \sigma = \sigma_I + \sigma_{IR} + \sigma_R, \quad \sigma_R = w,_{\nabla u} \tag{4}$$

where σ_I is the initial stress, σ_R and σ_{IR} are the reversible and irreversible stresses.

The dissipation is a product of forces and fluxes which are related by complementary laws. For example, for a visco-plastic solid admitting the dissipation potential $D(\nabla \dot{u}, \dot{\psi})$, the complementary laws are

$$\sigma_{IR} = D,_{\nabla \dot{u}}, \qquad -w,_\psi = D,_{\dot{\psi}}$$

In particular, if Fourier law of conduction is assumed:

$$q = -k\nabla T \tag{5}$$

the local equation of energy leads in this case to the classical heat equation

$$T\dot{s} - \nabla \cdot (k\nabla T) - d_i = 0 \tag{6}$$

For example, in a rigid body without internal parameter, the particular expression $w(T) = -aT(Ln(T/\tau) - 1)$, a and k are positive constants, leads to the equation of heat conduction

$$a\dot{T} - k\Delta T = 0 \tag{7}$$

This is the familiar framework of thermo-mechanics which are well presented in classical textbooks, cf. [9,10]. It is however well known that equation of diffusion (6) leads to an instantaneous diffusion of the information while the physics requires intuitively a finite velocity. This old question has been the subject of many discussions in the past in order to remove the paradox. For example, Cattaneo proposed a modification of Fourier law under the form

$$q + \eta\dot{q} = -k\nabla T, \quad \eta > 0$$

taking account of a memory effect [11]. In this case, Eq. (7) is replaced by

$$a\dot{T} + \eta a\ddot{T} - k\Delta T = 0 \tag{8}$$

Cattaneo equation (8) has been extended in several ways to describe the heat conduction with finite speed in media with memory [12–14].

3. Gradient thermodynamics

This section concerns with the introduction of ∇T as an additional state variable and pursues the description given in [5]. It is assumed here that the set of variables $(T, \nabla T, \nabla u, \psi)$ describes the local state and the expression of the free energy per unit reference volume is a given function $w(T, \nabla T, \nabla u, \psi)$. Under the basic relation (1) of Thermostatics and of Continuum Thermodynamics, it has been shown by Coleman and Noll argument that the free energy cannot depend on ∇T. It is then clear that this basic relation must be modified in order to include the temperature gradient.

3.1. Keeping the duality

In this approach, the basic point concerns with a new relationship between the internal energy and the free energy per unit reference volume. As in Classical Thermodynamics, this relationship is based again on Legendre transform with a slight modification. The duality is kept under the form [5]

$$\begin{cases} e(s, s', \nabla u, \psi) = sT + s' \cdot \nabla T + w(T, \nabla T, \nabla u, \psi) \\ s = -w,_T, \quad s' = -w,_{\nabla T}, \quad T = e,_s, \quad \nabla T = e,_{s'} \end{cases} \tag{9}$$

Thus, a new physical quantity, *the entropy vector s'*, is introduced. The introduction of the temperature gradient is followed by the introduction of the entropy vector s' in order to keep the concept of temperature–entropy duality in a global sense, e and $-w$ are related by Legendre transform, (s, s') and $(T, \nabla T)$ are dual variables, [5]. The internal energy is a convex and increasing function with respect to s as in Classical Thermodynamics. The convexity of the internal energy with respect to the independent variable ∇T is also assumed. It follows by this duality that w is a concave function with respect to T and ∇T.

This local relationship of energy and entropy leads also to a global definition of the entropy and the energy for a finite volume V as it has been shown in [5]:

$$\begin{cases} \mathbf{W}(\mathbf{T}, \mathbf{u}, \boldsymbol{\Psi}) = \int\limits_V w(T, \nabla T, \nabla u, \psi)\, dV \\ \mathbf{S}[\delta\mathbf{T}] = -\mathbf{W},_\mathbf{T} \cdot \delta\mathbf{T} \\ \mathbf{E}(\mathbf{S}, \mathbf{u}, \boldsymbol{\Psi}) = \mathbf{S}[\mathbf{T}] + \mathbf{W}(\mathbf{T}, \mathbf{u}, \boldsymbol{\Psi}) \end{cases} \tag{10}$$

Thus, the global entropy appears again as the derivative of the free energy functional with respect to the temperature field.

