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Thermodynamical description of running discontinuities.

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Abstract: Determination of the evolution of a system is studied through the definition of functionals presented here in the case of non linear dynamics. After a short account of the necessary notions for the description of the motion and of the mechanical interactions, the paper is devoted to the Hamiltonian functional of the system. The evolution of discontinuities along moving surfaces generally generates an entropy production which is a linear function of the speed of the moving interface. The thermodynamical force accompanying this motion is an energy release rate, the expression of which is related to the gradient of Hamiltonian of the system. The canonical equations of shock waves and moving discontinuities are established for any continuum. This provides a useful way of establishing constitutive laws for moving interfaces.

Keywords : Hamiltonian, shock-waves, jump, discontinuity, energy-release rate.

1. SOME GENERAL FEATURES

In order to explain and to predict the motion and the equilibrium of bodies or structures subjected to various physical interactions, a kinematical description of the motion is first performed. Usually one looks for the motion of a material point M from a reference configuration by describing its displacement $u(M, t)$.

After the kinematical description of the body, one has to deal with the mechanical interactions. Many statements permit the description of these interactions ; we can use for example the virtual-power statement. This describes the mechanical interaction between each material point of the body with respect to a given loading distribution. For sake of simplicity and conciseness of this presentation, a thermodynamical description of interaction is adopted.

First, the local state is defined by a set of state variables such as the strain $\boldsymbol{\varepsilon}$, a set of internal parameters $\boldsymbol{\alpha}$, and the absolute temperature θ . The local interaction is defined by a thermodynamical potential or the free energy $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, \theta)$ per unit of mass. The thermodynamical forces are defined by the state equations :

$$\boldsymbol{\sigma}_r = \rho \frac{\partial w}{\partial \boldsymbol{\varepsilon}}, \quad A = -\rho \frac{\partial w}{\partial \boldsymbol{\alpha}}, \quad s = -\frac{\partial w}{\partial \theta}$$

$\boldsymbol{\sigma}_r$ is the reversible stress, A is the thermodynamical forces associated to the internal vari-

ables, and \mathbf{s} is the entropy. In the case of reversibility, the knowledge of the free energy is sufficient to determine the local state of equilibrium defined by the stress $\boldsymbol{\sigma} = \boldsymbol{\sigma}_r$. In nonlinear mechanics, the internal state is generally associated with irreversibility. Then the fundamental inequality of thermodynamics implies that the internal production of entropy must be non negative. The equations of state do not provide the full constitutive equations; some complementary laws are necessary to describe the irreversibility. In the total dissipation, we distinguish the part due to the conduction and the part due to internal forces. The two parts are assumed to be separately non negative. The mechanical part has the form:

$$D_m = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \rho(\dot{w} + \mathbf{s}\dot{\theta}) = (\boldsymbol{\sigma} - \boldsymbol{\sigma}_r) : \dot{\boldsymbol{\varepsilon}} + \mathbf{A} \cdot \dot{\boldsymbol{\alpha}} \geq 0.$$

The state of stress during the evolution has been decomposed as $\boldsymbol{\sigma} = \boldsymbol{\sigma}_r + \boldsymbol{\sigma}_{ir}$. Let us assume that the behavior belongs to the class of the so-called *generalized standard materials*. This ensures the existence of a potential of dissipation $d(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}})$. The potential d is a convex function of the variables, with a minimum value at the origin. The evolution of the internal state is given by the normality rule :

$$(\boldsymbol{\sigma}_{ir}, \mathbf{A}) \in \partial d(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}}),$$

this means that the subdifferential $\partial d(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}})$ of d is the set of state $(\boldsymbol{\sigma}_{ir}, \mathbf{A})$ such that:

$$d(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}}) + \boldsymbol{\sigma}_{ir} : (\boldsymbol{\varepsilon}^* - \dot{\boldsymbol{\varepsilon}}) + \mathbf{A} \cdot (\boldsymbol{\alpha}^* - \dot{\boldsymbol{\alpha}}) \leq d(\boldsymbol{\varepsilon}^*, \boldsymbol{\alpha}^*),$$

for all admissible fields $\boldsymbol{\varepsilon}^*, \boldsymbol{\alpha}^*$. The existence of such a potential for the dissipation ensures the positivity of the entropy production:

$$\boldsymbol{\sigma}_{ir} : \dot{\boldsymbol{\varepsilon}} + \mathbf{A} \cdot \dot{\boldsymbol{\alpha}} \geq d(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}}) - d(0, 0) \geq 0.$$

