Mechanics of complex bodies: Commentary on the unified modeling of material substructures

Paolo Maria Mariano*

Abstract

Basic issues of the general model-building framework of the mechanics of complex bodies are discussed. Attention is focused on the representation of the material elements, the conditions for the existence of ground states in conservative setting and the interpretation of the nature of the various balance laws occurring.

Keywords: Complex bodies, material substructures, covariance

1 Introduction

Materials in which changes in the molecular or crystalline texture at various microscopic scales (substructure) influence the macroscopic behavior through peculiar interactions are commonly available. Liquid crystals, ferroelectrics, quasicrystals, polymeric fluids are paradigmatic examples. The attribute *complex* is assigned to bodies made of these materials in order to underline that significant substructural effects must be accounted for.

In complex bodies the prototype material element is a *system*. Often it is a perfectly identifiable Lagrangian system, like in nematic liquid crystals in which the characteristic stick molecules embedded in a soft matrix may be extracted and isolated from the rest. Sometimes it does not and the substructure is in a certain sense *virtual*, like in microcracked bodies: microcracks do not exist *per se*, rather they are determined only by the surrounding matter. On the other hand, the substructure can be procedural in the sense that it is a consequence of local rearrangements of the matter due to phase transitions from one energetic well to another as in martensite-austenite mixtures.

^{*}DICeA, University of Florence, via Santa Marta 3, I-50139 Firenze, Italy, email: paolo.mariano@unifi.it

Notwithstanding the variety of phenomena displayed by complex bodies and classified in condensed matter physics, there exists an abstract modelbuilding framework for the mechanics of complex bodies. It unifies in a unique format existing models of special classes of complex bodies and is a flexible tool for analyzing new materials.

Basic aspects of such a model-building framework are discussed here with pedagogical purposes and constructive criticism. Some appropriate references are scattered throughout the subsequent sections.

2 Representation of the morphology of material elements

In its primitive meaning, a body can be regarded as an abstract set \mathfrak{B} collecting material elements, each one being the smallest piece of matter characterizing the material composing the body. The basic issue is the 'representation' of such a set. In the standard format of continuum mechanics the geometrical representation adopted is the minimal one: each material element is mapped onto a place that it occupies in the ambient space \mathbb{R}^d . However, in the real world the material elements are groups of entangled molecules, simple or complex pieces of crystalline structures, stick molecules dispersed in a ground fluid etc., and substructural changes may generate actions that it is hard to identify only with perturbations of the standard stress. In all these cases the standard representation of bodies is too minimalist. The material element should be considered in essence a system rather than a windowless box so that, in the representation of the body, a map attributing to each material element a morphological descriptor ν of its (inner) substructure has to be defined. To construct the essential structures of the mechanics of complex bodies, at least at the level of first principles, it is not necessary to render precise the nature of the morphological descriptor except assuming that it is an element of a finitedimensional differentiable manifold \mathcal{M} with minimal geometrical properties (each property of \mathcal{M} has in fact physical meaning, see [11]). Once a reference place \mathcal{B} for the entire body is selected in \mathbb{R}^d , any other actual place \mathcal{B}_a (with the index a meaning actual) is considered to be achieved in an isomorphic copy $\hat{\mathbb{R}}^d$ of \mathbb{R}^d itself by means of a *transplacement* map

$$\mathcal{B} \ni x \mapsto y\left(x\right) \in \mathcal{B}_a$$

which is assumed to be one-to-one, differentiable and orientation preserving, with spatial derivative

$$F := Dy(x) \in Hom\left(T_x\mathcal{B}, T_{y(x)}\mathcal{B}_a\right).$$

The geometry of the inner structure of the material elements is described (at least at a coarse grained level) by a *morphological descriptor map*

$$\mathcal{B} \ni x \longmapsto \nu\left(x\right) \in \mathcal{M}$$

which is assumed differentiable with spatial derivative

$$N := D\nu(x) \in Hom\left(T_x\mathcal{B}, T_{\nu(x)}\mathcal{M}\right).$$

Motions are then time-parametrized families of transplacements and morphological descriptors, namely for $x \in \mathcal{B}$ and $t \in [0, \bar{t}] \subset \mathbb{R}$ the time

$$(x,t)\longmapsto y := y(x,t) \in \hat{\mathbb{R}}^d,$$
$$(x,t)\longmapsto \nu := \nu(x,t) \in \mathcal{M},$$

both fields assumed to be piecewise twice differentiable in time so that

$$\dot{y} := \frac{d}{dt} y(x,t)$$
 and $\dot{\nu} := \frac{d}{dt} \nu(x,t)$

represent the macroscopic velocity and the rate of change of the substructure respectively.

3 Standard and substructural actions

3.1 Observers

The description of material substructures constrains to give a detailed look to the essence of the notion of observer. I have discussed the point repeatedly (see e.g. [13] and references therein). The essential aspects of the discussion are summarized below (with additional remarks) as a preamble to the use of a weaker invariance requirement under changes in observers presented later. The aim is to underline how the geometrical features of the ambient space $\hat{\mathbb{R}}^d$ and the manifold of substructural shapes \mathcal{M} influence the structure of the integral balances of the interactions of macroscopic and substructural nature.

My point of view is that an observer should be considered as a representation of all geometrical environments necessary to describe the morphology of a given body and its motion. To this aim, in standard continuum mechanics one needs to select the reference place \mathcal{B} , the ambient space, say $\hat{\mathbb{R}}^d$, and the interval of time. They are all the geometrical environments needed. Different is the stage when substructural complexity arises and its changes influence the gross behavior. The manifold of substructural shapes comes into play in the way described above and one needs to represent it, specifically, one needs to select atlantes over \mathcal{M} .

