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The Method of Virtual Power in Continuum Mechanics. Application to Media Presenting Singular Surfaces and Interfaces

By

N. Daher, Besançon, and **G. A. Maugin**, Paris, France

With 2 Figures

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Summary

The work develops the principle of virtual power for finite velocity fields for so-called simple materials (or first-gradient theory) without further constitutive assumptions when the body is swept out by a singular surface which is either a *free* singular surface (such as usual strong discontinuities of continuum mechanics) or a *thermodynamical* singular surface (a so-called interface between phases). The formulation given on exemplary cases first shows how to systematically construct the new "internal" contact forces which exist at the discontinuity, as well as the new inertial contributions which arise from mass transfer across the singular surface and the acceleration of particles attached to it. Then it is shown how various virtual velocity fields generate all the dynamical field equations as well as transversality conditions when the description of external forces allows for them. The principle of virtual power here is so formulated that, when combined, for *real* velocity fields, with the first principle of thermodynamics in global form, it yields directly the so-called energy theorem both in the bulk and at the singular surface. Then the corresponding rates of entropy production are deduced after introduction of the second principle of thermodynamics. While one does not claim to obtain here essentially new equations, the present formulation of the principle of virtual power paves the way for useful complex extensions which are difficult to deal with through other avenues (e.g., electromagnetic continua with "junctions" such as piezoelectric semiconductors).

1. Introduction

Several authors [1], [2], [3] have pointed out the interest of using the energy method known as the "principle of virtual power" (for finite velocity fields rather than infinitesimal displacements) rather than the classical "vectorial approach" based on the statement of global or local balance laws, in the description of some phenomenological theories. This method of deducing field equations of a mechanistic nature is particularly suited to the case of complex continua such as those exhibiting a microstructure as also electromagnetic continua. However, this type of formulation does not seem to have been given for continuous media swept out by singular surfaces and/or lines. The aim of this paper is precisely the extension of the formulation of the principle of virtual power, using finite velocity fields, to describe this kind of situation, thus giving to that principle a range of application as wide as that of the classical vectorial approach while, of course, it retains all the advantages which it already owns in so far as field equations and further thermodynamical considerations are concerned.

It is salient to recall what do we understand here by a singular surface. It may be a strong discontinuity in the well known sense granted in continuum mechanics (e.g., a shock; this is a mathematical modelization of a thin transition zone across which steep gradients of field quantities accompanied by dissipative processes occur). More interesting for our purpose is the case of an *interface* between two phases which, in many cases, can also be conveniently simulated by a strong discontinuity, but the latter then has *material* properties (surface densities, velocity field, internal energy, temperature, entropy) in the same way as the bulk phases exhibit such material properties: a material surface is embedded in a three dimensional domain and splits it in two domains of which the material fields may suffer discontinuity across the said surface. In this case the balance equations for the surface material densities are also boundary conditions — jump relations — for the bulk parameters. These new balance equations can be stated by analogy with bulk balance equations, in addition accounting for fluxes from the adjacent three dimensional domains [4], [7]. Another method is to integrate bulk equations that describe the behavior of matter in the thin interphase layer over the thickness of the said layer and thereby obtain balance laws for so-called *true* and *excess* (surface) quantities [8] (also [13]).

The extension of the formulation of the principle of virtual power to the case of bodies swept out by strong discontinuities which model shock-like discontinuities or interfaces may be tackled from various sides, but we choose the one that seems the most natural. We shall not repeat here the basic arguments given elsewhere (e.g. in [3]). We only need to recall that a virtual power is a linear continuous form on a set of virtual velocities. The dual quantity to a "velocity" is a "force". The selection of a space of admissible velocities fixes, via this duality, the degree of refinement of the description of forces acting on the system. For so-called *internal forces* for which one ultimately needs to construct constitutive equations we suppose that the principle of objectivity applies, which, in turn, implies that the dual "velocity field" is objective [1], [2], [3]. This is what distinguishes "internal forces" from other types of forces in continuum mechanics. We start the present study by considering the simple purely mechanical quasistatic example (i.e., in the absence or neglect of acceleration in the bulk and mass transfer across the singular surface) and focus the attention on the double-faceted nature of the "new power" (internal or contact) due to the interaction between the three dimensional domain and the singular surface. Then we give a systematic procedure to construct the relevant virtual power by introducing a relative velocity field which, in a way, complements the objective velocity field (e.g., the rate-of-strain tensor) introduced in regular domains [3]. This procedure will allow one to enlarge, without further difficulty, the field of application of the principle to more involved mechanical and electromagnetic cases.

The first extension given here consists of the study of a purely mechanical continuum that contains a material deformable singular surface (which we later call a *thermodynamical singular surface* or *interface*). In this case the three surface balance laws or conditions (two jump conditions and one transversality condition) are deduced in a natural way from the principle of virtual power, while they must be somewhat postulated in the vectorial approach. Moreover, the combination of the principle of virtual power (for real velocity fields) with the global statement of the first principle of thermodynamics yields directly the *energy theorem* in global form, which exhibits the economy of thought in the present approach. We conclude with the thermodynamics that follows straigthforwardly thereoff. Although none of the resulting equations is new, we think that the methodology is very valuable and suits the mathematically oriented professional. Further works in fact will develop the usually messy case of electrodynamics (compare [9]) and the exemplary case of elastic piezoelectric semiconductors in which junctions are considered as thermodynamical singular surfaces and where the method proves its efficiency by providing heretofore unknown equations[1].

2. Notation

We use the classical notation of nonlinear continuum mechanics [3] either in rectangular tensor components or in intrinsic notation. The three dimensional body B occupies the simply connected open set D of physical Euclidean space E^3 at time t. An absolute Newtonian chronology is used. The unit outward normal to ∂D, the regular boundary of D, is noted $\boldsymbol{n}$. All subsequent reasonings are made in the present (Eulerian) configuration of the body.

Let $\Sigma(t)$ be a singular surface which sweeps out D, having absolute, non material (with respect to the matter of B), velocity $\boldsymbol{v}$ with respect to a fixed Galilean frame R_G and unit oriented normal $\boldsymbol{N}$. The unit binormal to $\partial\Sigma$, the boundary of $\Sigma(t)$ on ∂D (cf. Fig. 1), is noted $\boldsymbol{\tau}$. We indicate by $\gamma(t)$ a singular curve on $\Sigma(t)$ moving with the absolute velocity $\hat{\boldsymbol{v}}$ with respect to R_G and having unit binormal $\boldsymbol{\Lambda}$ and tangent $\boldsymbol{K}$.

[1] A brief note on the subject has already been published [10].

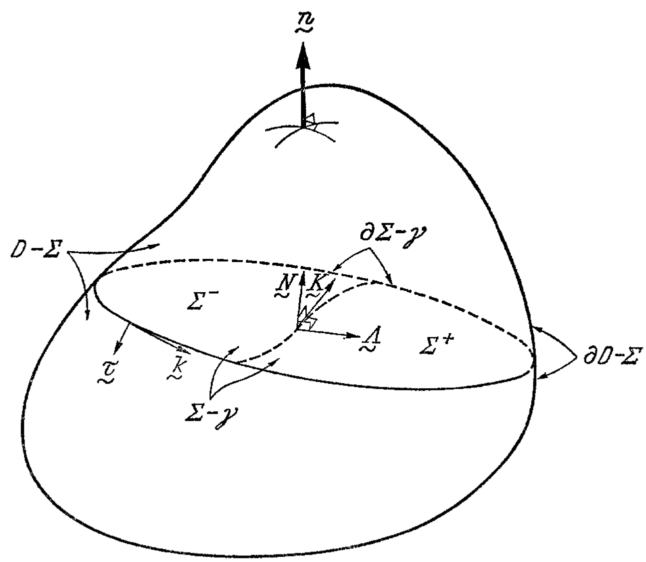


Fig. 1

The absolute particle velocities of "particles" belonging to D and $\Sigma(t)$ are noted $\boldsymbol{v}$ and $\hat{\boldsymbol{v}}$, respectively, or v_i and $\hat{v}_i$ in Cartesian components. The Einstein summation convention on dummy indices is understood. We have the

Definition. — A *singular surface* (line) *is called a* thermodynamical *singular surface* (line) *or* interface *if material quantities are attached to that surface* (line), *hence a surface* (line) *density of energy can be defined on it. Otherwise it is said to be* free.

Note that

$$\hat{v}_i - v_i = {}^{\Sigma}\hat{v}_i \tag{2.1}$$

is the velocity of a material "particle" that belongs to $\Sigma(t)$, with respect to $\Sigma(t)$, so that in the case of a free singular surface $\hat{\boldsymbol{v}}$ reduces to $\boldsymbol{v}$. On the other hand we always have

$$\hat{\boldsymbol{v}} \cdot \boldsymbol{N} = \boldsymbol{v} \cdot \boldsymbol{N} \tag{2.2}$$

since ${}^{\Sigma}\hat{\boldsymbol{v}}$ is tangent to Σ (equivalently, its normal component vanishes ${}^{\Sigma}\hat{\boldsymbol{v}} \cdot \boldsymbol{N} = 0$).