2. EQUILIBRIUM AND QUASISTATIC EVOLUTION

As time evolves the displacement field and the internal state must satisfy the following :

- the state equations :

$$\boldsymbol{\sigma}_r = \rho \frac{\partial w}{\partial \boldsymbol{\varepsilon}}, \quad \mathbf{A} = -\rho \frac{\partial w}{\partial \boldsymbol{\alpha}}, \quad \mathbf{s} = -\frac{\partial w}{\partial \theta},$$

- the conservation of the momentum:

$$\text{div } \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_r + \boldsymbol{\sigma}_{ir},$$

- the evolution equations of the state variables.
- all the boundary conditions.

For the overall system the rule of the free energy is replaced by the global free energy:

$$W(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\alpha}}, \bar{\theta}) = \int_{\Omega} \rho w(\boldsymbol{\varepsilon}(\mathbf{u}), \boldsymbol{\alpha}, \theta) d\omega$$

In a global description the equations of state possess the same form as in the local one, but

the state of the system is defined by *fields* of state variables. The equations of state are relationships between fields of state variables:

$$\tilde{\sigma}_r = \frac{\partial W}{\partial \tilde{\varepsilon}}, \quad \tilde{A} = -\frac{\partial W}{\partial \tilde{\alpha}}, \quad \tilde{s} = -\frac{\partial W}{\partial \tilde{\theta}},$$

These relations are obtained by the following definition: $\frac{\partial W}{\partial \tilde{q}} \bullet \tilde{q}^* = \int_{\Omega} \rho \frac{\partial w}{\partial q} q^* d\omega$. By using the properties of the characterization of the evolution of the internal state and integration over the body, we can define the dissipative function:

$$D(\tilde{\varepsilon}, \tilde{\alpha}) = \int_{\Omega} d(\dot{\varepsilon}, \dot{\alpha}) d\omega,$$

for which the evolution is given in terms of fields of state variables as :

$$(\tilde{\sigma}_{ir}, \tilde{A}) \in \partial D(\tilde{\varepsilon}, \tilde{\alpha}),$$

where the set $\partial D(\tilde{\varepsilon}, \tilde{\alpha})$ is defined obviously by :

$$D(\tilde{\varepsilon}, \tilde{\alpha}) - D(\tilde{\varepsilon}^*, \tilde{\alpha}^*) + \tilde{\sigma}_{ir} \bullet (\tilde{\varepsilon}^* - \tilde{\varepsilon}) + \tilde{A} \bullet (\tilde{\alpha}^* - \tilde{\alpha}) \leq 0, \quad \forall (\tilde{\varepsilon}^*, \tilde{\alpha}^*),$$

then we have for regular functions :

$$\frac{\partial D}{\partial \tilde{\varepsilon}} \bullet \tilde{\varepsilon}(\delta u) = \int_{\Omega} \sigma_{ir} : \varepsilon(\delta u) d\omega, \quad \frac{\partial D}{\partial \tilde{\alpha}} \bullet \delta \tilde{\alpha} = \int_{\Omega} A \cdot \delta \alpha d\omega.$$

Let us consider that the external loading derives from a potential given in terms of traction T^d applied on the external surface of the body. Then, the global free energy can be replaced by the potential energy of the system :

$$P(\tilde{u}, \tilde{\alpha}, \tilde{\theta}, T^d) = \int_{\Omega} w(\varepsilon(u), \alpha, \theta) \rho d\omega - \int_{\partial\Omega_T} T^d \cdot u da.$$

By combining all the equations in terms of fields of state variables, we can state the quasistatic evolution in a global manner by the variational system :

$$\frac{\partial P}{\partial \tilde{u}} \bullet \delta \tilde{u} + \frac{\partial D}{\partial \tilde{\varepsilon}} \bullet \tilde{\varepsilon}(\delta u) = 0, \quad \frac{\partial P}{\partial \tilde{\alpha}} \bullet \delta \tilde{\alpha} + \frac{\partial D}{\partial \tilde{\alpha}} \bullet \delta \tilde{\alpha} = 0.$$

These equations are defined on a set of admissible fields. The displacement is subject to boundary conditions $u = u^d$ over $\partial\Omega_u$. These equations are general; they contain the essential structure of a problem of quasistatic evolution. The first equation of this system explains the conservation of the momentum taking into account the constitutive law, the second explains the thermodynamic forces associated with the internal parameters.