Once \mathcal{M} is accounted for, the definition of changes in observers should involve the representations of $\hat{\mathbb{R}}^d$, \mathcal{B} , $[0, \bar{t}]$, \mathcal{M} . In particular, the attention is focused here on changes in observers leaving invariant \mathcal{B} and the interval of time. The last requirement defines synchronous changes in observers. Really, one could consider affine time rescaling: non essential consequences accrue so that they are not considered here.

• Changes in the ambient space are given by elements of $Diff(\hat{\mathbb{R}}^d, \hat{\mathbb{R}}^d)$, the group of diffeomorphisms of $\hat{\mathbb{R}}^d$ onto itself. Really one takes smooth curves

$$s \longmapsto \mathbf{f}_s \in Diff(\hat{\mathbb{R}}^d, \hat{\mathbb{R}}^d), \quad s \in \mathbb{R}^+,$$

with $\mathbf{f}_0 = id$, where id means identity. The parameter s can be identified with the time so that the curve $s \mapsto \mathbf{f}_s$ can be interpreted in the common way as the motion by which two observers differ as the time flows. In particular the vector field $y \mapsto v(y) := \frac{d\mathbf{f}_s}{ds}|_{s=0}$ can be considered as the (virtual) velocity of an observer moving with respect to another one, a velocity pulled back in the frame of the first observer.

• The material substructures are placed in the ambient space and the manifold \mathcal{M} collects only the elements of a concise description of the characteristic features of their geometry in space. Thus changes of frames in the ambient space alter in principle the geometry of the substructures and their consequent representation over \mathcal{M} . Disconnection between changes in the manifold of substructural shapes and changes of frames in space is admissible only when ν represents only a generic property of the substructures not associated with their geometry in space. Changes in the choice of atlantes over \mathcal{M} are governed by elements of the Lie group of diffeomorphisms of \mathcal{M} onto itself, namely

$$G := \{g : \mathcal{M} \longrightarrow \mathcal{M} \mid g \text{ a diffeomorphism}\}.$$

The link with changes in the ambient space are then assured by assuming the existence of a differentiable homeomorphism

$$h: Diff(\hat{\mathbb{R}}^d, \hat{\mathbb{R}}^d) \to G, \quad h(id) = id_G,$$

where id_G is the identity over G, so that a curve

$$s \mapsto \nu_g := h_s(\nu),$$

with $h_s = h(\mathbf{f}_s)$. By indicating by ξ the element of the Lie algebra \mathfrak{g} of G given by the derivative $\frac{dg_s}{ds}|_{s=0} = \frac{dh(\mathbf{f}_s)}{ds}|_{s=0}$, its value over a

given ν is indicated by $\xi_{\mathcal{M}}(\nu) := \frac{d\nu_s}{ds}|_{s=0}$. In particular, if the curve $s \mapsto \mathbf{f}_s$ is selected over the special orthogonal group SO(d), a subgroup of $Diff(\hat{\mathbb{R}}^d, \hat{\mathbb{R}}^d)$, for $\wedge q$ an element of the Lie algebra $\mathfrak{so}(d), q \in \hat{\mathbb{R}}^d$, it is possible (and also convenient) to write $\xi_{\mathcal{M}}(\nu)$ as the product $\mathcal{A}(\nu) q$ with $\mathcal{A}(\nu) \in Hom(\hat{\mathbb{R}}^d, T_{\nu}\mathcal{M})$.

Isometric semi-classical changes in observers are the ones that, by leaving invariant \mathcal{B} and $[0, \bar{t}]$, are characterized by the choice of the subgroup of $Diff(\hat{\mathbb{R}}^d, \hat{\mathbb{R}}^d)$ coinciding with the semi-direct product $\hat{\mathbb{R}}^d \ltimes SO(d)$.

Rotational semi-classical changes in observers are the ones in which the subgroup of $Diff(\hat{\mathbb{R}}^d, \hat{\mathbb{R}}^d)$ selected as ambient of $s \mapsto \mathbf{f}_s$ is just SO(d). In this case, by indicating by \dot{y}^* and $\dot{\nu}^*$ the rates evaluated after the change in observer (they are the pull-back in the frame of the first observer of the rates evaluated by the second observer), one gets

$$\dot{y}^* = \dot{y} + q \wedge (y - y_0),$$
 (3.1)

where y_0 is an arbitrarily fixed centre of rotation in the ambient space, and

$$\dot{\nu}^* = \dot{\nu} + \mathcal{A}\left(\nu\right)q. \tag{3.2}$$

Remind that q depends only on the parameter s that is identified here with the time, so that q = q(t).

3.2 Augmented external power and SO(d) invariance

A part of \mathcal{B} is any subset \mathfrak{b} of \mathcal{B} itself with non-vanishing volume measure and the same geometric 'regularity' of \mathcal{B} (that is the same topological properties). All parts of \mathcal{B} form an algebra $\mathfrak{P}(\mathcal{B})$ with respect to the operations of meet and join (see [2]).

Let Vel be the space of all rate fields $(x, t) \mapsto \dot{y}(x, t)$ and $(x, t) \mapsto \dot{\nu}(x, t)$ over the tube $\mathcal{B} \times [0, \bar{t}]$, rates calculated along possible motions $(x, t) \mapsto y(x, t)$ and $(x, t) \mapsto \nu(x, t)$.

A power along motions (y, ν) is a functional

$$\mathcal{P}:\mathfrak{P}\left(\mathcal{B}\right) imes Vel
ightarrow\mathbb{R}$$

which is additive over disjoint parts and linear in the rates.