The cut of the material body D by a singular surface $\Sigma(t)$ requires the introduction of the following notation. D^+ and D^- are two non-material subregions (cf. Fig. 1) such as $D = D^+ \oplus \Sigma \oplus D^-$. Then the material velocity $\boldsymbol{v}$ is defined as follows

$$\boldsymbol{v}^{\pm} = \begin{cases} \boldsymbol{v}H(D^{\pm}) & \text{if} \quad \boldsymbol{x} \in D^{\pm} \\ \boldsymbol{v} & \text{if} \quad \boldsymbol{x} \in \partial D^{\pm} \\ \text{uniform limit of } \boldsymbol{v}(D^{\pm}) \text{ for } D^{\pm} \ni \boldsymbol{x} \to \Sigma^{\pm} \text{ along } \boldsymbol{N}^{\pm} \end{cases} \tag{2.3}$$

where H is the characteristic (Heaviside) function of a set.

When the two subregions are glued back together we adopt the following notation which is self explanatory (cf. Fig. 2)

$$D^+ \oplus D^- \leftrightarrow D - \Sigma, \qquad \partial D^+ \oplus \partial D^- \leftrightarrow \partial D - \Sigma, \qquad \Sigma^\pm \leftrightarrow \Sigma \tag{2.4}$$

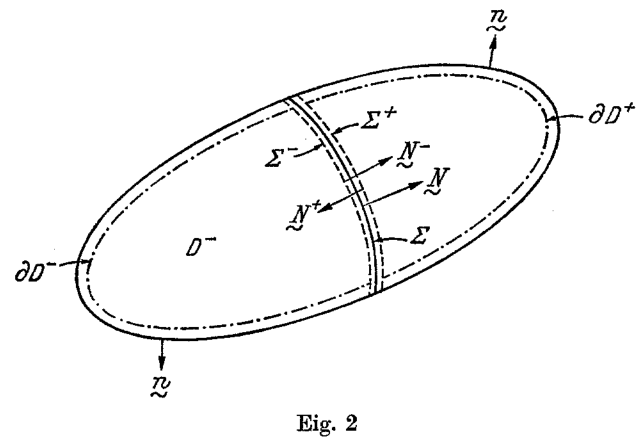
the latter with a unique choice of the normal oriented from the $(-)$ to the $(+)$ side of Σ, i.e., $\boldsymbol{N} = \boldsymbol{N}^- = -\boldsymbol{N}^+$.

The symbolisms $[\![\ldots]\!]$ and $\langle\ldots\rangle$ indicate, respectively, the jump and the mean value of their enclosures across, or at, $\Sigma(t)$, i.e.,

$$[\![A]\!] = A^+ - A^-, \qquad \langle A\rangle = \frac{1}{2}(A^+ + A^-) \tag{2.5}$$

where $A^\pm$ are the uniform limits of a field A ($\boldsymbol{x} \in D^\pm$) at $\boldsymbol{x} \in \Sigma(t)$ in approaching $\Sigma(t)$ on its faces $\Sigma^\pm$ along the normals $\boldsymbol{N}^\pm$.

When $\Sigma(t)$ presents a singular line we use the same notation as the one introduced above but we replace $\boldsymbol{v}^\pm$ by $\hat{\boldsymbol{v}}^\pm$, $A^\pm$ by $\hat{A}^\pm$, $D^\pm$ by $\Sigma^\pm$, $\partial D^\pm$ by $\partial\Sigma^\pm$, $\Sigma^\pm$ by $\gamma^\pm$ and $\boldsymbol{N}$ by Λ, where, if A denotes a field defined in the bulk, $\hat{A}$ is the equivalent field on the surface Σ.



Eig. 2

3. The Principle of Virtual Power in Presence of a Free Singular Surface

3.1 Quasi-Static Mechanical Example

In order to apply the principle of virtual power to a discontinuous material region we cut the medium in two subregions D^+ and D^- by the *non* material singular surface $\Sigma(t)$ having absolute velocity $\boldsymbol{v}$. We construct the expressions of virtual powers in D^+, D^- and on ∂D^+, ∂D^-, Σ^+ and Σ^- by using the method (the "recipes") known for regular three dimensional regions [3]. Then we glue back together the two subregions.

The expressions of various powers are (cf. [3] and note (ii) below)

$$P_i^*(D^-) = -\int_{D^-} \sigma_{ij}^- D_{ij}^{-*}\, dv, \qquad P_i^*(D^+) = -\int_{D^+} \sigma_{ij}^+ D_{ij}^{+*}\, dv \tag{3.1}$$

$$P_d^*(D^-) = \int_{D^-} (f_i^- v_i^{-*} + \phi_{ij}^- v_{i,j}^{-*})\, dv, \qquad P_d^*(D^+) = \int_{D^+} (f_i^+ v_i^{+*} + \Phi_{ij}^+ v_{i,j}^{+*})\, dv \tag{3.2}$$

$$P_c^*(\partial D^-) = \int_{\partial D^-} T_i^- v_i^{-*}\, da, \qquad P_c^*(\partial D^+) = \int_{\partial D^+} T_i^+ v_i^{+*}\, da \tag{3.3}$$

$$P_c^*(\Sigma^-) = \int_{\Sigma^-} \mathcal{T}_i^- (v_i^{-*} - \nu_i^*)\, da, \qquad P_c^*(\Sigma^+) = -\int_{\Sigma^+} \mathcal{T}_i^+ (v_i^{+*} - \nu_i^*)\, da \tag{3.4}$$

where we employed the convention (2.3) and correspondingly attributes a (+) or (−) superscript to the generalized forces introduced by duality. These forces, $\sigma_{ij}^\pm$, $f_i^\pm$, $\Phi_{ij}^\pm$, $T_i^\pm$ and $\mathcal{T}_i^\pm$, are, respectively, a symmetric intrinsic stress tensor, volume forces, volume "double" forces, and surface tractions at $\partial D^\pm$ or $\Sigma^\pm$. $(D_{ij}^\pm)^*$ is the strain tensor built from $(v_i^\pm)^*$ where an asterisk denotes a virtual field or the value of an expression in such a field. We have the following notes.

Note (i). — The choice of signs in the expression of powers is a question of convenience. Nevertheless, a simple physical interpretation may be given to justify this notation. Indeed, $P_i^*(D^\pm)$ is the power developed by the internal forces which are opposed to deformation ($P_i^* = -P_{\text{def}}^*$), while the opposite signs in the new contribution $P_c^*(\Sigma^\pm)$ are due to the fact that the traction forces are exerted on either side of Σ.

Note (ii). — The presence of relative velocities in the expression of $P_c^*(\Sigma^\pm)$ is due to the fact that the singular surface is *non* material. In the absence of $\Sigma(t)$ we have $\boldsymbol{v}^+ = \boldsymbol{v}^- = \boldsymbol{v}$ and $P_c^*(\Sigma^\pm) = 0$.

It is obvious that when we put the two subregions D^+ and D^- back together the contact forces on $\Sigma^\pm$ become *internal forces* for the whole system, so that the principle of virtual power, for an absolute Newtonian chronology but in quasi-statics (inertial terms discarded), takes the following form

$$0 = P_i^*(D^+ \oplus D^- \oplus \Sigma) + P_d^*(D^+ \oplus D^-) + P_c^*(\partial D^+ \oplus \partial D^-) \tag{3.5}$$

with

$$P_i^*(D^+ \oplus D^- \oplus \Sigma) = P_i^*(D^+ \oplus D^-) + P_i^*(\Sigma) \tag{3.6.1}$$

$$P_i^*(\Sigma) = P_c^*(\Sigma^+) + P_c^*(\Sigma^-) \tag{3.6.2}$$

$$\begin{gathered} P_k^*(\Omega^+ \oplus \Omega^-) = P_k^*(\Omega^+) + P_k^*(\Omega^-); \qquad k = i, d, c; \\ \Omega^\pm = (D^\pm \text{ or } \partial D^\pm). \end{gathered} \tag{3.6.3}$$

Accounting for the notation

$$\int_{D-\Sigma} A\, dv = \int_{D^+} A^+\, dv + \int_{D^-} A^-\, dv \tag{3.7}$$

$$\int_{\partial D-\Sigma} B\, da = \int_{\partial D^+} B^+\, da + \int_{\partial D^-} B^-\, da \tag{3.8}$$

$$\int_{\Sigma} [\![C]\!]\, da = \int_{\Sigma^-} [\![C]\!]\, da = -\int_{\Sigma^+} C^+\, da - \int_{\Sigma^-} C^-\, da = \int_{\Sigma^-} (C^+ - C^-)\, da, \tag{3.9}$$

the latter in reason of the fact that $\Sigma = \Sigma^-$ and $\boldsymbol{N} = \boldsymbol{N}^- = -\boldsymbol{N}^+$, we can transform Eq. (3.5) to

$$0 = P_i^*(D - \Sigma) + P_i^*(\Sigma) + P_d^*(D - \Sigma) + P_c^*(\partial D - \Sigma) \tag{3.10}$$

where

$$P_i^*(D - \Sigma) = -\int_{D-\Sigma} p_i^*\, dv, \qquad p_i^* = \sigma_{ij} D_{ij}^* \tag{3.11}$$

$$P_i^*(\Sigma) = -\int_{\Sigma} {}^{\Sigma}p_i^*\, da, \qquad {}^{\Sigma}p_i^* = [\![\mathcal{T}_i(v_i^* - \nu_i^*)]\!] \tag{3.12}$$

$$P_d^*(D - \Sigma) = \int_{D-\Sigma} (f_i v_i^* + \Phi_{ij} v_{i,j}^*)\, dv \tag{3.13.1}$$

$$P_c^*(\partial D - \Sigma) = \int_{\partial D-\Sigma} T_i v_i^*\, da. \tag{3.13.2}$$

In this latter formulation we see that the powers developed by at-a-distance (or body) and contact forces have the same form as in the absence of singular surface, the presence of the latter having only for effect to define these fields almost everywhere (hence the notation $D - \Sigma$ and $\partial D - \Sigma$) and to induce the additional virtual power (3.12) which accounts for the relative motion of the medium and the singularity.