3. THE DYNAMICAL CASE

The Hamiltonian is the total energy of the system [Stolz, 1988]:

$$H(\tilde{p}, \tilde{u}, \tilde{\alpha}, \tilde{s}, T^d) = \int_{\Omega} \frac{1}{2} \frac{p^2}{\rho} d\omega + \int_{\Omega} \rho e(u, \alpha, s) d\omega - \int_{\partial\Omega_T} T^d \cdot u da.$$

The first term is the kinetic energy $K(v) = \int_{\Omega} \frac{1}{2} p^2 / \rho \, d\omega = \int_{\Omega} \frac{1}{2} \rho v^2 \, d\omega$, $p = \rho v$ is the momentum, the second is the internal energy with the density: $e = w + \theta s$, and the last is the potential energy due to prescribed loading. The equation of motion are given by

$$\begin{aligned} \frac{\partial H}{\partial p} \bullet \delta p &= \int_{\Omega} \frac{p}{\rho} \cdot \delta p \, d\omega, \\ \frac{\partial H}{\partial u} \bullet \delta u &= \int_{\Omega} \rho \frac{\partial w}{\partial \varepsilon} : \varepsilon(\delta u) \, d\omega - \int_{\partial\Omega_T} T^d \cdot \delta u \, da \end{aligned}$$

Taking account of the decomposition of the stress $\sigma = \sigma_r + \sigma_{ir}$, of the conservation of the momentum inside the volume and of the boundary conditions

$$\operatorname{div} \sigma = \rho \gamma \text{ over } \Omega, \quad \sigma \cdot n = T^d \text{ over } \partial\Omega_T$$

we modify the expressions :

$$\frac{\partial H}{\partial u} \bullet \delta u = - \int_{\Omega} \sigma_{ir} : \varepsilon(\delta u) \, d\omega - \int_{\Omega} \rho \gamma \cdot \delta u \, d\omega,$$

then with the relations :

$$\frac{d}{dt} \int_{\Omega} p \cdot \delta u \, d\omega = \int_{\Omega} \rho \gamma \cdot \delta u \, d\omega.$$

we obtain the conservation of momentum in the Hamiltonian form:

$$\frac{\partial H}{\partial u} \bullet \delta u = - \frac{\partial D}{\partial \dot{\varepsilon}} \bullet \varepsilon(\delta u) - \frac{d}{dt} \int_{\Omega} p \cdot \delta u \, d\omega,$$

Finally, the Hamiltonian formulation of the evolution of the system is obtained:

$$\begin{aligned} \frac{\partial H}{\partial p} \bullet \delta p &= \frac{d}{dt} \int_{\Omega} u \cdot \delta p \, d\omega, \\ \frac{\partial H}{\partial u} \bullet \delta u &= - \frac{\partial D}{\partial \dot{\varepsilon}} \bullet \varepsilon(\delta u) + \frac{d}{dt} \int_{\Omega} p \cdot \delta u \, d\omega, \\ \frac{\partial H}{\partial \alpha} \bullet \delta \alpha &= - \frac{\partial D}{\partial \dot{\alpha}} \bullet \delta \alpha, \\ \frac{\partial H}{\partial s} \bullet \delta s &= \int_{\Omega} \rho \theta \delta s \, d\omega. \end{aligned}$$

A conduction law must be given and the positivity of the entropy production must be verified to determine the evolution of the system :

$$\frac{d}{dt} \int_{\Omega} \rho s \, d\omega + \int_{\partial\Omega} \frac{q \cdot n}{T} \, da \geq 0.$$

For the real motion, the value of the Hamiltonian is the sum of the kinetic energy, of the internal energy and of the potential energy of the external (given) load. The conservation of the energy of the system can be easily rewritten as

$$\frac{dH}{dt} - \frac{\partial H}{\partial T^d} \cdot \dot{T}^d = - \int_{\partial\Omega} q \cdot n \, da,$$

where q is the heat flux, and we consider that no external volume heat source are prescribed.