The explicit representation of a given \mathcal{P} requires classification of the interactions occurring in a body. The interest here is on the expression of the power of all *external* actions over a generic part \mathfrak{b} and along a motion (y, ν) , a functional indicated from now on by $\mathcal{P}_{\mathfrak{b}}^{ext}(\dot{y}, \dot{\nu})$. Once \mathfrak{b} is selected arbitrarily, interactions with the rest of the power and the external environment are classified in two main subclasses: (1) standard actions power conjugated with the macroscopic deformation, (2) substructural actions associated with the rate of change of the substructure inside the material elements. Each subclass is further subdivided into bulk and contact actions which admit densities with respect to volume and surface measures, dx and $d\mathcal{H}^{d-1}$, respectively.

The natural expression of the external power satisfying previous assumptions is then given by

$$\mathcal{P}_{\mathfrak{b}}^{ext}(\dot{y},\dot{\nu}) := \int_{\mathfrak{b}} (b \cdot \dot{y} + \beta \cdot \dot{\nu}) \ dx + \int_{\partial \mathfrak{b}} (\mathbf{t} \cdot \dot{u} + \boldsymbol{\tau} \cdot \dot{\nu}) \ d\mathcal{H}^{d-1},$$

a power written in referential form. The term 'augmented' in the title of this section underlines the presence of the power densities of the substructural actions. At any x in \mathfrak{b} one gets

$$b := b(x) \in T_{y(x)}^* \mathcal{B}_a \simeq \mathbb{R}^d, \ \beta := \beta(x) \in T_{\nu(x)}^* \mathcal{M},$$

while, for $x \in \partial \mathfrak{b}$,

$$\mathbf{t} := \mathbf{t} (x) \in T_{y(x)}^* \mathcal{B}_a \simeq \hat{\mathbb{R}}^d, \ \boldsymbol{\tau} := \boldsymbol{\tau} (x) \in T_{\nu(x)}^* \mathcal{M}.$$

Cauchy theorem indicates that the standard traction \mathbf{t} can be expressed in Lagrangian representation by means of the first Piola-Kirchhoff stress tensor P, so that $\mathbf{t} = Pn$ at any $x \in \partial \mathbf{b}$ where n is defined. P(x) belongs to $Hom(\mathbb{R}^d, T^*_{y(x)}\mathcal{B}_a)$ and also it is natural to consider it as the density of a form over \mathcal{B} . The argument of the proof is the standard Cauchy's one based on the tetrahedron, or subtle refinements of it (see the results in [20]). In analogous way one may presume that $\boldsymbol{\tau} = \mathcal{S}n$ with $\mathcal{S}(x) \in Hom(\mathbb{R}^d, T^*_{\boldsymbol{\nu}(x)}\mathcal{M})$. Of course, even the microstress \mathcal{S} can be considered as the density of a form over \mathcal{B} . The standard tetrahedron argument does not apply here because the field $x \mapsto \boldsymbol{\tau}(x)$ takes values on the whole cotangent bundle $T^*\mathcal{M} = \bigcup_{\nu \in \mathcal{M}} T^*_{\nu}\mathcal{M}$ so that its total over a generic side of the tetrahedron is not defined, as pointed out more in general later. To prove the existence of \mathcal{S} by using the tetrahedron argument, it is necessary to embed \mathcal{M} in a linear space (the relevant proof is in [2]). The embedding always exists since \mathcal{M} is assumed here to be finitedimensional (Whitney theorem) and can be selected to be also isometric (Nash theorem), this choice having the advantage to preserve the quadratic part of the independent kinetic energy that can be sometimes attributed to the material substructure (see relevant comments in [13]). However, the theorems indicating the availability of the embedding of \mathcal{M} in a linear space do not assure the uniqueness of the embedding itself. More precisely, the embedding

is neither unique nor rigid (\mathcal{M} can be at the end folded in various manners in the process). Additionally, the dimension of the target linear space depends on the regularity of the embedding (Nash theorem). In all cases, if one finds convenient embedding \mathcal{M} in a linear space for technical purposes, for example for constructing appropriate finite elements for some special model of complex bodies, the choice of the embedding becomes strictly a matter of modelling. Of course, such a peculiarity disappears when the complex material under examination admits a manifold of substructural shapes which is coincident with a linear space, as in the case of micromorphic or, more generally, affine bodies (see [18]).

One might naïvely claim that \mathcal{M} is always a linear space so that the scheme of affine bodies (the one discussed for example in [7], [9]) is sufficient for analyzing the material complexity at substructural level.

Solids with distributed magnetic spins in conditions of magnetic saturation $(\mathcal{M} \text{ coincides with } S^2)$ and the superfluid helium 4He (where $\mathcal{M} = S^1 \subset \mathbb{C}$) are elementary counterexamples to the claim. With the aim of unifying the treatment of as many special cases of physical interest as possible, it is then necessary to consider \mathcal{M} as an abstract manifold prescribing only the minimal geometrical properties necessary to build up the essential objects which are useful for constructing the mechanics of complex bodies. In this case the existence of the microstress $\mathcal{S}(x) \in Hom(\mathbb{R}^d, T^*_{\nu(x)}\mathcal{M})$ can be assumed a priori (an intrinsic representation of \mathcal{S} in terms of measures is presented in [19] where the primary object considered is the inner power, instead of the external one).

Without investigating further on the question, I assume here that τ depends linearly on the normal at x to $\partial \mathfrak{b}$ so that the natural expression of the external power of all actions over the generic part \mathfrak{b} along y and ν is then

$$\mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{y},\dot{\nu}\right) := \int_{\mathfrak{b}} \left(b\cdot\dot{y} + \beta\cdot\dot{\nu}\right) \ dx + \int_{\partial\mathfrak{b}} \left(Pn\cdot\dot{y} + \mathcal{S}n\cdot\dot{\nu}\right) \ d\mathcal{H}^{d-1}.$$

A crucial axiom is the requirement that the power $\mathcal{P}_{\mathfrak{b}}^{ext}$ is invariant under isometric changes in observers, that is under the action of the semi-direct product $\mathbb{R}^d \ltimes SO(d)$ over the ambient space and the action of elements of G over \mathcal{M} induced by the homeomorphism h introduced above (see also additional remarks in [11], [13], [15]). Here, a weaker axiom is used, namely invariance of the power under the sole action of SO(d) in space and the corresponding action of G over \mathcal{M} through h. It is thus required that observers differing only by a proper rotation evaluate the same power.