Introduction of the set of relative velocity field: $\mathcal{V}_{\mathrm{rel}}(\Sigma)$

The construction of the power of "internal" forces on both sides of $\Sigma(t)$ may be performed following a systematic procedure analogous to the one used for a regular body $P_i^*(D - \Sigma)$ [3]. In fact, the introduction of a *relative* velocity field at points on Σ extends the objective velocity field $\mathcal{V}_{\mathrm{obj}}$ introduced for points in $D - \Sigma$ in [3]. We can define the set of virtual relative velocity fields.

$$\mathcal{V}_{\mathrm{rel}}(\Sigma) = \{v_j^+ - \nu_j,\ v_j^- - \nu_j\} \tag{3.14}$$

at all $\boldsymbol{x} \in \Sigma(t)$ [see Appendix A: General method]. The two fields which span $\mathcal{V}_{\mathrm{rel}}(\Sigma)$ are *objective*. Let $\mathcal{T}_j^+$ and $\mathcal{T}_j^-$ be the internal forces introduced by duality so that we can write

$${}^{\Sigma}p_i^* = \mathcal{T}_j^+(v_j^+ - \nu_j)^* - \mathcal{T}_j^-(v_j^- - \nu_j)^* = [\![\mathcal{T}_j(v_j^* - \nu_j^*)]\!]. \tag{3.15}$$

Then we can say that ${}^{\Sigma}P_i$ is built by imposing the principle of objectivity to the "internal" forces $\mathcal{T}^{\pm}$ in the same way as P_i is built by requiring that $P_i(D)$ be a linear form on a set of *objective* generalized velocities. The condition equivalent to the rigidifying of the virtual velocity field ($D_{ij}^* = 0$ in the bulk) is $(\boldsymbol{v}^+)^* = (\boldsymbol{v}^-)^* = \boldsymbol{\nu}^*$, hence the free singular surface becomes a material surface in a rigidifying virtual motion.

3.2 Application of the Principle of Virtual Power and Local Equations

On assuming that Eq. (3.10) holds good for all virtual velocity fields $\boldsymbol{v}^*$, $(\boldsymbol{v}^{\pm})^*$ and $\boldsymbol{\nu}^*$ and any element of volume and surface in $D - \Sigma$ and on $\partial D - \Sigma$ and Σ, we obtain the following local field equations after using the generalized divergence theorem (see Appendix B)

$$0 = t_{ij,j} + f_i \quad \text{in } D - \Sigma \tag{3.16}$$

$$T_i = t_{ij} n_j \quad \text{on } \partial D - \Sigma \tag{3.17}$$

$$\mathcal{T}_i^{\pm} = t_{ij}^{\pm} N_j \quad \text{on } \Sigma^{\pm} \tag{3.18.1, 2}$$

$$0 = [\![\mathcal{T}_i]\!] \quad \text{across } \Sigma \tag{3.19}$$

where the a priori nonsymmetric Cauchy stress tensor is defined by

$$t_{ij} = \sigma_{ij} - \Phi_{ij} \tag{3.20}$$

and the local statement of the balance of angular momentum is simply obtained by taking the skewsymmetric part of (3.20), hence

$$t_{[ij]} = \Phi_{[ji]} . \tag{3.21}$$

The *jump condition* (3.19) is generated by arbitrary $\boldsymbol{\nu}^*$ (which are obviously continuous across Σ). In the present case Eq. (3.19) means that the *internal* contact forces $\mathcal{T}^{\pm}$ on either side of Σ are *equal*; but this is due to the fact that we discarded inertial effects (see next paragraph).

The combination of Eqs. (3.18.1, 2) and (3.19) here yields the *continuity* of the *traction* across Σ:

$$[\![t_{ij}]\!] \, N_j = 0 \quad \text{across } \Sigma. \tag{3.22}$$

3.3 Dynamical Mechanical Example

The study of the dynamical case requires the construction of the virtual power of *inertial forces* due, on the one hand, to *material particle acceleration* in $D - \Sigma$ and, on the other hand, to *mass transfer* across $\Sigma(t)$. As emphasized in [3] the very expression of inertial forces is given by Newton's expression. For the quantity due to mass transfer across the singularity a little work is needed (see Appendix D for detail). In the present case (*free* singular surface), the expression of the inertial power of inertial forces takes on the following form

$$P_a^*(D) = P_a^*(D - \Sigma) + P_a^*(\Sigma) \tag{3.23}$$

where

$$P_a^*(D - \Sigma) = \int\limits_{D-\Sigma} \varrho \frac{dv_i}{dt} v_i^* \, dv \tag{3.24.1}$$

$$P_a^*(\Sigma) = \int\limits_{\Sigma} m[\![v_i]\!] \, \nu_i^* \, da \tag{3.24.2}$$

with the normal mass flux or *mass transfer*

$$m = \varrho(\boldsymbol{v} - \boldsymbol{\nu}) \cdot \boldsymbol{N}. \tag{3.25}$$

The principle of virtual power in global form is then stated as follows

$$\begin{aligned} P_a^*(D - \Sigma) + P_a^*(\Sigma) = P_i^*(D - \Sigma) + P_i^*(\Sigma) \\ + P_d^*(D - \Sigma) + P_c^*(\partial D - \Sigma). \end{aligned} \tag{3.26}$$

The application of this for any virtual velocity fields $\boldsymbol{v}^*$, $(\boldsymbol{v}^\pm)^*$ and $\boldsymbol{\nu}^*$ and any element of volume and surface leads to the following dynamical set of local equations

$$\varrho \frac{dv_i}{dt} = t_{ij,j} + f_i \qquad \text{in } D - \Sigma \tag{3.27}$$

$$T_i = t_{ij} n_j \qquad \text{on } \partial D - \Sigma \tag{3.28}$$

$$\mathcal{T}_i^\pm = t_{ij}^\pm N_j \qquad \text{on } \Sigma^\pm \tag{3.29}$$

and

$$m[\![v_i]\!] = [\![\mathcal{T}_i]\!] \qquad \text{across } \Sigma(t). \tag{3.30}$$

On combining (3.29.1, 2) and (3.30) we obtain the jump condition

$$[\![\varrho v_i(v_j - \nu_j) - t_{ij}]\!]\, N_j = 0 \quad \text{across } \Sigma(t). \tag{3.31}$$

We note that the dynamical state across Σ — here, the mass transfer — is responsible for the inequality of "internal contact forces" on the two sides of Σ, so that only the contribution present in Eq. (3.31) is continuous across the singularity and *not* the traction $\mathcal{T}$ alone.

4. The Principle of Virtual Power in Presence of a Thermodynamical Singular Surface

4.1 Dynamical Mechanical Example

The method of constructing virtual powers due to *material quantities* attached to, or defined on, a singular surface is quite identical to that used for material quantities defined in the bulk. The fields defined on Σ are denoted by a superimposed caret (ˆ) in order to distinguish them from those defined in the bulk, e.g., $\hat{\varrho}$ is a mass density per unit area on Σ, etc. The statement of the principle of virtual power may now be written in a compact manner as

$${}^tP_a^* = {}^tP_i^* + {}^tP_d^* + {}^tP_c^* \tag{4.1}$$

where the left superscript t stands for "total". More precisely,

$$^{t}P_a^* = P_a^*(D - \Sigma) + P_a^*(\Sigma) + \hat{P}_a^*(\Sigma), \tag{4.2}$$

$$^{t}P_i^* = P_i^*(D - \Sigma) + P_i^*(\Sigma) + \hat{P}_i^*(\Sigma), \tag{4.3}$$

$$^{t}P_d^* = P_d^*(D - \Sigma) + \hat{P}_d^*(\Sigma), \tag{4.4}$$

$$^{t}P_c^* = P_c^*(\partial D - \Sigma) + \hat{P}_c^*(\partial\Sigma), \tag{4.5}$$

where $P(D - \Sigma)$, $P(\Sigma)$ and $\hat{P}(\Sigma)$ denote, respectively, powers developed in the bulk, on either side of Σ and on Σ, with the following expressions (see Appendices C and D)

$$P_a^*(\Sigma) = \int_\Sigma [\![m(v_i - \hat{v}_i)]\!] \, \hat{v}_i^* \, da, \tag{4.6}$$

$$P_i^*(\Sigma) = -\int_\Sigma {}^{\Sigma}p_i^* \, da, \tag{4.7}$$

$$P_a^*(D - \Sigma) = \int_{D-\Sigma} \varrho \frac{dv_i}{dt} v_i^* \, dv, \tag{4.8}$$

$$\hat{P}_a^*(\Sigma) = \int_\Sigma \hat{\varrho} \frac{\hat{d}\hat{v}_i}{dt} \hat{v}_i^* \, da, \tag{4.9}$$