3.2. The two principles

In this description, the energy balance remains unchanged while an additional entropy source is assumed. The two thermodynamic principles are written as

$$\begin{cases} \dot{E} = P_i + P_{cal} \\ P_V^{entr} = \int\limits_V \left(\dot{s} + \frac{\nabla T}{T} \cdot \dot{s}' \right) dV + \int\limits_{\partial V} \frac{q}{T} \cdot n\, da \geqslant 0 \end{cases} \tag{11}$$

Thus, an additional term in the entropy production, the entropy source $\frac{\nabla T}{T} \cdot \dot{s}'$, is proposed. This differs in spirit from the possibility of extra-entropy fluxes which has been introduced by many authors in the study of gradient models for solids with micro-structures, cf. [15,8,16]. Such entropy source seems to be natural from the non-equilibrium of the local state. The following equations result after some calculation

$$\begin{cases} T\dot{s} + \nabla T \cdot \dot{s}' + \nabla q - d_i = 0 \quad \text{(local equation of energy)} \\ d_{total} = d_i + d_T \geqslant 0, \quad d_i = \sigma_{IR} : \nabla \dot{u} - w,_\psi \cdot \dot{\psi}, \quad d_T = -\frac{\nabla T}{T} \cdot q \end{cases} \tag{12}$$

3.3. The heat equation

The local equation of energy leads to the following heat equation when the Fourier law of conduction is assumed:

$$-\nabla \cdot (k\nabla T) + T\dot{s} + \nabla T \cdot \dot{s}' - d_i = 0 \tag{13}$$

with classical mixed boundary conditions (prescribed temperature or given heat flux).

4. The paradox of instantaneous conduction

Let us consider a simple example of conduction in a rigid solid with the following expression of the free energy:

$$w(T, \nabla T) = -aT\big(Ln(T/\tau) - 1\big) - \frac{b}{2}\nabla T \cdot \nabla T \quad \Rightarrow \quad e(s, s') = a\tau e^{s/a} + \frac{1}{2b}s' \cdot s'$$

where $a > 0$ and $b > 0$ are two constants, τ is a given temperature. The derived thermal equation is

$$-k\Delta T + a\dot{T} + b\nabla T \cdot \nabla\dot{T} = 0 \tag{14}$$

The interest of this heat equation is especially clear regarding to the classical paradox of instantaneous conduction of the classical thermal equation (6). The proposed equation (14) differs clearly from Cattaneo equation (8).

For example, the small perturbation $\theta(x, t) = T(x, t) - T_o(x)$ of a stationary temperature $T_o(x) = \tau + gx/L$, in a rigid rod $[0, L]$ is considered. The temperature variation $\theta(x, t)$ is governed by the associated linearized equation:

$$F[\theta] = A\theta_{,t} + B\theta_{,tx} - \theta_{,xx} = 0 \quad \text{with } A = \frac{a}{k} > 0 \quad \text{and} \quad B = \frac{bg}{kL} \tag{15}$$

This equation is associated with finite velocity of propagation. Indeed, elementary solutions of the form $\theta = \exp(rx + \omega t)$, where $r = i/\ell$ and ω are complex numbers, are searched for. The condition $F[\theta] = 0$ leads to the solution

$$\theta(x, t) = e^{i(x-ct)/\ell}e^{-\gamma t} \quad \text{with } c = -\frac{B}{A^2\ell^2 + B^2}, \quad \gamma = \frac{A}{A^2\ell^2 + B^2}$$

It is concluded that an elementary solution of wave length $2\pi\ell$ propagates at celerity c with damping coefficient γ. The wave propagates with finite velocity c in the opposite direction of the thermal gradient T as expected.

5. A micro–macro modeling

The expressions (9) of the entropy s and of the internal energy e in terms of the free energy w can be illustrated in the modeling of the macroscopic conduction in a rigid composite composed of periodic cells V of dimension ℓ.

If T^* denotes the local temperature at a point in V of local coordinates y, it is assumed that the classical framework of thermodynamics is satisfied in the cell, i.e. $s^* = -w_{,T^*}$ and $e^* = T^*s^* + w^*$ where $w^*(T^*)$ is the free energy density, s^* is the entropy and e^* is the internal energy of the material. The local law of conduction is $q^* = -k^*\nabla_y T^*$.