The definition of the Hamiltonian can be extended to generalized media. The proposed description can be performed in all the cases in which we can define the behavior by two potentials: a global free energy and a dissipative function. If some particular internal constraints exist, this description must be revised.

4. MECHANICAL TRANSFORMATIONS ALONG MOVING SURFACES

We consider a moving interface along which mechanical transformation occurs [Pradeilles-Duval et al, 1995]. Two materials coexist at any time in the structure and the body is heterogeneous. The evolution of the surface along which the transformation takes place is characterized in the energy analysis. Some connections can be made with the notion of configurational forces, [Gurtin, 1995, Maugin, 1995, Truskinovski, 1987, Grinfeld, 1980, 1991].

Let Ω denote the domain, composed of two distinct volumes Ω_1 and Ω_2 which are occupied by two materials with different mechanical properties. The perfect interface between them is assumed to be regular and is denoted by Γ . Material 1 changes to material 2 along Γ by an irreversible process. Hence Γ moves with a normal velocity ϕ positive along Γ . The state of the system is characterized by the displacement field u , from which a strain field is derived ϵ . The other parameters are the temperature θ , the internal parameters α and the position of the boundary Γ .

When the surface Γ propagates, with velocity $c = \phi N$, (N normal outward to Ω_2), mechanical quantities can have a jump, ($[f] = f_1 - f_2$) and all volume integrals ($F = \int_{\Omega} f d\omega$) have rates defined by :

$$\dot{F} = \int_{\Omega} \dot{f} d\omega - \int_{\Gamma} [f] c \cdot N da.$$

The mass conservation is defined by the continuity of the mass flux :

$$m = \rho c \cdot N = \rho \phi.$$

Then the conservation of energy and the entropy production are rewritten as

$$\int_{\Omega} (\dot{e} + \gamma \cdot v) \rho d\omega - \int_{\Gamma} [e + \frac{1}{2} v^2] m da = - \int_{\partial\Omega} q \cdot n da + P_{ext},$$

$$\int_{\Omega} \rho \dot{s} d\omega - \int_{\Gamma} [s] m da + \int_{\partial\Omega} \frac{q \cdot n}{T} da \geq 0.$$

By the momentum conservation we have

$$P_{ext} = \int_{\Omega} \sigma : \dot{\epsilon} d\omega + \int_{\Gamma} N \cdot [\sigma \cdot v] da + \int_{\Omega} \rho \gamma \cdot v d\omega.$$

This is true for all volume Ω then we deduce the local equations of conservation :

$$\rho \dot{e} = \sigma : \dot{\epsilon} - \text{div} q,$$

$$0 = m[e + \frac{1}{2}v^2] + N \cdot [\sigma \cdot v] - [q] \cdot N.$$

The entropy production takes the form:

$$\int_{\Omega} (\rho \dot{s} + \frac{\text{div} q}{\theta}) - \frac{q \cdot \nabla \theta}{\theta^2} d\omega + \int_{\Gamma} (-[s] m + [\frac{q}{\theta}] \cdot N) da \geq 0.$$

The interface is perfect, then the displacement is continuous along the interface $[u] = 0$, and the temperature is assumed to be continuous $[\theta] = 0$.

Some dissipation can occur along the moving surface. The mechanical discontinuities must satisfy some constraints, they must be kinematically admissible and ensure the positivity of the entropy production. The jumps of the mechanical quantities must verify the Hadamard equations:

$$[v] + [\nabla u] \cdot c = 0, [\dot{\theta}] + [\nabla \theta] \cdot c = 0,$$

and the momentum equation:

$$[\sigma] \cdot N + m[v] = 0.$$

Combining the local equations of conservation, we rewrite the production of entropy in terms of volume and surface contribution:

$$D_{\Omega} = \sigma : \dot{\varepsilon} - \rho(\dot{w} + s\dot{\theta}) - \frac{q \cdot \nabla \theta}{\theta^2}, \forall x \in \Omega,$$

$$D_{\Gamma} = \frac{1}{\theta}(\rho[w]c \cdot N - N \cdot \bar{\sigma} \cdot [\nabla u] \cdot c) = \frac{G_s}{\theta} \phi, \forall x \in \Gamma,$$

where the quantity $\bar{\sigma}$ is $\frac{1}{2}(\sigma_1 + \sigma_2)$. Along the surface, the production of entropy is defined in a similar form as in a quasistatic thermomechanical coupled evolution by replacing the tension along the surface by the mean tension, and as in an isothermal analysis the results of Abeyaratne and Knowles [Abeyaratne et al.,1990].