$$P_i^*(D - \Sigma) = -\int_{D-\Sigma} p_i^* \, dv, \tag{4.10}$$

$$\hat{P}_i^*(\Sigma) = -\int_\Sigma \hat{p}_i^* \, da, \tag{4.11}$$

$$P_d^*(D - \Sigma) = \int_{D-\Sigma} (f_i v_i^* + \phi_{ij} v_{i,j}^*) \, dv, \tag{4.12}$$

$$\hat{P}_d^*(\Sigma) = \int_\Sigma (\hat{f}_i \hat{v}_i^* + \hat{\phi}_{ij} \hat{v}_{i,j}^*) \, da, \tag{4.13}$$

$$P_c^*(\partial D - \Sigma) = \int_{\partial D-\Sigma} T_i v_i^* \, da, \tag{4.14}$$

$$\hat{P}_c^*(\partial\Sigma) = \int_{\partial\Sigma} \hat{T}_i \hat{v}_i^* \, dl, \tag{4.15}$$

where

$$p_i^* = \sigma_{kj} D_{kj}^*, \qquad {}^{\Sigma}p_i^* = [\![\mathscr{T}_j (v_j^* - \hat{v}_j^*)]\!], \qquad \hat{p}_i^* = \hat{\sigma}_{kj} \hat{D}_{kj}^* \tag{4.16}$$

where $\hat{D}_{kj}$ is the strain rate tensor constructed from $\hat{\boldsymbol{v}}$ for "particles" belonging to Σ, and $\frac{\hat{d}}{dt} = \frac{\partial}{\partial t} + \hat{\boldsymbol{v}} \cdot \boldsymbol{\nabla} = \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} + {}^{\Sigma}\hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{\nabla}}$.

With the usual arguments of localization, hence for any virtual fields $\boldsymbol{v}^*$, $(\boldsymbol{v}^{\pm})^*$, $\hat{\boldsymbol{v}}^*$ and $D\hat{\boldsymbol{v}}^*$ and any element of volume, surface and line, accounting for the change from volume to surface gradients, (Ω is the mean curvature of Σ)

$$\begin{gathered}
\nabla = \hat{\nabla} + \boldsymbol{N}D, \qquad D = \boldsymbol{N}\cdot\nabla \\
\hat{\nabla}_i = P_{ij}\nabla_j, \qquad P_{ij} = \delta_{ij} - N_iN_j, \qquad \Omega = -\frac{1}{2}\nabla\cdot\boldsymbol{N}
\end{gathered} \tag{4.17}$$

projecting when needed on Σ or on its normal and using the various generalizations of Stokes' theorem (Appendix B), we obtain from (4.1) the following local equations, first in the form

$$\varrho\frac{dv_i}{dt} = t_{ij,j} + f_i \quad \text{in } D - \Sigma \tag{4.18}$$

$$T_i = t_{ij}n_j \qquad \text{on } \partial D - \Sigma \tag{4.19}$$

$$\hat{\varrho}\frac{\hat{d}\hat{v}_i}{dt} + [\![m(v_i - \hat{v}_i)]\!] = [\![\mathcal{T}_i]\!] + (\hat{\nabla}_j + 2\Omega N_j)\,\hat{t}_{ij} + \hat{f}_i \quad \text{on } \Sigma \tag{4.20}$$

$$\hat{T}_i = \hat{t}_{ij}\tau_j \quad \text{on } \partial\Sigma, \qquad \hat{t}_{ij} = \hat{\sigma}_{ij} - \hat{\phi}_{ij} \tag{4.21}$$

along with [for all $(\boldsymbol{v}^\pm)^*$ and $(D\hat{\boldsymbol{v}})^*$] the "internal" traction

$$\mathcal{T}_i^\pm = t_{ij}^\pm N_j \quad \text{on } \Sigma^\pm \tag{4.22}$$

and the transversality condition

$$\hat{t}_{ij}N_j = 0 \quad \text{on } \Sigma. \tag{4.23}$$

On account of Eqs. (4.22) and (4.23) we can also write Eq. (4.20) in the more usual form

$$\hat{\varrho}\frac{\hat{d}\hat{v}_i}{dt} + [\![\varrho(v_i - \hat{v}_i)(v_j - \nu_j) - t_{ij}]\!]\,N_j = \hat{\nabla}_j\hat{t}_{ij} + \hat{f}_i \quad \text{on } \Sigma(t). \tag{4.24}$$

4.2 *Remarks*

a) On setting $\hat{\varrho} = 0$ or $\hat{d}\hat{v}_i/dt = 0$ and $\hat{f}_i = 0$, and the constitutive equations of the "hydrostatic" type

$$t_{ij} = -p\delta_{ij}, \qquad \hat{t}_{ij} = -\sigma P_{ij} \tag{4.25}$$

with $\hat{\nabla}\sigma = 0$, in the absence of mass transfer, Eq. (4.24) provides Laplace's equation

$$[\![p]\!] + 2\Omega\sigma = 0 \tag{4.26}$$

where the surface tension σ is the two dimensional analog of a pressure.

b) If we do not account for a gradient-theory on Σ, i.e., we take $\hat{v}_{i,j} \equiv 0$, then we may say that the thermodynamical singular surface is *rigid* since $\hat{D}_{ij} = 0$. In this case $\hat{t}_{ij}$ disappears from the local equations.

c) If Σ is nothing but a *free* singular surface (no material quantities with a superimposed caret) we have $\hat{\boldsymbol{v}} = \boldsymbol{v}$ continuous across Σ and $[\![m]\!] = 0$ so that Eq. (4.20) reduces to

$$[\![m(\boldsymbol{v} - \boldsymbol{\nu})]\!] = m[\![\boldsymbol{v}]\!] = [\![\mathcal{T}]\!] \tag{4.27}$$

which is none other than Eq. (3.30).

d) Notice that the more complex is the medium considered, the more "advantageous" is the principle of virtual power as compared to the classical vectorial approach. Indeed, in order to obtain the above-deduced local equations from the vectorial approach one needs to postulate

(i) in a global form the equation of balance of momentum and angular momentum inside the volume as well as at the singular surface.

(ii) in local form, Cauchy's lemma on a surface cut and its two dimensional equivalent, as also the transversality condition for $\hat{t}_{ij}$.

e) The systematic procedure based on the principle of objectivity for "internal forces" allows one to treat more involved mechanical cases such as the possibility of having a singular line γ on the singular surface, without further difficulties. In fact, for a *free* singular line, ${}^tP_d{}^*$ and ${}^tP_c{}^*$ are not altered. We just have to add the contributions due to the inertial forces, here, precisely, the mass transfer across $\gamma(t)$ — see Appendix D — for ${}^tP_a{}^*$ and those due to the relative velocity of the singular surface and the free singular line $\left({}^\gamma p_i{}^* = {}^\gamma[\![\hat{\mathcal{T}}_j(\hat{v}_j{}^* - \hat{\nu}_j{}^*)]\!]\right)$. We thus obtain the additional equations

$$\hat{\mathcal{T}}_i{}^\pm = \hat{t}_{ij}^\pm \Lambda_j \quad \text{along } \gamma^\pm \tag{4.28}$$

$$\hat{m}[\![\hat{v}_i]\!] = [\![\hat{\mathcal{T}}_i]\!] \quad \text{across } \gamma \tag{4.29}$$

where

$$\hat{m} = \hat{\varrho}(\hat{v}_i - \hat{\nu}_i)\,\Lambda_i. \tag{4.30}$$

The combination of (4.28) and (4.29) then yields

$$[\![\hat{\varrho}\hat{v}_i(\hat{v}_j - \hat{\nu}_j) - \hat{t}_{ij}]\!]\,\Lambda_j = 0 \quad \text{across } \gamma. \tag{4.31}$$

The similarity between the structure of this last equation and Eq. (3.31) for a free singular surface must be emphasized. The "internal contact" forces $\hat{\mathcal{T}}^\pm$ are equal if there is no mass transfer across the singular line $\gamma(t)$.

f) If we wish to render our description finer, we may alter ${}^tP_d{}^*$ by introducing a traction $\hat{R}_i$ on $\Sigma - \gamma$ and a lineal force $\bar{f}_i$ on γ, so that

$$P_d{}^* = \int\limits_{D-\Sigma} (f_i v_i{}^* + \phi_{ij} v_{i,j}^*)\, dv + \int\limits_{\Sigma-\gamma} (\hat{f}_i \hat{v}_i{}^* + \hat{\phi}_{ij} \hat{v}_{i,j}^* + \hat{R}_i D\hat{v}_i{}^*)\, da + \int\limits_{\gamma} \bar{f}_i \bar{v}_i{}^*\, dl \tag{4.32}$$

where $\bar{v}_i = \hat{\nu}_i$ for a free singular line in the same way as $\hat{v}_i = v_i$ for a free singular surface. Accounting for these additional terms, the transversality condition (4.23) and the local line Eq. (4.31) are replaced by

$$\hat{R}_i = \hat{t}_{ij} N_j \quad \text{on } \Sigma - \gamma \tag{4.33}$$

and

$$[\![\hat{\varrho}\hat{v}_i(\hat{v}_j - \hat{\nu}_j) - \hat{t}_{ij}]\!] \Lambda_j = \bar{f}_i \quad \text{along } \gamma. \tag{4.34}$$

In these conditions Eq. (4.20) is replaced by

$$\hat{\varrho}\,\frac{\hat{d}\hat{v}_i}{dt} + [\![\varrho(v_i - \hat{v}_i)\,(v_j - \nu_j) - t_{ij}]\!]\,N_j = \hat{V}_j\hat{t}_{ij} + \hat{f}_i + 2\Omega\hat{R}_i \quad \text{on } \Sigma - \gamma. \tag{4.35}$$

The vector field $\hat{R}$ is a so-called double normal traction in certain theories of membranes and second-gradient theories of continua (see [3, pp. 48—49]). If we let the singular surface coincide with the boundary of the three dimensional domain then using appropriate notations we deduce equations similar to those obtained from a second-gradient theory in the bulk (compare [1] and [11])!