Axiom 1 (SO(d) invariance) At mechanical equilibrium the external power of all actions on any part of \mathcal{B} is invariant under rotational semi-classical

changes in observers, namely

$$\mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{y}^{*},\dot{\nu}^{*}\right) = \mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{y},\dot{\nu}\right) \tag{3.3}$$

for any choice of the rotational velocity $q(t) \in \hat{\mathbb{R}}^d$ and any $\mathfrak{b} \in \mathfrak{P}(\mathcal{B})$.

Theorem 1 (i) If for any \mathfrak{b} the vector fields $x \mapsto Pn$ and $x \mapsto \mathcal{A}^*Sn$ are defined over $\partial \mathfrak{b}$ and are integrable there, the integral balances of actions on \mathfrak{b} hold:

$$\int_{\mathfrak{b}} b \, dx + \int_{\partial \mathfrak{b}} Pn \, d\mathcal{H}^{d-1} = 0, \qquad (3.4)$$

$$\int_{\mathfrak{b}} \left((y - y_0) \wedge b + \mathcal{A}^* \beta \right) \, dx + \int_{\partial \mathfrak{b}} \left((y - y_0) \wedge Pn + \mathcal{A}^* \mathcal{S}n \right) \, d\mathcal{H}^{d-1} = 0.$$
(3.5)

(ii) Moreover, if the tensor fields $x \mapsto P$ and $x \mapsto S$ are of class $C^1(\mathcal{B}_0) \cap C^0(\bar{\mathcal{B}}_0)$ then

$$DivP + b = 0 \tag{3.6}$$

and there exist a covector field $x \mapsto z \in T_{\nu(x)}\mathcal{M}$ such that

$$skw\left(PF^*\right) = \frac{1}{2}e\left(\mathcal{A}^*z + \left(D\mathcal{A}^*\right)\mathcal{S}\right)$$
(3.7)

and

$$Div\mathcal{S} - z + \beta = 0, \tag{3.8}$$

with $z = z_1 + z_2$, $z_2 \in Ker\mathcal{A}^*$. (iii) If the rate fields $(x, t) \mapsto \dot{y}(x, t) \in \hat{\mathbb{R}}^d$ and $(x, t) \mapsto \dot{\nu}(x, t) \in T_{\nu(x)}\mathcal{M}$ are differentiable in space, the local balances imply

$$\mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{y},\dot{\nu}\right) = \mathcal{P}_{\mathfrak{b}}^{int}\left(\dot{y},\dot{\nu}\right) \tag{3.9}$$

where

$$\mathcal{P}_{\mathfrak{b}}^{int}\left(\dot{y},\dot{\nu}\right) := \int_{\mathfrak{b}} \left(P \cdot \dot{F} + z \cdot \dot{\nu} + \mathcal{S} \cdot \dot{N}\right) \, dx.$$

Above **e** is Ricci's alternating index. $\mathcal{P}_{\mathfrak{b}}^{int}(\dot{y}, \dot{\nu})$ is called an inner (or internal) power.

PROOF: The immediate consequence of the axiom of SO(d) invariance is the integral balance of moments (3.5) obtained by using (3.1) and (3.2) in (3.3). In (3.1) the point y_0 is arbitrary. As a consequence, by taking an arbitrary vector $w \in \mathbb{R}^d$, one can substitute y_0 with $y_0 + w$ in (3.5). Such a substitution corresponds to a simple shift of the centre of the rotation of one

observer with respect to the other. By subtracting (3.5) from its counterpart calculated at $y_0 + w$, one then gets

$$w \cdot (\int_{\mathfrak{b}} b \, dx + \int_{\partial \mathfrak{b}} Pn \, d\mathcal{H}^{d-1}) = 0,$$

which corresponds to (3.4) as a consequence of the arbitrariness of w. Note that the substitution $y_0 \longrightarrow y_0 + w$ is possible due to the linear structure of $\hat{\mathbb{R}}^d$, a structure that is in general not available over the manifold of substructural shapes \mathcal{M} . Under the regularity hypotheses above, the local balance (3.6) follows as usual by exploiting Gauss theorem and the arbitrariness of \mathfrak{b} . The same localization procedure applied to the integral balance (3.5) and the validity of (3.6) imply the local balance

$$ePF^* - (D\mathcal{A}^*)\mathcal{S} = \mathcal{A}^*(Div\mathcal{S} + \beta)$$

Since $\mathcal{A}^*(\nu) \in Hom(T_v^*\mathcal{M}, \hat{\mathbb{R}}^d)$, two information are available from this equation: (1) At each $\nu \in \mathcal{M}$ the difference $ePF^* - (D\mathcal{A}^*)\mathcal{S}$ is the image in $\hat{\mathbb{R}}^d$ of a covector in $T_v^*\mathcal{M}$, let say z. (2) Such a covector is just equal to $Div\mathcal{S} + \beta$. The equation (3.9) follows by direct calculation under the validity of the pointwise balances (3.6) and (3.8).

Of course, the balance equations above include the dynamic case because the bulk actions can be decomposed additively in their inertial and non-inertial parts, the latter being identified by requiring that their power balances the rate of change of the kinetic energy. In this procedure it is assumed that the energy is the sum of macroscopic and substructural contributions. For the sake of conciseness the topic is not developed here (see [13] for the details).