The behavior of each phase is defined by the free energy w_i as a function of strain ε , temperature θ and a set of internal variables α , the evolution of which is governed by a pseudo potential of dissipation $d_i(\dot{\alpha})$, a convex function of $\dot{\alpha}$. As before, the state equations are

$$\sigma = \rho \frac{\partial w_i}{\partial \varepsilon}, s = -\frac{\partial w_i}{\partial \theta}, A = -\rho \frac{\partial w_i}{\partial \alpha},$$

where A , the thermodynamical forces associated with the internal parameter α satisfies : $A = \partial d_i / \partial \dot{\alpha}$. The dissipation due to conduction is given by a conduction law.

As before, the variation of the Hamiltonian H determines the power heat supply. We decompose the volume Ω into the two volumes Ω_i (n_i the normal outward to Ω_i), the position Γ of the surface is an internal variable and the Hamiltonian takes the form:

$$H(\bar{u}, \bar{p}, \bar{\alpha}, \bar{s}, \Gamma, T^d) = H_1 + H_2 - \int_{\partial \Omega_T} T^d \cdot u da,$$

$$\text{where } H_i = \int_{\Omega_i} \frac{1}{2} \frac{p^2}{\rho} d\omega + \int_{\Omega_i} \rho e(\varepsilon(u), \alpha, s) d\omega,$$

The equations of motion are then

$$\begin{aligned}\frac{\partial H_i}{\partial p} \cdot \delta p &= \int_{\Omega_i} \mathbf{v} \cdot \delta \mathbf{p} \, d\omega, \\ -\frac{\partial H_i}{\partial \mathbf{u}} \cdot \delta \mathbf{u} &= \int_{\Omega_i} \rho \boldsymbol{\gamma} \cdot \delta \mathbf{u} \, d\omega + \int_{\partial \Omega_i} \mathbf{n}_i \cdot \boldsymbol{\sigma} \cdot \delta \mathbf{u} \, da.\end{aligned}$$

Each volume has a contribution to the global Hamiltonian:

$$\frac{dH_i}{dt} = \int_{\partial \Omega_i} \mathbf{n}_i \cdot \boldsymbol{\sigma} \cdot \mathbf{v} \, da - \int_{\Omega_i} (-A \cdot \dot{\boldsymbol{\alpha}} + \rho \theta \dot{s}) \, d\omega + \int_{\Gamma} \left(\frac{1}{2} \frac{p^2}{\rho} + \rho e \right) \mathbf{c} \cdot \mathbf{n}_i \, da.$$

And for the overall system we obtain the equation:

$$\begin{aligned}\frac{dH}{dt} - \frac{\partial H}{\partial T^d} \cdot \dot{T}^d &= \frac{\partial H}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} + \frac{\partial H}{\partial s} \cdot \dot{s} - \int_{\Gamma} [e + \frac{1}{2} v^2] \mathbf{m} \, da - \int_{\Gamma} N \cdot [\boldsymbol{\sigma} \cdot \mathbf{v}] \, da \\ &= - \int_{\Omega} \text{div} \mathbf{q} \, d\omega - \int_{\Gamma} [q] \cdot N \, da.\end{aligned}$$

Making the distinction between volume and surface terms, we find

$$\begin{aligned}\frac{\partial H}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} + \frac{\partial H}{\partial s} \cdot \dot{s} &= - \int_{\Omega} A \cdot \dot{\boldsymbol{\alpha}} \, d\omega + \int_{\Omega} \rho \theta \dot{s} \, d\omega = - \int_{\Omega} \text{div} \mathbf{q} \, d\omega, \\ \frac{\partial H}{\partial T} \cdot \dot{T} &= - \int_{\Gamma} G_{th} \phi \, da = - \int_{\Gamma} [q] \cdot N \, da.\end{aligned}$$