5. Thermodynamics

5.1 The Energy Equation

Whenever there exists a thermodynamical singular surface in D we can state the first principle of thermodynamics in global form as

$$\frac{d}{dt}\,(E + K) + \frac{\hat{d}}{dt}\,(\hat{E} + \hat{K}) = P_e + \dot{Q}_h \tag{5.1}$$

with the self-evident definitions

$$E(D - \Sigma) = \int\limits_{D-\Sigma} \varrho e\, dv, \qquad \hat{E}(\Sigma) = \int\limits_{\Sigma} \hat{\varrho}\hat{e}\, da \tag{5.2}$$

$$K(D - \Sigma) = \int\limits_{D-\Sigma} \frac{1}{2}\,\varrho v^2\, dv, \qquad \hat{K}(\Sigma) = \int\limits_{\Sigma} \frac{1}{2}\,\hat{\varrho}\hat{v}^2\, da \tag{5.3}$$

$$P_e = \int\limits_{D-\Sigma} (f_i v_i + \phi_{ij} v_{i,j})\, dv + \int\limits_{\partial D-\Sigma} T_i v_i\, da + \int\limits_{\Sigma} (\hat{f}_i \hat{v}_i + \hat{\phi}_{ij}\hat{v}_{i,j})\, da + \int\limits_{\partial\Sigma} \hat{T}_i \hat{v}_i\, dl \tag{5.4}$$

and

$$\dot{Q}_h = \int\limits_{D-\Sigma} \varrho h\, dv - \int\limits_{\partial D-\Sigma} \boldsymbol{q}\cdot\boldsymbol{n}\, da + \int\limits_{\Sigma} \hat{\varrho}\hat{h}\, da - \int\limits_{\partial\Sigma} \hat{\boldsymbol{q}}\cdot\boldsymbol{\tau}\, dl \tag{5.5}$$

where e, $\hat{e}$, h, $\hat{h}$, $\boldsymbol{q}$ and $\hat{\boldsymbol{q}}$ are, respectively, the internal energy per unit mass in $D - \Sigma$ and on Σ, the heat supplies per unit mass in $D - \Sigma$ and on Σ, and the heat flux vectors at $\partial D - \Sigma$ and across $\partial\Sigma$.

Accounting for the transport theorems recalled in Appendix B and *combining the first principle of thermodynamics with the principle of virtual power* (4.1) *written for* real *velocity fields,* we obtain the so-called *energy theorem* in the following global form

$$\frac{dE}{dt} + \frac{\hat{d}\hat{E}}{dt} + {}^{t}P_i + \dot{\mathcal{K}}_{ex}(\Sigma) = \dot{Q}_h \tag{5.6}$$

where we have defined the *excess rate of kinetic energy* $\dot{\mathcal{K}}_{ex}$ by

$$\dot{\mathcal{K}}_{ex}(\Sigma) \equiv \left(\frac{dK}{dt} + \frac{\hat{d}\hat{K}}{dt}\right) - {}^{t}P_a = \int_{\Sigma} \left[\!\left[\frac{1}{2}\, m(\boldsymbol{v} - \hat{\boldsymbol{v}})^2 \right]\!\right] da. \tag{5.7}$$

After localization Eq. (5.6) yields the equations

$$\varrho\,\frac{de}{dt} = p_i + \varrho h - \nabla \cdot \boldsymbol{q} \quad \text{in } D - \Sigma \tag{5.8}$$

$$\begin{aligned} &\hat{\varrho}\,\frac{\hat{d}\hat{e}}{dt} + \left[\!\left[m \left\{ (e - \hat{e}) + \frac{1}{2}\,(\boldsymbol{v} - \hat{\boldsymbol{v}})^2 \right\} \right]\!\right] + [\![q_j]\!]\, N_j \\ &= {}^{\Sigma}p_i + \hat{p}_i + \hat{\varrho}\hat{h} - (\hat{\nabla} + 2\Omega \boldsymbol{N}) \cdot \hat{\boldsymbol{q}} \quad \text{on } \Sigma \end{aligned} \tag{5.9}$$

On assuming, as it looks natural, the transversality condition

$$\hat{\boldsymbol{q}} \cdot \boldsymbol{N} = 0 \tag{5.10}$$

and accounting for Eqs. (3.25) and (4.16), instead of Eqs. (5.8) and (5.9) we have

$$\varrho\,\frac{de}{dt} = \sigma_{ij} D_{ij} + \varrho h - \nabla \cdot \boldsymbol{q} \quad \text{in } D - \Sigma \tag{5.11}$$

$$\begin{aligned} &\hat{\varrho}\,\frac{\hat{d}\hat{e}}{dt} + \left[\!\left[\varrho \left\{ (e - \hat{e}) + \frac{1}{2}\,(\boldsymbol{v} - \hat{\boldsymbol{v}})^2 \right\} (v_j - \nu_j) - t_{ij}(v_i - \hat{v}_i) + q_j \right]\!\right] N_j \\ &= \hat{\sigma}_{ij}\hat{D}_{ij} + \hat{\varrho}\hat{h} - \hat{\nabla} \cdot \hat{\boldsymbol{q}} \quad \text{on } \Sigma. \end{aligned} \tag{5.12}$$

These equations are the same as those deduced in other works based on the vectorial approach (cf. [4], [5], [6]).

Whenever Σ is a free singular surface, on account of Eq. (3.31) the local equation (5.12) reduces to

$$\left[\!\left[\varrho \left(e + \frac{v^2}{2}\right)(v_j - \nu_j) - t_{ij} v_i + q_j \right]\!\right] N_j = 0 \quad \text{across } \Sigma \tag{5.13}$$

or

$$m \left[\!\left[e + \frac{v^2}{2} \right]\!\right] = [\![t_{ij} v_i - q_j]\!]\, N_j \quad \text{across } \Sigma \tag{5.14}$$

which is the classical jump relation from which the Hugoniot equation follows in the study of hydrodynamics or elastic shocks when $\boldsymbol{q} = \boldsymbol{0}$; see [12, Eqs. (4.4.2) and (7.4.10)].

5.2 Second Principle of Thermodynamics

This is naturally expressed in global form as

$$\frac{dN}{dt} + \frac{\hat{d}\hat{N}}{dt} \geqq \mathcal{N} \tag{5.15}$$

with

$$N(D - \Sigma) = \int_{D-\Sigma} \varrho\eta \, dv, \qquad \hat{N}(\Sigma) = \int_{\Sigma} \hat{\varrho}\hat{\eta} \, da \tag{5.16}$$

and

$$\mathcal{N} = \int_{D-\Sigma} \varrho \frac{h}{\theta} \, dv - \int_{\partial D-\Sigma} \frac{1}{\theta} \boldsymbol{q} \cdot \boldsymbol{n} \, da + \int_{\Sigma} \hat{\varrho} \frac{\hat{h}}{\hat{\theta}} \, da - \int_{\partial\Sigma} \frac{1}{\hat{\theta}} \hat{\boldsymbol{q}} \cdot \boldsymbol{\tau} \, dl \tag{5.17}$$

where η and $\hat{\eta}$ are, respectively, the entropies per unit mass in $D - \Sigma$ and on Σ while θ and $\hat{\theta}$ are thermodynamical temperatures attributed to the bulk and the surface, respectively. The second assumption holds only when Σ is a *thermodynamical* singular surface (in particular when Σ possesses an internal energy and an entropy so that $\hat{\theta} = \partial\hat{e}/\partial\hat{\eta}$). In writing (5.17) we have also assumed that the entropy fluxes are nothing but heat fluxes divided by the corresponding temperature, although this is certainly not true in general, but for so-called simple thermodynamic processes (see [12, p. 129]).