Theorem 1 is the same that can be obtained by imposing as an axiom the invariance of the external power under isometric semi-classical changes in observers mentioned earlier (see [11]). Such an equivalence underlines that the integral balance of standard forces is a peculiar consequence of the 'rigid' structure of $\hat{\mathbb{R}}^d$ (its linear structure) and is associated with one of the Killing fields of the metric in the ambient space (see [21] for the analogous observation in the case of simple bodies). The same property is not available over \mathcal{M} straight away. In fact, it has been assumed here that the manifold of substructural shapes is abstract so that it does not coincide with a linear space in general. For this reason the totals of the substructural actions are not defined a priori, as mentioned above in discussing the possible path toward the proof of the existence of the microstress \mathcal{S} . Consider, for example, the field $x \mapsto \beta(x) \in T^*_{\nu(x)}\mathcal{M}$ that is $\beta : \mathcal{B} \longrightarrow T^*\mathcal{M}$. The target space $T^*\mathcal{M}$ is not a linear space so that the integral of β on any part \mathfrak{b} of \mathcal{B} is not defined unless \mathcal{M} itself is a linear space. Analogous remarks hold for the fields $x \mapsto z(x) \in T^*_{\nu(x)}\mathcal{M}$ and $x \mapsto (\mathcal{S}n)(x) \in T^*_{\nu(x)}\mathcal{M}$. As a consequence, not only an integral balance of substructural actions does not follow from the requirement of invariance of the power under changes in observers but it is even not defined. Moreover, the fact that β and \mathcal{S} appear only in the balance of moments does not means that they represent (micro) couples because in the integral balance of moments they are multiplied by the the formal adjoint of \mathcal{A} which maps at each ν elements of $T_{\nu}\mathcal{M}$ onto elements of \mathbb{R}^d .

Various alternative paths can be followed to get pointwise balances of actions. The comments below apply to them.

- 1. One could postulate the integral balances of standard and substructural actions as first principles. However, as pointed out above, such a point of view can be adopted only in the (very) special case in which \mathcal{M} is a linear space. When it is not the case, the balance of substructural actions cannot be postulated, because the integrals appearing are not defined.
- 2. One could adopt the virtual power procedure proposed in [7] for affine bodies, by postulating in fact the weak form of the balance equations. In this case one must postulate not only the expression of the external power but also the internal power, the power of the inner actions. In this way one should postulate the existence of the inner self-action z. In contrast, in Theorem 1 the existence of z is proven.
- 3. One could adopt the point of view by Green, Rivlin and Naghdi along the path indicated by Marsden's and Hughes's theorem in [16] by postulating the expression of the first principle of thermodynamics (a point of view exploited in [3] with reference to isometric changes in observers). In this case, however, one is forced not only to postulate the existence of the energy but also to prescribe its functional dependence on the state variables, in contrast with the minimalist approach followed in Theorem 1. Such a point of view is however one of the manners useful to prove the covariance of the pointwise balance of actions (that is the invariance under the action of the entire group of diffeomorphisms on the ambient space and the action of G on \mathcal{M}). The other ways are given by the exploitation of Noether theorem and/or d'Alembert-Lagrange type principles in presence of viscous-type dissipation at macroscopic and/or substructural level (see [4] and [13] for the relevant results). A requirement of covariance allows one to eliminate the indetermination given by $z_2 \in Ker\mathcal{A}^*$: in this case z_2 vanishes identically.

When ν represents only a generic property of the substructures not associated with their geometry in space, changes of frame in the ambient space

and over \mathcal{M} can be considered disconnected. By imposing invariance of the external power with respect to isometric semi-classical changes in observers, one gets two distinct integral balances of moments:

$$\int_{\mathfrak{b}} (y - y_0) \wedge b \, dx + \int_{\partial \mathfrak{b}} (y - y_0) \wedge Pn \, d\mathcal{H}^{d-1} = 0$$

and

$$\int_{\mathfrak{b}} \mathcal{A}^* \beta \ dx + \int_{\partial \mathfrak{b}} \mathcal{A}^* \mathcal{S}n \ d\mathcal{H}^{d-1} = 0.$$

Theorem 1 can be rewritten. The sole difference in this case is that 3.7 splits in the two equations

$$skw\left(PF^*\right) = 0, \quad skw\left(\mathcal{A}^*z + \left(D\mathcal{A}^*\right)\mathcal{S}\right) = 0. \tag{3.10}$$

4 The energetic scenario and the existence of ground states

4.1 A priori restrictions on constitutive structures.

After describing the morphology of the generic material element and representing the actions along a motion, the local energetic scenario must be specified.

At the macroscopic scale, since deformation is accounted for, each material element (considered as a whole) is assumed in energetic contact with the neighboring fellows. The consequent interactions are standard tensions.

At the scale of the substructure, i.e. within each material element, some alternatives are possible (see additional remarks in [14]). They are classified under suggestion of the common path followed in statistical physics.

- 1. The generic material element is a closed system with respect to its substructure: there is no migration of substructures out of the material element, and the substructure itself does not interact energetically with the neighboring fellows.
- 2. The substructure of the generic material element is in energetic contact with the substructures of the neighboring elements. No migration occur.
- 3. The material element is an open system: both energetic contact and migration of substructures are possible.

Here the attention is focused on case 2 mainly. Remarks are added on case 1. Case 3 is not touched here for the sake of brevity (see [12] for relevant developments).

