

# MECHANICS OF MATERIAL MUTATIONS

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ABSTRACT. Mutations in solids are intended here as dissipative reorganizations of the material texture at different spatial scales. We discuss possible views on the description of material mutations with special attention to the interpretations of the idea of multiple reference shapes for mutant bodies. In particular, we analyze the notion of *relative power* – it allows us to derive standard, microstructural and configurational actions from a unique source – and the description of crack nucleation in simple and complex materials in terms of a variational selection in a family of bodies differing one another by the defect pattern, a family parameterized by vector-valued measures. We also show that the balance equations can be derived by imposing structure invariance to the mechanical dissipation inequality.

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<sup>1</sup>Here, the word *shape* can refer to topological and/or geometrical aspects, depending on the specific circumstances.

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## 1. A GENERAL VIEW

**1.1. A matter of terminology.** The word *mutation* appearing in the title indicates the occurrence of changes in the material structure of a body, a *reorganization of matter* with dissipative nature. Implicit is the idea of considering mutations that

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<sup>2</sup>In principle, the reader could jump such a section during a first reading, coming back to it just before beginning the last section.

have a non-trivial influence on the gross behavior of a body under external actions – the adjective *non-trivial* being significant time to time. I use the word mutation here in this sense, relating it to dissipation, although not strictly to irreversible paths in state space<sup>3</sup> – mentioning dissipation appears necessary because even a standard elastic deformation implies a “reorganization” of the matter (think for example to deformation-induced anisotropies).

Mutation implies relation with some reference configuration or state; in general a mutation is *with respect to* a setting that we take as a paragon. Such a setting does not necessarily coincide *only* with the reference place of a continuum body. In fact, affirming that a mutation is macroscopic or microscopic implies the selection of spatial scales that we consider in representing the characteristic geometric features of a body morphology. Not all these features are entirely described by the assignment of a macroscopic reference place. To clarify the point, it can be useful to recall a few basic issues in continuum mechanics, which is – we remind – the mechanics of tangible bodies, leaving a part corpuscular phenomena adequately treated by using concepts and methods pertaining to quantum theories, or considering just the effects of such phenomena emerging at long wavelength approximation.<sup>4</sup>

**1.2. Material elements: monads or systems?** In the first pages of classical basic treatises in continuum mechanics, we read that a body is a set of not further specified *material elements* (let us say ordered sets of atoms and/or entangled molecules) that we represent just mapping the body in the three-dimensional Euclidean point space. Then we consider how bodies deform along motions, imposing conditions that select among possible changes of place. Strain tensors indicate just how and how much lines, areas and volumes are stretched, i.e. the way neighboring material elements go near or away with each other. They do not give information on how the matter at a point changes its geometry – in the case it does it – along a motion. In other words, we consider commonly the material element at a point as an indistinct piece of matter, a black box without further structure. We introduce information on the material texture at the level of constitutive relations – think for example to the material symmetries in the case of simple bodies. However, the parameters that the constitutive relations introduce refer to peculiar material features averaged over a piece of matter *extended* in space, what we use to call, in homogenization procedures, *representative volume element*<sup>5</sup>. In other words, in assigning constitutive relations we implicitly specify what we intend for material element, and this is matter of modeling in the specific case considered time to time. This way we include a length-scale in the continuum scheme, even when we do not declare it explicitly. The remark is rather clear already in linear elasticity. In fact, when in the linear setting we assign to a point a fourth-rank constitutive tensor, declaring some material symmetry (say cubic, for example), the symmetry at hands is associated with a subclass of rotations, and they are referred to the point considered. A point, however, does not rotate around itself. Hence, in speaking of material symmetries at a point we are implicitly attributing to it the characteristic

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<sup>3</sup>Solid-to-solid second-order phase transitions, like the ones in shape memory alloys, are a typical example of mutations involving dissipation but not irreversibility.

<sup>4</sup>The mechanics of quasicrystals is a paradigmatic example of emergence at gross scale of the effects of atomistic events (see [63] and [76]).

<sup>5</sup>D. Krajcinovic’s treatise [59] contains extended remarks on the definition of representative volume elements and the related problems.

features of a piece of matter extended in space, with finite size. For example, in the case of cubic symmetry mentioned above, we imagine that a material point represents at least a cubic crystal, but we do not declare its size that is this way an implicit material length-scale. We need not to render explicit the size of the material element in traditional linear elasticity but, nevertheless, such a material length scale does exist. The events occurring above a length-scale scale, whatever is its origin, are described by relations among neighboring material elements. The ones below are collapsed at a point. Hence, in thinking of mutations, we can grossly distinguish between rearrangements of matter

- *among* material elements, and
- *inside* them.