Accounting for the generalized divergence and transport theorems of Appendix B, we deduce from (5.15) the following local inequalities

$$\varrho \frac{d\eta}{dt} \geqq \frac{1}{\theta} (\varrho h - \nabla \cdot \boldsymbol{q}) - \boldsymbol{q} \cdot \nabla \left(\frac{1}{\theta}\right) \quad \text{in } D - \Sigma \tag{5.18}$$

and

$$\hat{\varrho} \frac{\hat{d}\hat{\eta}}{dt} \geqq \frac{1}{\hat{\theta}} (\hat{\varrho}\hat{h} - \hat{\nabla} \cdot \hat{\boldsymbol{q}}) - \hat{\boldsymbol{q}} \cdot \hat{\nabla} \left(\frac{1}{\hat{\theta}}\right) - \left[\!\left[\varrho(\eta - \hat{\eta}) (v_j - \nu_j) + \frac{q_j}{\theta} \right]\!\right] N_j \quad \text{on } \Sigma. \tag{5.19}$$

When Σ is a free singular surface the latter reduces to the classical "jump inequality" (cf. [12, Eq. (4.6.10)]).

$$\left[\!\left[\varrho\eta(v_j - \nu_j) + \frac{q_j}{\theta} \right]\!\right] N_j \geqq 0 \quad \text{across } \Sigma. \tag{5.20}$$

5.3 Clausius-Duhem Inequality

We introduce Helmholtz free energies Ψ and $\hat{\Psi}$ such that

$$\Psi = e - \eta\theta \quad \text{in} \quad D - \Sigma, \qquad \hat{\Psi} = \hat{e} - \hat{\eta}\hat{\theta} \quad \text{on} \quad \Sigma. \tag{5.21}$$

Accounting now for the local equation of energy and Eqs. (5.18), (5.19) we obtain the so-called Clausius-Duhem inequalities

$$-\varrho\left(\frac{d\Psi}{dt}+\eta\frac{d\theta}{dt}\right)+\sigma_{ij}D_{ij}-\frac{1}{\theta}\,\boldsymbol{q}\cdot\nabla\theta\geqq 0\quad\text{in } D-\Sigma \tag{5.22}$$

$$\begin{aligned}&-\hat{\varrho}\left(\frac{\hat{d}\hat{\Psi}}{dt}+\hat{\eta}\frac{\hat{d}\hat{\theta}}{dt}\right)+\hat{\sigma}_{ij}\hat{D}_{ij}-\frac{1}{\hat{\theta}}\,\hat{\boldsymbol{q}}\cdot\hat{\nabla}\hat{\theta}\\&-\left[\!\left[m\left\{\eta(\theta-\hat{\theta})+(\Psi-\hat{\Psi})+\frac{1}{2}(\boldsymbol{v}-\hat{\boldsymbol{v}})^2\right\}\right]\!\right]\\&+\left[\!\left[t_{ij}(v_i-\hat{v}_i)-q_j\left(1-\frac{\hat{\theta}}{\theta}\right)\right]\!\right]N_j\geqq 0\quad\text{on }\Sigma.\end{aligned} \tag{5.23}$$

When Σ is a *free* singular surface these reduce to

$$\begin{aligned}&m\left[\!\left[\eta\theta\left(\frac{1}{\theta}-\left\langle\frac{1}{\theta}\right\rangle\right)-\left\langle\frac{1}{\theta}\right\rangle\left(\Psi+\frac{v^2}{2}\right)\right]\!\right]\\&+\left[\!\left[\left\langle\frac{1}{\theta}\right\rangle t_{ij}v_i+q_j\left(\frac{1}{\theta}-\left\langle\frac{1}{\theta}\right\rangle\right)\right]\!\right]N_j\geqq 0.\end{aligned} \tag{5.24}$$

This is obtained by eliminating the fields which carry a superimposed caret except for $\hat{\boldsymbol{v}}$ that we must set equal to $\boldsymbol{v}$ and $\hat{\theta}^{-1}$ which we must set equal to $\langle\theta^{-1}\rangle$. The same equation can be obtained by straightforward combination of Eqs. (5.14) and (5.20). This shows that the identification $\hat{\theta}^{-1}=\langle\theta^{-1}\rangle$ for a *free* singular surface is a *necessity*.

For illustration purposes and further comparison with other works it is salient to consider the special case of the hydrostatic type of behaviour for the nondissipative contributions in Eqs. (5.22) and (5.23). That is, we consider

$$\Psi=\Psi_B(\varrho^{-1},\theta),\qquad\hat{\Psi}=\Psi_S(\hat{\varrho}^{-1},\hat{\theta}) \tag{5.25}$$

with

$$\phi_{ij}=\hat{\phi}_{ij}=0,\qquad\text{hence}\qquad t_{ij}=\sigma_{ij}=t_{ji},\ \hat{t}_{ij}=\hat{\sigma}_{ij}=\hat{t}_{ji}$$

and

$$\sigma_{ij}={}^D\sigma_{ij}-p\delta_{ij},\qquad\hat{\sigma}_{ij}={}^D\hat{\sigma}_{ij}-\sigma P_{ij} \tag{5.26}$$

$$p=-\frac{\partial\Psi_B}{\partial\varrho^{-1}},\qquad\sigma=-\frac{\partial\Psi_S}{\partial\hat{\varrho}^{-1}} \tag{5.27}$$

$$\eta=-\frac{\partial\Psi}{\partial\theta},\qquad\hat{\eta}=-\frac{\partial\hat{\Psi}}{\partial\hat{\theta}}. \tag{5.28}$$

Then Eqs. (5.22) and (5.23) yield the remaining *entropy productions*

$$\gamma_B=\frac{1}{\theta}\,{}^D\sigma_{ij}D_{ij}+\boldsymbol{q}\cdot\nabla\left(\frac{1}{\theta}\right)\geqq 0 \tag{5.29}$$

and

$$\gamma_S = \frac{1}{\hat{\theta}}\, {}^D\hat{\sigma}_{ij}\hat{D}_{ij} + \hat{\boldsymbol{q}} \cdot \hat{\nabla}\left(\frac{1}{\hat{\theta}}\right) - \left[\frac{m}{\hat{\theta}}\left\{(\Psi - \hat{\Psi}) + \eta(\theta - \hat{\theta}) + \frac{1}{2}(\boldsymbol{v} - \hat{\boldsymbol{v}})^2\right\} - \frac{1}{\hat{\theta}}\,\sigma_{ij}N_j(v_i - \hat{v}_i) + q_j N q_j\left(\frac{1}{\hat{\theta}} - \frac{1}{\theta}\right)\right] \geqq 0 \tag{5.30}$$

where ${}^D\hat{\sigma}_{ij}$ is transverse, i.e., satisfies ${}^D\hat{\sigma}_{ij}N_j = 0$. Equation (5.30) can be written in several forms. In particular because of the continuity of $\hat{\theta}$ at Σ we have

$$\left[\!\!\left[q_j\left(\frac{1}{\hat{\theta}} - \frac{1}{\theta}\right)\right]\!\!\right] N_j = -\langle q_{(N)}\rangle \left[\!\!\left[\frac{1}{\theta}\right]\!\!\right] + [\![q_{(N)}]\!]\left(\frac{1}{\hat{\theta}} - \left\langle\frac{1}{\theta}\right\rangle\right), \qquad q_{(N)} = q_j N_j. \tag{5.31}$$

Similarly, because of the continuity of both $\hat{\theta}$ and $\hat{\boldsymbol{v}}$

$$\left[\!\!\left[\frac{1}{\hat{\theta}}\, {}^D\sigma_{ij}(v_i - \hat{v}_i)\right]\!\!\right] N_j = \frac{1}{\hat{\theta}}\langle {}^D\sigma_{ij}N_j\rangle [\![v_i]\!] + \frac{1}{\hat{\theta}}[\![{}^D\sigma_{ij}N_j]\!]\left(\langle v_i\rangle - \hat{v}_i\right) \tag{5.32}$$

and this shows that the velocities and the temperature inverses of the bulk and the surface intervene in a very similar way in combinations which involve either the jump of the bulk quantity (e.g. $[\![\boldsymbol{v}]\!]$ or $\left[\!\!\left[\frac{1}{\theta}\right]\!\!\right]$) or the difference between the mean of the bulk quantity (e.g., $\langle \boldsymbol{v}\rangle$ or $\left\langle\frac{1}{\theta}\right\rangle$) and the surface quantity (e.g., $\hat{\boldsymbol{v}}$ or $\frac{1}{\hat{\theta}}$). On account of previous remarks we note that as the *thermodynamical singular surface* reduces to a *free* singular surface, these differences must vanish i.e.,

$$\langle \boldsymbol{v}\rangle = \hat{\boldsymbol{v}} = \boldsymbol{v}, \qquad \left\langle\frac{1}{\theta}\right\rangle = \frac{1}{\hat{\theta}}. \tag{5.33}$$

Equations (5.29) and (5.30) agree with the entropy production established by other authors by different means (e.g., [6], [7], [8]). Authors who define the fields attached to the singular surface by means of an average through a layer thickness may find richer possibilities (in this regard see [13] where an additional term involving $\boldsymbol{N}. (\hat{\boldsymbol{v}} - \boldsymbol{v})$ appears in (5.30)). This cannot be the case here since ${}^\Sigma\hat{\boldsymbol{v}} \cdot \boldsymbol{N} = 0$ (Eq. 2.2)). However if we assume that $\hat{\boldsymbol{v}}$ has such a normal component in addition to $\boldsymbol{v}$, without changing the previous notation, instead of (2.1) we may write

$$\hat{\boldsymbol{v}} = \boldsymbol{v} + {}^\Sigma\hat{\boldsymbol{v}} + \hat{v}_N\boldsymbol{N}, \qquad {}^\Sigma\hat{\boldsymbol{v}} \cdot \boldsymbol{N} = 0, \tag{5.34}$$

and look at the thermodynamical dual of the normal component $\hat{v}_N$ (obviously an objective quantity). It is possible from Eq. (5.12) to show that the power developed by $\hat{v}_N$ reads

$$p(\hat{v}_N) = -\left\{[\![N_i t_{ij} N_j]\!] + (\hat{\nabla}_j \hat{t}_{ij})\, N_i\right\} \hat{v}_N. \tag{5.35}$$

For the simple case (4.25), this transforms to

$$p(\hat{v}_N) = \mathscr{L}\hat{v}_N, \qquad \mathscr{L} = [\![p]\!] + 2\Omega\sigma. \tag{5.36}$$

Obviously, $\mathscr{L} = 0$ corresponds to Laplace's equation (4.26). If $\hat{v}_N \neq 0$, by arguments of irreversible thermodynamics then $\mathscr{L}$ is generally nonzero and there is a deviation from Laplace's equation. This is a result obtained by R. Gatignol [13] using the average through a transition layer.