Under the macroscopic data $(T, \nabla T)$, it is assumed that the temperature field $T^*(y)$ is in a steady state:

$$\nabla_y \cdot q^* = 0, \quad q^* = k^*\nabla_y T^* \quad \forall y \in V$$

such that

$$\langle T^* \rangle = \frac{1}{V}\int_V T^*(y)\,dV = T, \qquad \langle \nabla_y T^* \rangle = \nabla T$$

with periodic boundary conditions for $\nabla_y T^*$ and q^*. Thus, it can be written as

$$T^*(y) = T + \nabla T \cdot \phi(y) \tag{16}$$

where the vector $\phi(y)$, of components $\phi_i(y)$, $i = 1, 3$ satisfies

$$\begin{cases} \nabla_y \cdot \big(k^*\nabla_y\phi_i\big) = 0 \quad \forall y \in V \\ \langle\phi_i\rangle = 0, \quad \left\langle\dfrac{\partial\phi_i}{\partial y_j}\right\rangle = \delta_{ij} \\ + \text{ appropriated boundary conditions} \end{cases} \tag{17}$$

With the decomposition $\phi(y) = y + \varphi(y)$, the boundary conditions are

$$\varphi \text{ periodic}, \quad (k^*\nabla_y\varphi) \cdot n \text{ anti-periodic on } \partial V \tag{18}$$

It is well known in the homogenization analysis of periodic media that the system of Eqs. (17) defines a unique solution $\phi(y)$.

Since energy and entropy are additive, the macro free energy, entropy and internal energy per unit volume are:

$$w(T, \nabla T) = \langle w^* \rangle, \qquad s = \langle s^* \rangle, \qquad e = \langle e^* \rangle$$

From the expression (16), it is clear that

$$s = \langle s^* \rangle = \langle -w^*_{,T^*} \rangle = -w_{,T}$$

In the same spirit:

$$\begin{cases} w_{,\nabla T} \cdot \delta(\nabla T) = \langle w^*_{,T^*} \phi \cdot \delta(\nabla T) \rangle \\ \quad = \langle -s^* \phi \rangle \cdot \delta(\nabla T) = -s' \cdot \delta(\nabla T) \\ \quad \text{thus } s' = -w_{,\nabla T} \text{ with } s' = \langle s^* \phi \rangle \end{cases}$$

The expression (9) of the internal energy follows:

$$\begin{cases} e = \langle T^* s^* + w^* \rangle = \langle s^*(T + \nabla T \cdot \phi) + w^* \rangle \\ \quad = Ts + \langle s^* \cdot \phi \rangle \cdot \nabla T + w = Ts + s' \cdot \nabla T + w \end{cases}$$

Let q be by definition $q = \langle q^* \rangle$. Thus, q and ∇T are related by the homogenized law of conduction

$$q = \langle -k^* \nabla_y T^* \rangle = -\langle k^* \nabla_y \phi \rangle \cdot \nabla T = -k \nabla T \quad \text{with } k = \langle k^* \nabla_y \phi \rangle$$

and the following expression holds in the same spirit as Hill–Mandel relationship:

$$q \cdot \nabla T = \langle q^* \cdot \nabla T^* \rangle$$

By definition, the macroscopic heat supply per unit time and per unit volume $\nabla \cdot q$ is the heat produced per unit macroscopic volume and unit time

$$\nabla \cdot q = \frac{\int_{\partial V} q^* \cdot n \, da}{\int_V dV} \quad \text{thus } \nabla \cdot q = \langle \nabla_y \cdot q^* \rangle$$

From the local energy balance, the macroscopic balance follows

$$0 = \langle \dot{e}^* - \nabla_y \cdot q^* \rangle = \dot{e} - \nabla \cdot q$$

The macroscopic intrinsic dissipation per unit volume is

$$\langle \theta \dot{s}^* - \nabla_y \cdot q^* \rangle = \langle T \dot{s}^* + \nabla T \cdot \phi \dot{s}^* \rangle - \nabla \cdot q = T\dot{s} + \nabla T \cdot \dot{s}' - \nabla \cdot q$$

Thus, the expressions of the first and second principles (11) are fully justified from the homogenized behavior of a solid with substructures as well as the macroscopic thermal conduction (14).