The gradient of the Hamiltonian with respect to the position of the moving surface determines the intensity of the heat source due to the propagation of mechanical discontinuities. This gradient takes the form of a release rate of internal energy :

$$\mathbf{G}_{th} = \rho [e] - N \cdot \bar{\boldsymbol{\sigma}} \cdot [\nabla \mathbf{u}] \cdot N.$$

The production of entropy has a surface term which is explained as

$$\int_{\Gamma} (-[s] \mathbf{m} + [\frac{q}{\theta}] \cdot N) \, da = \int_{\Gamma} \frac{G_s}{\theta} \phi \, da.$$

In the same spirit, the intensity of the source of entropy production is a release rate of free energy $\mathbf{G}_s = \rho [w] - N \cdot \bar{\boldsymbol{\sigma}} \cdot [\nabla \mathbf{u}] \cdot N$, divided by the temperature. Without more hypotheses this term is not directly connected with the variation of the Hamiltonian.

In the isothermal case, the dissipation and the heat sources are related by the uniform temperature, the heat flux is zero and $\mathbf{G}_{th} = \mathbf{0}$. The dissipation is a jump of entropy along the moving surface given by \mathbf{G}_s ; defining the isothermal Hamiltonian by

$$\hat{H} = \int_{\Omega} \frac{p^2}{\rho} \, d\omega + \int_{\Omega} \rho (w(\boldsymbol{\varepsilon}(\mathbf{u}), \boldsymbol{\alpha})) \, d\omega - \int_{\partial \Omega_T} T^d \cdot \mathbf{u} \, da;$$

the dissipation is expressed by the variation of the isothermal Hamiltonian:

$$\frac{d\hat{H}}{dt} - \frac{\partial \hat{H}}{\partial T^d} \cdot \dot{T}^d = \frac{\partial \hat{H}}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} - \int_{\Gamma} \{ [w + \frac{1}{2} v^2] \mathbf{m} + [N \cdot \boldsymbol{\sigma} \cdot \mathbf{v}] \} \, da.$$

By considering the surface and volume terms, we see that the energy release rate is the ther-

modynamical force associated with the velocity of Γ , and is the derivative of the Hamiltonian with respect to the position of the surface. The expression G_s is recovered.

5. QUASISTATIC EVOLUTION

In isothermal evolution, complementary relations must be considered to describe irreversibility. An energy criterion is chosen as a generalized form of the well known Griffith theory. Then, we assume

$$\phi \geq 0, \text{ if } G = G_c \text{ on } \Gamma, \phi = 0, \text{ otherwise.}$$

This is a local energy criterion. At each equilibrium state, the interface Γ can be decomposed into two subsets where the propagation is either possible or not. Let denote by Γ^+ , the subset of Γ where the critical value G_c is reached. The evolution of the interface is governed by the consistency condition, during the evolution of Γ ; if, at the geometrical point $\mathbf{x}_\Gamma(t)$, the criterion is reached

$$G(\mathbf{x}_\Gamma(t), t) = G_c,$$

then the derivative of G following the moving surface vanishes $D_\phi G = 0$. This leads to the consistency condition written for all point inside Γ^+ :

$$(\phi - \phi^*) D_\phi G \geq 0, \forall \phi^* \geq 0, \text{ over } \Gamma^+;$$

otherwise $\phi = 0$. With Hadamard relations this derivative takes on the final form

$$D_\phi G = [\sigma] : \nabla v_1 - \dot{\sigma}_2 : [\nabla u] - \phi K$$

$$K = t \cdot \text{div}_\Gamma \sigma_2 \cdot [\nabla u] \cdot N - t \cdot \sigma_2 \cdot \nabla([\nabla u] \cdot N) + [\sigma : \nabla \varepsilon \cdot N] - N \cdot \sigma \cdot (\nabla \nabla u \cdot N) \cdot N,$$

where $\text{div}_\Gamma \sigma_2 = \text{div} \sigma_2 - N \cdot \nabla \sigma_2 \cdot N$. In that case, the evolution is determined by the functional :

$$\begin{aligned} F(v, \phi, \dot{T}^d) &= \int_\Omega \frac{1}{2} \varepsilon(v) : \frac{\partial^2 w}{\partial \varepsilon \partial \varepsilon} : \varepsilon(v) \, d\omega - \int_{\partial \Omega_T} \dot{T}^d \cdot v \, da \\ &\quad + \int_\Gamma \phi [\sigma] : \nabla v_1 + \frac{\phi^2}{2} K \, da \end{aligned}$$