Appendix A: Virtual Power of Tractions at a Free Singular Surface

A.1 Indirect Method (reminder)

The medium is cut in thought in two subregions D^+ and D^- separated by a free singular surface. The whole velocity field at Σ is characterized by three independent and continuous velocity fields which are $\boldsymbol{v}^+$, $\boldsymbol{v}^-$ and $\boldsymbol{\nu}$. The virtual powers are constructed for both subregions and these are then glued back together. We obtain thus

$$P_i^*(\Sigma) = -\int_{\Sigma(t)} [\![\mathscr{T}_j(v_j^* - \nu_j^*)]\!]\, da. \tag{A 1}$$

A.2 General Method

This formulation relies on the construction of a set of relative velocity fields $\mathcal{V}_{\text{rel}}$ at Σ in the same manner as the objective set $\mathcal{V}_{\text{obj}}$ is introduced for internal forces in the bulk [3] and for the same reason (objectivity of internal forces).

The three absolute velocities $\boldsymbol{v}^+$, $\boldsymbol{v}^-$ and $\boldsymbol{\nu}$ may be combined to generate

$${}^T\mathcal{V}_{\text{rel}}(\Sigma) = \left\{\boldsymbol{v}^+ - \boldsymbol{\nu},\ \boldsymbol{v}^- - \boldsymbol{\nu},\ [\![\boldsymbol{v}]\!]\right\}. \tag{A 2}$$

Only two of the three relative velocity fields thus introduced are linearly independent and are therefore sufficient to construct $P_i(\Sigma)$. Two cases seem natural and deserve special attention

(i) $[\![\boldsymbol{v}]\!]$ is eliminated from the set (A 2) leaving

$$\mathcal{V}_{\text{rel}}(\Sigma) = \{\boldsymbol{v}^+ - \boldsymbol{\nu},\ \boldsymbol{v}^- - \boldsymbol{\nu}\}. \tag{A 3}$$

By duality we thus have

$$P_i^*(\Sigma) = -\int_{\Sigma(t)} [\![\mathscr{T}_j(v_j^* - \nu_j^*)]\!]\, da \tag{A 4}$$

which is none other than Eq. (A 1).

(ii) $[\![\boldsymbol{v}]\!]$ is kept. In order not to favor $\boldsymbol{v}^+$ or $\boldsymbol{v}^-$ in taking one of the remaining two relative velocities in the set (A 2) we consider their mean value at Σ and, instead of (A 3), consider the linearly independent set,

$$\overline{\mathscr{V}}_{\text{rel}}(\Sigma) = \{[\![\boldsymbol{v}]\!], \langle \boldsymbol{v} \rangle - \boldsymbol{v}\}. \tag{A 5}$$

By duality we thus write

$$P_i^*(\Sigma) = -\int_\Sigma \{K_j[\![v_j^*]\!] + F_j(\langle v_j^* \rangle - v_j^*)\}\, da. \tag{A 6}$$

The equivalence of (A 4) and (A 6) is obtained whenever

$$\boldsymbol{K} = \langle \mathscr{T} \rangle, \qquad \boldsymbol{F} = [\![\mathscr{T}]\!]. \tag{A 7}$$

If one uses (A 6) directly in the principle of virtual power (3.5) then one can show that the local equations deduced will be *exactly* the same as those deduced in section 3 once the "intermediate", internal contact forces $\boldsymbol{K}$ and $\boldsymbol{F}$ have been eliminated from the final equations (without using (A 7) obviously!).

Note. — Let $\boldsymbol{A} \cdot \mathcal{V}$ be the inner product where $\boldsymbol{A}$ is introduced by duality with $\mathcal{V}$. It is obvious that the absence of $\mathcal{V}$ implies automatically the absence of $\boldsymbol{A}$ in the subsequent formulation. The very form of the expression (A 6) incites us to look for the physical situation for which $\langle \boldsymbol{v} \rangle = \boldsymbol{v}$ at Σ. On account of the brief remark just made, $\boldsymbol{v}^* = \langle \boldsymbol{v}^* \rangle$ implies $\boldsymbol{F} = \boldsymbol{0}$ and then the local equations on Σ are shown to reduce to

$$[\![t_{ij}]\!]\, N_j = 0, \qquad m[\![v_i]\!] = 0 \tag{A 8}$$

separately. The second of Eqs. (A 8) offers two alternatives:

(α) either $m \neq 0$ and $[\![\boldsymbol{v}]\!] = 0$. In this case $P_i^*(\Sigma) \equiv 0$ after Eq. (A 6) and the singular surface cannot be of the shock type.

(β) or $[\![\boldsymbol{v}]\!] \neq 0$ and $m = 0$. Then we have no mass transfer across the discontinuity which may be called a *discontinuity of contact.*[2]

In brief we have just shown that for a continuous medium presenting a discontinuity, $\boldsymbol{v} = \langle \boldsymbol{v} \rangle$ is valid only in the absence of transfer of mass. It is not difficult to prove the reciprocal statement. Indeed, $m^\pm = 0$ gives $\boldsymbol{v}^\pm \cdot \boldsymbol{N} = \boldsymbol{v} \cdot \boldsymbol{N}$ which, in turn, yields $\boldsymbol{v} \cdot \boldsymbol{N} = \langle \boldsymbol{v} \rangle \cdot \boldsymbol{N}$ and since the tangential component may be chosen arbitrarily, then without loss in generality we may write $\boldsymbol{v} = \langle \boldsymbol{v} \rangle$ (compare [6]).

[2] Such a case where $P_i^*(\Sigma)$ reduces to

$$P_i^* = -\int_\Sigma K_j[\![v_j^*]\!]\, da = -\int_\Sigma K[\![v^*]\!]\, da,$$

is standard in the extremum energy principles used for rigid-plastic bodies where K is the scalar tangential stress (cf. [16, sec. 64]).

Appendix B: Generalized Divergence and Transport Theorems

We recall that

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla}, \qquad \frac{\hat{d}}{dt} = \frac{\partial}{\partial t} + \hat{\boldsymbol{v}} \cdot \boldsymbol{\nabla} = \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} + {}^{\Sigma}\hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{\nabla}}. \tag{B 1}$$

Then we have (for the proofs see [4] and [15])

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$$\frac{d}{dt} \int\limits_{D-\Sigma} \phi \, dv = \int\limits_{D-\Sigma} \left\{ \frac{d\phi}{dt} + \phi(\boldsymbol{\nabla} \cdot \boldsymbol{v}) \right\} dv + \int\limits_{\Sigma} [\![\phi(\boldsymbol{v} - \boldsymbol{\nu})]\!] \cdot \boldsymbol{N} \, da \tag{B 2}$$

$$\frac{\hat{d}}{dt} \int\limits_{\Sigma} \hat{\phi} \, da = \int\limits_{\Sigma-\gamma} \left\{ \frac{\hat{d}\hat{\phi}}{dt} + \hat{\phi}(\hat{\boldsymbol{\nabla}} \cdot \hat{\boldsymbol{v}}) \right\} da + \int\limits_{\gamma} [\![\hat{\phi}(\hat{\boldsymbol{v}} - \boldsymbol{\nu})]\!] \cdot \boldsymbol{\Lambda} \, dl \tag{B 3}$$

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$$\int\limits_{D-\Sigma} \boldsymbol{\nabla} \cdot \boldsymbol{A} \, dv + \int\limits_{\Sigma} [\![\boldsymbol{A}]\!] \cdot \boldsymbol{N} \, da = \int\limits_{\partial D-\Sigma} \boldsymbol{A} \cdot \boldsymbol{n} \, da \tag{B 4}$$

$$\int\limits_{\Sigma-\gamma} (\hat{\boldsymbol{\nabla}} + 2\Omega \boldsymbol{N}) \cdot \hat{\boldsymbol{A}} \, da + \int\limits_{\gamma} [\![\hat{\boldsymbol{A}}]\!] \cdot \boldsymbol{\Lambda} \, dl = \int\limits_{\partial\Sigma-\gamma} \hat{\boldsymbol{A}} \cdot \boldsymbol{\tau} \, dl \tag{B 5}$$

where

$$\hat{\nabla}_i = P_{ij} \nabla_j, \qquad P_{ij} = \delta_{ij} - N_i N_j, \qquad 2\Omega = -\boldsymbol{\nabla} \cdot \boldsymbol{N}. \tag{B 6}$$

We also note that

$$\frac{\partial}{\partial t} \int\limits_{D-\Sigma} \phi \, dv = \int\limits_{D-\Sigma} \frac{\partial \phi}{\partial t} \, dv - \int\limits_{\Sigma} [\![(\boldsymbol{\nu} \cdot \boldsymbol{N}) \, \phi]\!] \, da. \tag{B 7}$$