The procedure to establish a priori constitutive restrictions is the standard one, based on the Clausius-Duhem inequality which is written here in isothermal form as a mechanical dissipation inequality. It prescribes that

$$\frac{d}{dt}\Psi\left(\mathfrak{b}\right) - \mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{y}, \dot{\nu}\right) \le 0,\tag{4.1}$$

for any choice of the rate fields. $\Psi(\mathfrak{b})$ is the total *free energy* of \mathfrak{b} along $(x,t) \longmapsto (y(x,t), \nu(x,t))$. The standard assumption is that $\Psi(\mathfrak{b})$ is absolutely continuous with respect to the volume measure so that there is a density ψ such that

$$\Psi\left(\mathfrak{b}\right) = \int_{\mathfrak{b}} \psi \ dx.$$

The constitutive dependence on the state variables must then be assigned not only for ψ but also for the stress measures (namely P, z and S). Simple assumptions are as follows:

$$\psi = \psi(F, \nu, N), \quad P = P(F, \nu, N), \quad z = z(F, \nu, N), \quad \mathcal{S} = \mathcal{S}(F, \nu, N).$$

If ψ admits partial derivatives with respect to its entries, the arbitrariness of **b** and equation (3.9) imply the local dissipation inequality

$$(\partial_F \psi - P) \cdot \dot{F} + (\partial_\nu \psi - z) \cdot \dot{\nu} + (\partial_N \psi - S) \cdot \dot{N} \le 0.$$
(4.2)

The possibility to choose arbitrarily the rate in (4.2) from any given state (F, ν, N) implies the classical relations (see also [1])

$$P = \partial_F \psi \left(F, \nu, N \right), \quad z = \partial_\nu \psi \left(F, \nu, N \right), \quad \mathcal{S} = \partial_N \psi \left(F, \nu, N \right).$$
(4.3)

The mechanical dissipation inequality (4.1) forbids the dependence of ψ on the rate of the fields involved. In fact, if ψ would depend on (let say) $\dot{\nu}$, in the reduced version of the mechanical dissipation inequality a term of the type $\partial_{\dot{\nu}}\psi(F,\nu,N,\dot{\nu})\cdot\ddot{\nu}$ would appear with no correspondence in the structure of the internal power $\mathcal{P}_{\mathfrak{b}}^{int}(\dot{y},\dot{\nu})$ where no action developing power in $\ddot{\nu}$ is presented. The arbitrariness of $\ddot{\nu}$ would imply then $\partial_{\dot{\nu}}\psi = 0$. In contrast, P, z and \mathcal{S} may depend on the rates of the state variables when *viscous-like effects occur* at various scales. The dependence on the the rate of the state variables is compatible with the mechanical dissipation inequality 4.1, provided that one assumes the validity of an additive decomposition of P, z and \mathcal{S} into conservative and dissipative parts. By indicating the triple (F,ν,N) by ς , one then presumes that

$$P = P^{c}(\varsigma) + P^{d}(\varsigma, \dot{\varsigma}), \quad z = z^{c}(\varsigma) + z^{d}(\varsigma, \dot{\varsigma}), \quad \mathcal{S} = \mathcal{S}^{c}(\varsigma) + \mathcal{S}^{d}(\varsigma, \dot{\varsigma}).$$

Such decompositions must be supplemented by the assumption that the conservative components are determined by the free energy. The use of (4.1) implies once more the relations (4.3) for the conservative addenda and the reduced dissipation inequality

$$P^d \cdot \dot{F} + z^d \cdot \dot{\nu} + \mathcal{S}^d \cdot \dot{N} \ge 0. \tag{4.4}$$

Consequently, P^d , z^d and S^d are linear in \dot{F} , $\dot{\nu}$ and \dot{N} . Additional assumptions on the structure of the dissipation can be made.

1. One may presume that strong dissipation conditions are satisfied a priori (that is independently of 4.1), namely

$$P^d \cdot \dot{F} \ge 0, \quad z^d \cdot \dot{\nu} \ge 0, \quad \mathcal{S}^d \cdot \dot{N} \ge 0.$$

Then one may write

$$P^d = a_P \dot{F}, \quad z^d = a_z \dot{\nu}, \quad \mathcal{S}^d = a_S \dot{N},$$

with a_P , a_z and a_S positive definite (scalar valued) state functions.

2. One could consider a strong condition for the macroscopic dissipation, namely

$$P^d \cdot \dot{F} \ge 0$$

and a weaker dissipation condition for the substructure:

$$z^d \cdot \dot{\nu} + \mathcal{S}^d \cdot \dot{N} \ge 0.$$

In this case, P^d is equal to $a_P \dot{F}$ while z^d and \mathcal{S}^d are linear functions of $\dot{\nu}$ and \dot{N} .

3. Other conditions can be presumed to hold. They may describe different viscous-like effects. Dissipative effects of plastic-like type can be accounted for. The standard plasticity theory and its strain gradient version fall within this scheme, when one identifies ν with the plastic strain. In all cases of plastic-like behavior a flow condition in terms of the subdifferential of some admissible region in the state space must be involved (here the existence of a dissipation pseudo-potential is assumed). Energetic solutions to the resulting evolutionary problem can be obtained under appropriate hypotheses (relevant analytical tools can be found in [17], [6]). One may ask what is the relation with standard internal variable schemes. In their initial formulation, such schemes have been proposed with the aim of describing the removal from thermodynamical equilibrium (see [5], [10]). In this (historical) sense internal variables are by definition not observable and play a parametric role at equilibrium, in contrast with the approach proposed here. The derivatives of the energy with respect to the internal variables and their derivatives are not considered true interactions, rather they are thermodynamic affinities (see once more [17], [6]). They do not appear in the expression of the external power. In contrast, I consider ν as an observable quantity the variations of which contribute to the equilibrium by means of true interactions. This is the reason for which I call ν morphological descriptor rather than internal variable. Connections are possible between the internal variable scheme and the multifield scheme that I discuss here. Assumptions should be necessary in order to avoid to render the comparison only formal.