Then the evolution is given by

$$\frac{\partial F}{\partial v} * (v - v^*) + \frac{\partial F}{\partial \phi} \cdot (\phi - \phi^*) \geq 0$$

for all v^* kinematically admissible field, and $\phi^*(s) \geq 0$ along Γ^+ . The discussion of the stability and bifurcation along an evolution process can be now investigated as proposed by Pradeilles and Stolz [Pradeilles et al, 1995]. Consider the rate of displacement v solution of the boundary value problem for any given velocity ϕ of propagation, v satisfies:

$$\text{div} \dot{\sigma} = 0, \dot{\sigma} = \frac{\partial^2 w}{\partial \varepsilon \partial \varepsilon} : \varepsilon(v), \text{ inside } \Omega,$$

$$v = v^d, \text{ on } \partial\Omega_u, \dot{\sigma}.N = \dot{T}^d \text{ on } \partial\Omega_\sigma,$$

and non classical boundary conditions on Γ :

$$D_\phi(\sigma.N) = 0, D_\phi[u] = [v] + \phi[\nabla u].N = 0.$$

Consider the value W of F for this solution $v(\phi, \dot{T}^d)$ then $W(\phi, \dot{T}^d) = F(v(\phi, \dot{T}^d), \phi, \dot{T}^d)$, and the stability of the actual state is determined by the condition of the existence of a solution

$$\delta\phi \cdot \frac{\partial^2 W}{\partial\phi\partial\phi} \cdot \delta\phi \geq 0, \delta\phi \geq 0 \text{ on } \Gamma^+, \delta\phi \neq 0,$$

and the uniqueness and non bifurcation is characterized by

$$\delta\phi \cdot \frac{\partial^2 W}{\partial\phi\partial\phi} \cdot \delta\phi \geq 0, \delta\phi \neq 0 \text{ on } \Gamma^+.$$

6. THE CANONICAL EQUATIONS OF SHOCK WAVES.

The local equations of shock waves will be derived from a thermodynamical potential and a dissipation pseudopotential. The canonical equations rule the jump relations and the constitutive behavior in a section of the shock [Germain, 1972]. Let us consider a shock wave, we propose to study the evolution of the shock. Locally the surface of discontinuity is replaced by its tangent plane, and one considers a frame moving with a velocity ϕ which is the normal speed of the shock. Along the line of discontinuities, some relationships between the jumps of quantities must be verified:

- for the momentum :

$$[\sigma].N + m[v] = 0,$$

- for the energy :

$$-[q].N + m[\frac{1}{2}v^2 + e] + N.[\sigma.v] = 0,$$

- for the entropy production :

$$-m[s] + [\frac{q}{\theta}].N \geq 0.$$

The quantity m denotes the mass flux and accounts for the mass conservation. The shock is governed by the constants mV^d, mQ^d which are related respectively to the flux of momentum and to the flux of energy. The jump conditions are rewritten as

$$\begin{aligned} mV^d &= \sigma^\pm.N - mv^\pm, \\ -mQ^d &= -q^\pm.N + m(\frac{1}{2}v^2 + e)^\pm - N.\sigma^\pm.v^\pm. \end{aligned}$$

The main problem is to determine the state (-) if the state(+) and the constant mV^d, mQ^d are given while respecting the positivity of the entropy production in an anelastic material. The jump conditions give us only the jump of entropy, but no direct relation between this

discontinuity and the jump of internal parameters. One must determine the loading path or the history of all the quantities inside the shock; this describes the internal structure of the shock.

To solve this problem we can consider the discontinuity surface as a layer normal to the direction of the propagation of the shock ; one has to study the inner expansion of all the quantities in a continuous process in the frame translating with the shock surface, assuming that all quantities depend only on the local normal coordinate $X = x - \phi t$. For the inner expansion, X varies from $-\infty$ to $+\infty$. We are interested in a one dimensional motion.