When we restrict the description of the body morphology to the sole choice of the place occupied by the body (the standard approach, indeed), mutations *inside* material elements appear just in the selection of constitutive equations – material symmetry breaking in linear elasticity is an example – and possible flow rules. However, such mutations can generate interactions which can be hardly described by using only the standard representation of contact actions in terms of the Cauchy or Piola-Kirchhoff stresses. Examples follow.

- Local couples orient the stick molecules that constitute liquid crystals in nematic order.
- In solid-to-solid phase transition (e.g. austenite-martensite), micro-actions occur between the different phases.
- Micro-actions of different type appear in ferroelectrics, produced by neighboring different polarizations and even inside a single crystal by the electric field generated by the local dipole.
- Another example is rather evident when we think of a material constituted by entangled polymers scattered in a soft melt. External actions may produce indirectly local polymer disentanglements or entanglements without altering the connection of the body. Moreover, in principle every molecule might deform with respect to the surrounding matter, independently of what is placed around it, due to mechanical, chemical or electrical effects, the latter occurring when the polymer can suffer polarization. The common limit procedure defining the standard (canonical) traction at a point does not allow us to distinguish between the contributions of the matrix and the polymer. Considering explicitly the local stress fluctuations induced by the polymer would, however, require a refined description of the mechanics of the composite, which could be helpful in specific applications.
- Finally (but the list would not end here), we can think of the actions generated in the quasicrystals by atomic flips.

However, beyond the examples, the issue is essentially connected with the standard definition of tractions. At a given point and with respect to an assigned (smooth) surface crossing that point, the standard traction is a force developing power in the velocity of that point, i.e. the local rate material element are crowded or sheared to. And the velocity vector does not bring with it explicit information on what happens *inside* the material element at that point, even relatively to the events *inside* the surrounding elements. When physics suggests us to account for the effects of microscopic events, we generally need a representation of the contact actions refined with respect to the standard one. In these cases, the quest does

not reduce exclusively to the proposal of an appropriate constitutive relation (often obtained by data-fitting procedures) in the standard setting. We have often to start from the description of the morphology of a body, inserting fields that may bring at continuum level information on the microstructure. In this sense we can call them *descriptors of the material morphology* (or inner degrees of freedom, even if to me the first nomenclature could be more clear at times). This way, at the level of geometrical description of body morphology we are considering every material element as a *system* that can have its own (internal) evolution with respect to the surrounding elements, rather than a *monad*, which is, in contrast, the view adopted in the traditional setting. I use here the word monad (coming from the ancient Greek) to indicate *an ultimate unit that cannot be divided further into pieces*. Hence, I use *system* as opposite to monad, intending in short to indicate an articulate structure, a micro-world from which we select the features that are of a certain prominence, even essential (at least we believe that they are so), in the specific investigation that we are pursuing, and that define what we call *microstructure*.

**1.3. Manifold of microstructural shapes**<sup>6</sup>. A wide list of possible examples of material morphology descriptors emerges from the current literature: scalars, vectors, tensors of various ranks, combinations of them, etc. However, in checking the examples, we can realize that for the construction of the *basic structures* of a mechanical models, we do not need to specify the nature of the descriptor of the material morphology (*descriptor*, in short). What we need is

- the possibility of representing these descriptors in terms of components – a number list, indeed – and
- the differentiability of the map assigning the descriptor to each point in the reference place.

The former requirement is necessary in numerical computations. The prominence of the latter appears when we try to construct balance equations or to evaluate how much microstructural shapes vary from place to place. We do not need much more to construct the skeletal format of a model-building framework. We have just to require that the descriptors of the finer spatial scale material morphology are selected over a differentiable manifold<sup>7</sup> – it is a set admitting a covering of intersecting subsets which can be mapped by means of homeomorphisms into Euclidean spaces, assumed here all with a certain dimension; let us assume it *finite*, for the sake of simplicity.<sup>8</sup>

The choice of assigning to every point of the place occupied by a body – say  $\mathcal{B}$ , a fit region of the three-dimensional Euclidean point space – a descriptor of the material microstructure, selected in a manifold  $\mathcal{M}$ , is a way to introduce a *multi-scale* representation since  $\nu \in \mathcal{M}$  brings at macroscopic scales information on the microscopic structure of the matter. Time-variations of  $\nu$  account for both reversible and irreversible changes in the material microstructure at the scale (or scales) the choice of  $\nu$  is referred to. Moreover, when  $\nu$  is considered a differentiable

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<sup>6</sup>Here, the word *shape* can refer to topological and/or geometrical aspects, depending on the specific circumstances.