From (16) and (17), the difference of temperature $T^* - T$ is of order $\nabla T \ell$. Thus, if $\ell \ll T/\nabla T$, the contribution of additional terms involving ∇T in the expression of the energy, the entropy and in the heat equation (14) can be neglected and the classical results of Continuum Thermodynamics and of Homogenization, cf. for example [17], are recovered. The proposed framework is thus interesting for solids with micro-structures when the temperature gradient is very strong, so that ℓ is not small compared to $T/\nabla T$.

6. Comparison with existing results

Different discussions have also been given in the literature on this subject, cf. [3,4,16]. In particular, Forest et al.'s discussion [3] followed an approach due to Frémond [6], Maugin cf. for example [8], or Gurtin [7], denoted here as the FGM-approach, to include the gradient of the internal parameter as state variable. The entropy and the internal energy have been defined as

$$\begin{cases} s(T, \nabla T, \nabla u, \psi) = -w_{,T} + \nabla \cdot w_{,\nabla T} = -\dfrac{\delta w}{\delta T} \\ e(T, \nabla T, \nabla u, \psi) = Ts + w(T, \nabla T, \nabla u, \psi) \end{cases} \tag{19}$$

It is clear from this definition (19) that the internal energy e and the free energy w are no longer dual functions as in classical thermodynamics. The energy balance is modified while the entropy production remains unchanged, as shown in [3]

$$\begin{cases} \dot{E} + \dot{K} = P_{ext} + P_{cal} + P_T \\ P_T = \displaystyle\int_{\partial V} f_T \cdot \dot{T} \, da \\ P_{entr} = \displaystyle\int_V \dot{s} \, dV + \int_{\partial V} \frac{q}{T} \cdot n \, da \geqslant 0 \end{cases} \tag{20}$$

where P_T denotes an extra energy supply due to the neighboring exchanges. In [3], an additional virtual equation is also introduced in the spirit of FGM-approach under the form

$$\int_V \gamma \cdot \nabla \delta T \, dV = \int_{\partial V} f_T \delta T \, da \quad \forall \delta T$$

the force γ plays the role of a micro-force. The following expression of the additional force has been derived

$$f_T = w,_{\nabla T} \cdot n \tag{21}$$

If the Fourier law of conduction is assumed, the proposed heat equation is

$$-k\Delta T + T\dot{s} - d_i = 0 \quad \text{with } s = -\frac{\delta w}{\delta T} \tag{22}$$

For the considered simple example, the heat equation is thus:

$$-k\Delta T + a\dot{T} - bT\Delta\dot{T} = 0 \tag{23}$$

A complementary description starting from the expression of the internal energy in terms of the entropy and the entropy gradient has also been given by Forest and Amestoy [4]:

$$e = e(s, \nabla s, \nabla u, \psi) \tag{24}$$

In this case, $T = e,_s$ and the vector $\theta = e,_{\nabla s}$ has been denoted by the authors as the *hyper-temperature*. The FGM-approach is again followed to include the entropy gradient. For example, if

$$e = \frac{\xi}{2}s^2 + \frac{\zeta}{2}\nabla s \cdot \nabla s \tag{25}$$

the following heat equation is then derived under Fourier law of conduction

$$T(s)\dot{s} - k\xi\Delta s + k\zeta\Delta^2 s = 0 \tag{26}$$

The paradox of instantaneous propagation remains with Eqs. (23) and (26) as with the classical one (6) since only the value $c = 0$ can be found and the information is thus instantaneous.

7. Conclusion

To include the temperature gradient, an original expression of the internal energy and of the entropy respecting the duality by Legendre transform has been proposed and gives a consistent extension of the classical framework of continuum thermodynamics when the local state is in a steady state. This description can be understood from a micro–macro modeling of the heat conduction in a non-homogeneous rigid solid.

Our discussion is given with a special emphasis on the associated heat equation. The proposed heat equation (13) is interesting since it removes the paradox of instantaneous propagation. A refined comparison on the pertinence of the heat equations (6), (8), (23), (26) and (13) appears to be a useful subject for practical applications.

Acknowledgements

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