A constitutive law and a pseudo-potential of dissipation being given to describe the internal behavior, the dissipation is known inside the shock and therefore the jump of entropy is given as

$$-m[s] + \left[\frac{q}{\theta}\right].N = \int_{-\infty}^{+\infty} \left(\frac{D_m}{\theta} - \frac{q \cdot \text{grad}\theta}{\theta^2}\right) dx \geq 0.$$

Using the other jump conditions expressed in terms of the given constant of the shock, we can rewrite the jump of entropy as

$$mQ^d \left[\frac{1}{\theta}\right] + mV^d \cdot \left[\frac{v}{\theta}\right] + m \left[\frac{(w - \frac{1}{2}v^2)}{\theta}\right] = \int_{-\infty}^{+\infty} \left(\frac{D_m}{\theta} - q \cdot \frac{\text{grad}\theta}{\theta^2}\right) d\omega.$$

This defines the shock generating function P :

$$P = \frac{mQ^d}{\theta} + mV^d \cdot \frac{v}{\theta} + m \frac{(w - \frac{1}{2}v^2)}{\theta},$$

in the steady state analysis, $\dot{f} = \phi f_{,x}$, and P has the following form:

$$P(u_{,x}, \alpha, \theta) = \frac{mQ^d}{\theta} + mV^d \cdot \frac{\phi u_{,x}}{\theta} + m \frac{(w - \frac{1}{2}\phi^2 u_{,x}^2)}{\theta}.$$

The jump of P is the total dissipation:

$$P(x^+) - P(x^-) = \int_{-\infty}^{+\infty} \left(\frac{D_m}{\theta} - q \cdot \frac{\text{grad}\theta}{\theta^2}\right) dX$$

The function P is supposed to be a continuous function of X , and the value of P on a section dX has the following form:

$$PdX = m \frac{Q}{\theta} dX + \frac{mV^d}{\theta} \cdot (v(X + dX) - v(X)) + \frac{1}{\theta} m (w - \frac{1}{2}v^2) dX.$$

Then P is related to the Lagrangian defined on the section dX :

$$L = \left(\frac{1}{2}v^2 - w\right) m dX - mV^d \cdot [v]_X^{X+dX}$$

Defining the dissipative function D as previously :

$$D(\varepsilon(X), \alpha(X), \theta(X)) = \frac{1}{\theta} (d(\phi \varepsilon_{,x}, \phi \alpha_{,x}) + \frac{1}{2} \frac{K}{\theta} (\theta_{,x})^2),$$

we adopt a Fourier law for the thermal conduction $q = -K \cdot \text{grad}\theta$.

The shock structure is determined by the canonical equations :

$$\frac{\partial P}{\partial \theta} = \frac{\partial D}{\partial \theta_{,x}}, \quad \frac{\partial P}{\partial u} = \frac{\partial D}{\partial u_{,x}}, \quad \frac{\partial P}{\partial \alpha} = \frac{\partial D}{\partial \alpha_{,x}},$$

and we obtain the local property

$$\frac{dP}{dX} = \frac{D_m}{\theta} - q \cdot \frac{\text{grad}\theta}{\theta^2}.$$

If the temperature is continuous i.e. $[\theta] = 0$, the jump of P is exactly related to the definition of G_s . If a continuous process governs the internal structure of the discontinuity, the quantity G_s is a global characteristic of the moving discontinuity. When local behavior is given in term of w and D , the behavior of all the jumps are given. This is a way to build global behavior for shock waves or moving discontinuities inside a continuum. It is the analogue of homogenization for dynamical behavior.

A typical example has been given in plasticity. In this case the determination of compatible states (+) and (-) is not easily studied from a general viewpoint. For propagation of longitudinal waves, if we suppose that the loading process is monotonic, we obtain a curve which gives the relation between the jump of the quantities, as in the adiabatic Hugoniot curve in gas dynamics [Mandel, 1978]. This result is obtained by the assumption of a radial loading path during the shock. This is the structure of the shock. But in a general case, the internal structure for shock wave in plasticity must be studied as proposed by Germain and Lee [Germain et al., 1973].

7. CONCLUSIONS

We have studied the thermodynamics of running discontinuities from a global point of view and related all the quantities to a Hamiltonian principle generalized to nonlinear behavior. In quasistatic evolution we have given a boundary value problem for the evolution of a moving surface, the motion being governed by an energy criterion. Some connections with fracture mechanics can be also given in the same formalism [Stolz et al, 1996; Bui et al, 1987]. Finally the internal structure of discontinuities has been investigated to provide a global behavior of the moving surface in agreement with the positivity of the production of entropy.

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