4.2 Ground states

Consider a complex body displaying a pure conservative behavior. In this case one may identify the free energy with the elastic one. In absence of inertia, the energy of the whole body is then

$$\mathcal{E}(y,\nu) := \int_{\mathcal{B}} e(x, y(x), F(x), \nu(x), N(x)) dx,$$

where the density e is the difference between the elastic energy e^i and the potential of body forces $e_1^e + e_2^e$, the latter being decomposed in the part associated with standard gravitational forces (e_1^e) and the potential of possible external fields acting directly over the substructure (e_2^e) , namely $e = e^i (x, F, \nu, N) - (e_1^e (u) + e_2^e (\nu))$, with e^i the elastic energy.

A pair of fields (u, ν) satisfying the variational principle

$$\min_{y,\nu} \mathcal{E}\left(y,\nu\right)$$

is called *ground state*. Conditions for the existence of ground states follow constitutive assumptions on (i) the nature of the functional classes in which one places y and ν , (ii) the 'structural' properties of e.

Let $y : \mathcal{B} \to \hat{\mathbb{R}}^d$ be a Sobolev map, namely an element of $W^{1,1}(\mathcal{B}, \hat{\mathbb{R}}^d)$. Denote first by M(F) the *d*-vector in $\hat{\mathbb{R}}^{2d}$ collecting all the minors of F (i.e. of Dy). M(F) is then an element of $\Lambda_d(\mathbb{R}^d \times \hat{\mathbb{R}}^d)$.

It is possible to construct the d-current integration G_y over the graph of y. Precisely, G_y is the linear functional on smooth d-forms ω with compact

support in $\mathcal{B} \times \hat{\mathbb{R}}^d$ defined by

$$G_{y} := \int_{\mathcal{B}} \left\langle \omega\left(x, y\left(x\right)\right), M\left(Dy\left(x\right)\right) \right\rangle \ dx.$$

The boundary current associated with G_y is indicated by ∂G_y and defined by $\partial G_y(\omega) := G_u(d\omega), \ \omega \in \mathcal{D}^{d-1}(\mathcal{B} \times \hat{\mathbb{R}}^d)$ with $\mathcal{D}^{d-1}(\mathcal{B} \times \hat{\mathbb{R}}^d)$ the space of (d-1)-forms with compact support in $\mathcal{B} \times \hat{\mathbb{R}}^d$ (details on the nature and the properties of Cartesian currents can be found in [8]).

The functional spaces in which the existence of minima is investigated must be specified. Their choice has constitutive nature.

1. The macroscopic deformation y is assumed to be a weak diffeomorphism (in symbols $y \in dif^{1,1}(\mathcal{B}, \hat{\mathbb{R}}^d)$). In fact, y is considered a $W^{1,1}(\mathcal{B}, \hat{\mathbb{R}}^d)$ map such that (i) $|M(Dy)| \in L^1(\mathcal{B})$, (ii) $\partial G_y = 0$ on $\mathcal{D}^{d-1}(\mathcal{B} \times \hat{\mathbb{R}}^d)$, (iii) det Dy(x) > 0 for almost every $x \in \mathcal{B}$, (iv) for any $f \in C_c^{\infty}(\mathcal{B} \times \hat{\mathbb{R}}^d)$

$$\int_{\mathcal{B}} f(x, y(x)) \det Dy(x) \ dx \le \int_{\hat{\mathbb{R}}^d} \sup_{x \in \mathcal{B}} f(x, w) \ dw.$$

In particular, the subspace

$$dif^{r,1}(\mathcal{B},\hat{\mathbb{R}}^d) := \left\{ y \in dif^{1,1}(\mathcal{B},\hat{\mathbb{R}}^d) | |M(Dy)| \in L^r(\mathcal{B}) \right\},\$$

for some r > 1, is of special interest below.

2. It is assumed that (i) \mathcal{M} has Riemannian structure with (at least) C^1 -metric $g_{\mathcal{M}}$, and (ii) covariant derivatives are explicitly calculated by making use of the natural Levi-Civita connection. The C^1 -Riemannian structure implies that \mathcal{M} can be isometrically embedded in a linear space isomorphic to \mathbb{R}^M (for some M) by Nash theorem: it is then considered as a closed submanifold of \mathbb{R}^M . It is then assumed that $\nu \in W^{1,s}(\mathcal{B}_0, \mathcal{M})$, s > 1, with

$$W^{1,s}\left(\mathcal{B},\mathcal{M}\right) := \left\{ \nu \in W^{1,s}\left(\mathcal{B},\mathbb{R}^{M}\right) \mid \nu\left(x\right) \in \mathcal{M} \text{ for a.e. } x \right\}.$$

The energy functional \mathcal{E} is then extended to

$$\mathcal{W}_{r,s} := dif^{r,1}(\mathcal{B}, \mathbb{R}^d) \times W^{1,s}(\mathcal{B}, \mathcal{M}).$$

Assumptions on the structural properties of the energy density e must also be specified. e cannot be convex in F for the standard objectivity argument but it can be convex in N.