Appendix C: Balance of Mass

The mass contained in a material volume is constant with time. Mathematically this may be expressed in the following manner

(a) *in the absence of a thermodynamical singular surface*

$$\frac{d}{dt} \int\limits_{D} \varrho \, dv = 0 \quad \text{or} \quad \frac{d}{dt} \int\limits_{D-\Sigma} \varrho \, dv = 0$$

(b) *in the presence of a thermodynamical singular surface*

$$\frac{d}{dt}\int\limits_{D-\Sigma} \varrho \, dv + \frac{\hat{d}}{dt}\int\limits_{\Omega} \hat{\varrho} \, da = 0 \quad \text{with} \quad \Omega = \Sigma - \gamma \quad \text{or } \Sigma.$$

Accounting for volume and surface transport theorems we obtain:

In the absence of singularity

$$\frac{d\varrho}{dt} + \varrho \nabla \cdot \boldsymbol{v} = 0 \quad \text{in } D. \tag{C 1}$$

In the presence of a free singular surface $\left(m \equiv \varrho(\boldsymbol{v} - \boldsymbol{\nu}) \cdot \boldsymbol{N}\right)$

$$\frac{d\varrho}{dt} + \varrho \nabla \cdot \boldsymbol{v} = 0 \quad \text{in } D - \Sigma, \qquad [\![m]\!] = 0 \qquad \text{across } \Sigma. \tag{C 2}$$

In the presence of a regular thermodynamical singular surface

$$\frac{d\varrho}{dt} + \varrho \nabla \cdot \boldsymbol{v} = 0 \quad \text{in } D - \Sigma, \qquad \frac{\hat{d}\hat{\varrho}}{dt} + \hat{\varrho}(\hat{\nabla} \cdot \hat{\boldsymbol{v}}) + [\![m]\!] = 0 \quad \text{on } \Sigma. \tag{C 3}$$

In the presence of a free discontinuity line on the thermodynamical singular surface $\left(\hat{m} \equiv \hat{\varrho}(\hat{\boldsymbol{v}} - \hat{\boldsymbol{\nu}}) \cdot \boldsymbol{\Lambda}\right)$

$$\begin{gathered} \frac{d\varrho}{dt} + \varrho \nabla \cdot \boldsymbol{v} = 0 \quad \text{in } D - \Sigma, \qquad \frac{\hat{d}\hat{\varrho}}{dt} + \hat{\varrho}(\hat{\nabla} \cdot \hat{\boldsymbol{v}}) + [\![m]\!] = 0 \quad \text{on } \Sigma - \gamma \\ [\![\hat{m}]\!] = 0 \qquad \text{across } \gamma. \end{gathered} \tag{C 4}$$

Appendix D: Virtual Power of Inertial Forces

The total inertial quantity is defined as follows

(a) *in the absence of singularity*

$$\boldsymbol{I}(D) = \frac{d}{dt}\int\limits_{D} \varrho \boldsymbol{v} \, dv \tag{D 1}$$

(b) *in the presence of a thermodynamical singular surface*

$$\boldsymbol{I}(D \oplus \Sigma) = \frac{d}{dt}\int\limits_{D-\Sigma} \varrho v \, dv + \frac{\hat{d}}{dt}\int\limits_{\Sigma} \hat{\varrho}\hat{\boldsymbol{v}} \, da. \tag{D 2}$$

Accounting for volume and surface transport theorems as well as for the balance of mass (Appendix C) we obtain the inertial quantities as

(a) *in the absence of singularity*

$$\boldsymbol{I}(D) = \int_D \boldsymbol{f}^{\text{inert}}\, dv \tag{D 3}$$

(b) *in the presence of a thermodynamical singular surface*

$$\boldsymbol{I}(D \oplus \Sigma) = \int_{D-\Sigma} \boldsymbol{f}^{\text{inert}}\, dv + \int_{\Sigma} \hat{\boldsymbol{f}}^{\text{inert}}\, da \tag{D 4}$$

where we have defined the following inertial forces per unit volume or surface

* inertial force per unit volume due to the acceleration of particles

$$\boldsymbol{f}^{\text{inert}} = \varrho \frac{d\boldsymbol{v}}{dt} \quad \text{in} \quad D - \Sigma \tag{D 5}$$

* inertial force per unit surface on Σ (two contributions)

$${}^{\Sigma}\hat{\boldsymbol{f}}^{\text{inert}} = {}^{\Sigma}\boldsymbol{f}^{\text{inert}} + \hat{\boldsymbol{f}}^{\text{inert}} \tag{D 6}$$

* contribution due to mass transfer across $\Sigma(t)$

$${}^{\Sigma}\boldsymbol{f}^{\text{inert}} = [\![m(\boldsymbol{v} - \hat{\boldsymbol{v}})]\!] \tag{D 7}$$

* contribution due to acceleration of the "particles" attached to Σ

$$\hat{\boldsymbol{f}}^{\text{inert}} = \hat{\varrho} \frac{\hat{d}\hat{\boldsymbol{v}}}{dt}. \tag{D 8}$$

We note that for a free singular surface ($\hat{\varrho} = 0$, $\hat{\boldsymbol{v}} = \boldsymbol{v}$, $[\![m]\!] = 0$) the expression (D 6) reduces to

$${}^{\Sigma}\hat{\boldsymbol{f}}^{\text{inert}} = m[\![\boldsymbol{v}]\!]$$

since both m and $\boldsymbol{v}$ are continuous across Σ.

The virtual power per unit volume (surface) of inertial volume (surface) forces is the scalar product of inertial forces and the virtual velocity fields of the *corresponding* media. In global form this may be expressed as follows

$${}^{t}P_a{}^* = P_a{}^*(D - \Sigma) + P_a{}^*(\Sigma) + \hat{P}_a{}^*(\Sigma) \tag{D 9}$$

$$P_a{}^*(D - \Sigma) = \int_{D-\Sigma} \boldsymbol{f}^{\text{inert}} \cdot \boldsymbol{v}^*\, dv, \tag{D 10}$$

$$P_a{}^*(\Sigma) = \int_{\Sigma} {}^{\Sigma}\boldsymbol{f}^{\text{inert}} \cdot \hat{\boldsymbol{v}}^*\, da, \tag{D 11}$$

$$\hat{P}_a{}^*(\Sigma) = \int_{\Sigma} \hat{\boldsymbol{f}}^{\text{inert}} \cdot \hat{\boldsymbol{v}}^*\, da. \tag{D 12}$$

Accounting for Eqs. (D 5), (D 7) and (D 8) we thus have

(i) *in the absence of discontinuity* ([1]—[8])

$$ {}^tP_a^*(D) = \int_D \varrho \frac{d\boldsymbol{v}}{dt} \cdot \boldsymbol{v}^* \, dv; \tag{D 13}$$

(ii) *in the presence of a free singular surface* ($\hat{\boldsymbol{v}}^* = \boldsymbol{v}^*$)

$$ {}^tP_a^*(D \oplus \Sigma) = \int_{D-\Sigma} \varrho \frac{d\boldsymbol{v}}{dt} \cdot \boldsymbol{v}^* \, dv + \int_\Sigma m[\![\boldsymbol{v}]\!] \cdot \boldsymbol{v}^* \, da, \tag{D 14}$$

(iii) *in the presence of a thermodynamic singular surface*

$$ {}^tP_a^*(D \oplus \Sigma) = \int_{D-\Sigma} \varrho \frac{d\boldsymbol{v}}{dt} \cdot \boldsymbol{v}^* \, dv + \int_\Sigma \left\{ [\![m(\boldsymbol{v} - \hat{\boldsymbol{v}})]\!] + \hat{\varrho} \frac{\hat{d}\hat{\boldsymbol{v}}}{dt} \right\} \cdot \hat{\boldsymbol{v}}^* \, da. \tag{D 15}$$

The extension of this construction with a view to accounting for an eventual free discontinuity line γ requires no further difficulty and yields the following expression

$$ \begin{aligned} {}^tP_a^*(D \oplus \Sigma \oplus \gamma) = \int_{D-\Sigma} \varrho \frac{d\boldsymbol{v}}{dt} \cdot \boldsymbol{v}^* \, dv + \int_{\Sigma-\gamma} \left\{ [\![m(\boldsymbol{v} - \hat{\boldsymbol{v}})]\!] + \hat{\varrho} \frac{\hat{d}\hat{\boldsymbol{v}}}{dt} \right\} \cdot \hat{\boldsymbol{v}}^* \, da \\ + \int_\gamma \hat{m}[\![\hat{\boldsymbol{v}}]\!] \cdot \hat{\boldsymbol{v}}^* \, dl. \end{aligned} \tag{D 16}$$

Notice the analogy between the last terms of Eqs. (D 14) and (D 16) where Σ and γ are a free singular surface and line, respectively.

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N. Daher
Laboratoire de Physique et Métrologie
des Oscillateurs du C.N.R.S.
associé à l'Université de Franche-Comté-Besançon
32 avenue de l'Observatoire
F-25000 Besançon
France

G. A. Maugin
Laboratoire de Mécanique Théorique
associé au C.N.R.S.
Université Pierre et Marie Curie, tour 66
4 place Jussieu
F-75230 Paris Cedex 05
France