- *e* is assumed to be polyconvex in *F* and convex in *N*. There exists a Borel function $Pe : \mathcal{B} \times \hat{\mathbb{R}}^d \times \mathcal{M} \times \Lambda_d(\mathbb{R}^d \times \hat{\mathbb{R}}^d) \times M_{M \times d} \to \overline{\mathbb{R}}^+$, with values $Pe(x, y, \nu, \xi, N)$, which is (*i*) l. s. c. in (y, ν, ξ, N) for a.e. $x \in \mathcal{B}$, (*ii*) convex in (ξ, N) for any (x, y, ν) , (*iii*) and also such that $Pe(x, y, \nu, \mathcal{M}(F), N) = e(x, y, \nu, F, N)$ for any (x, y, ν, F, N) with det F > 0.
- By assumption *e* satisfies the growth condition

$$e(x, y, \nu, F, N) \ge C_1 \left(\left| M(F) \right|^r + \left| N \right|^s \right) + \vartheta \left(\det F \right)$$

for any (x, y, ν, F, N) with det F > 0, r, s > 1 and $C_1 > 0$ constants, and $\vartheta : (0, +\infty) \to \mathbb{R}^+$ a convex function such that $\vartheta (t) \to +\infty$ as $t \to 0^+$.

Theorem 2 ([15]) The functional \mathcal{E} achieves the minimum value in the classes

$$\mathcal{W}_{r,s}^d := \{(y,\nu) \in \mathcal{W}_{r,s} | y = y_0 \text{ on } \partial \mathcal{B}_y, \nu = \nu_0 \text{ on } \partial \mathcal{B}_\nu\}$$

and

$$\mathcal{W}_{r,s}^c := \left\{ (y,\nu) \in \mathcal{W}_{r,s} \mid \partial G_y = \partial G_{y_0} \text{ on } \mathcal{D}^2(\mathbb{R}^d \times \hat{\mathbb{R}}^d), \nu = \nu_0 \text{ on } \partial \mathcal{B}_{\nu} \right\}.$$

In the theorem above $\partial \mathcal{B}_y$ and $\partial \mathcal{B}_\nu$ are the portions of the boundary $\partial \mathcal{B}$ where boundary data are assigned in terms of y and ν respectively. Details and comments on the physical consequences of the assumptions above can be found in [15].

5 Notes and complements

The first variation of the energy functional $\mathcal{E}(y,\nu)$ along C^1 minimizers allows one to obtain the balances of standard and substructural actions (3.6) and (3.8). The condition (3.7) is a consequence of a requirement of objectivity for the elastic energy e^i . Remarks leading to (3.10) also apply. In addition, horizontal variations can be made by altering the reference place by means of the diffeomorphism $\Phi_{\varepsilon}(x) := x + \varepsilon \phi(x), \phi \in C_0^1(\mathcal{B}, \mathbb{R}^3), \varepsilon$ a real parameter. $\Phi_{\varepsilon}(x)$ leaves unchanged the boundary $\partial \mathcal{B}$ for ε sufficiently small. In fact, horizontal variations can be considered as a sort of relabeling of the reference place. One then defines $y_{\varepsilon}(x) := y(\Phi_{\varepsilon}^{-1}(x))$ and $\nu_{\varepsilon}(x) := \nu(\Phi_{\varepsilon}^{-1}(x))$, and obtains a mapping $\varepsilon \longmapsto \mathcal{E}(y_{\varepsilon}, \nu_{\varepsilon})$. In case of appropriate smoothness, differentiation with respect to ε gives rise to the configurational balance

$$Div\mathbb{P} + \partial_x e = 0. \tag{5.1}$$

where $\mathbb{P} = e^i I - F^* P - N^* S \in Aut(\mathbb{R}^d)$ is the extended Hamilton-Eshelby tensor in the mechanics of complex bodies (see [11]). In the smooth case (5.1) is essentially the pull back in \mathcal{B} of the balance of standard forces (3.6).

Different is the stage when the variation is calculated on non-smooth minimizers, namely on $\mathcal{W}_{r,s}^d$ where it is sure by Theorem 2 that ground states exist. The main difficulty is that Sobolev maps may not admit tangential derivatives so that the balance of standard forces in terms of first Piola-Kirchhoff stress (3.6) cannot be derived. One may compute horizontal variations, variations over \mathcal{M} and the variation of the actual shape \mathcal{B}_a . I summarize here the relevant results (see for details [15]).

- 1. Under appropriate growth conditions for the polyconvex extension of the energy and its derivatives with respect to x, M(F) and N, one proves that (i) F^*P and N^*S belong to $L^1(\mathcal{B})$ and (ii) the balance (5.1) holds in terms of distributions.
- 2. An additional assumption on the growth of $|\partial_y Pe|$ implies that (i) $\sigma := (\det F)^{-1} PF^* \in L^1_{loc}(\tilde{y}(\mathcal{B}_0), \hat{\mathbb{R}}^3 \otimes \hat{\mathbb{R}}^3)$, with $x \longmapsto \tilde{y}(x)$ the Lusin representative of y and (ii) the balance of standard forces hold in distributional sense in terms of the Cauchy stress σ .
- 3. Variations over \mathcal{M} , obtained by means of smooth curves $\varepsilon \to \overline{\varphi}_{\varepsilon} \in Aut(\mathcal{M}), \ \overline{\varphi} \in C^1(\mathcal{M})$, and an additional assumption on the growth of $|\partial_{\nu}Pe|$, allow one to show that $\mathcal{S} \in L^1(\mathcal{B}_0, \mathbb{R}^{3*} \otimes T^*\mathcal{M})$ and (*ii*) the balance of substructural actions (3.8) holds in the sense of distributions. Such a result excludes the interpretation (suggested by some author) of the balance of substructural actions as a sort of balance of configurational actions, unless the word configurational is used in a sense a little bit far from the current one.

The remarks in this section contribute to the current debate on the nature of configurational actions.

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Mehanika kompleksnih tela: komentar o unificiranom modelovanju materijalnih podstruktura

Diskutuju se osnovne postavke opšteg okvira za gradjenje modela mehanike kompleksnih tela. Posebna pažna se poklanja reprezentaciji materijalnih elemenata, uslovima postojanja nosećih stanja u konzervativnom ustrojstvu kao i interpretaciji raznih zakona balansa koji se pojavljuju.

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