<sup>7</sup>The idea of using just a generic differentiable manifold as a space for the descriptors of material microstructure appeared first variously in solid state physics literature (see the extended review [80]), while its use in conjunction with the description of macroscopic strain is due to Capriz (see [13] and references therein).

<sup>8</sup>Additional details will appear in subsequent sections.

function of time, its time-derivative  $\dot{\nu}$  enters the expression of the power of actions associated with microstructural changes. They can be classified essentially into two families: *self-actions* occurring inside what is considered material element in the continuum modeling and *micro-stresses*, which are contact actions between neighboring material elements, due to microstructural changes that differ with each other from place to place.

**1.4. Caution.** The selection of a generic differentiable manifold as the ambient hosting the finer scale geometry of the matter unifies classes of available models. However, we could ask the reason of working with an abstract manifold when, at the end, we select it to be finite-dimensional, and we know that any finite-dimensional, differentiable manifold can be embedded in a linear space with appropriate dimension – it is Whitney theorem [120]. Moreover, in the special case where  $\mathcal{M}$  is selected to be Riemannian<sup>9</sup>, Nash theorems (see [88] and [89]) assure that the embedding in a linear space can be even isometric. Hence, we could select a linear space from the beginning, instead of starting with  $\mathcal{M}$ , which is in general non-linear for no special restrictions appear in its definition. The choice would surely simplify the developments: formally, the resulting mechanical structures would appear as the canonical ones *plus* analogous constructs linked with the microstructure description. Examples of schemes admitting naturally a linear space as a manifold of microstructural shapes are the ones describing the so-called micromorphic continua (an appropriate format for polymeric structures), nematic elastomers, quasicrystals.

A convenient choice like that, however, would erode generality of the resulting mechanical structures. The reason is that both Whitney and Nash theorems do not assure at all uniqueness of the embedding in a linear space. In particular, Nash theorems state that the regularity of the embedding determines the dimension of the target linear space. The recourse to an embedding would be necessary essentially when physics would suggest not precisely an element of a linear space as a descriptor of the material morphology. There are intermediate examples: when a body admits polarization under certain conditions, a  $3D$  vector naturally describes at a point the electric or magnetic dipole created there. However, in saturation conditions (the maximum admissible polarization for the material is reached), an instinctive choice for  $\mathcal{M}$  would be a sphere in  $\mathbb{R}^3$ , i.e. a non-linear manifold obtained by imposing a constraint into a linear space. For this reason, in developing formal mechanical structures, we could work in  $\mathbb{R}^3$  directly, with the care to add a constraint limiting the values of the polarization vector. This way we have the advantage of working at the beginning in a linear space, meeting certain difficulties at a later stage. The alternative would be to consider the sphere just mentioned not as a portion of  $\mathbb{R}^3$  but as an independent manifold, accepting its intrinsic non-linearity.

To maintain generality and with the aim of indicating tools that could be sufficiently flexible to be adapted to several situations, it could be preferable to consider  $\mathcal{M}$  as a non-linear manifold from the beginning. The additional effort should also be to introduce the smallest possible number of assumptions on the geometrical nature of  $\mathcal{M}$ . Every geometrical property brings possible physical meaning, so, not all properties are generically appropriate.

The embedding of  $\mathcal{M}$  in a linear space appears expedient when we want to construct finite element schemes for numerical computations.

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<sup>9</sup>It means that  $\mathcal{M}$  is endowed by a metric  $g$ , which is at every  $\nu \in \mathcal{M}$  a positive-definite quadratic form in the tangent space to  $\mathcal{M}$  at  $\nu$ .

**1.5. Refined descriptions of the material texture.** The assignment of a single  $\nu$  to a point  $x \in \mathcal{B}$  as a representative of the material microstructure implies one of the two following options:

- $\nu$  refers to a single microstructural individual – an example is when we consider the material element of a polymer-reinforced composite as a patch of matter containing a single macromolecule embedded in a matrix, and  $\nu$  describes only the molecule.
- We consider the material element as a container of a family of distinct microstructural entities. In this case,  $\nu$  is a sort of *average* over the family in a sense that must be specified time to time. Nematic liquid crystals constitute an example:  $\nu$  represents at a point the prevalent orientation direction of a family of stick molecules with head-to-tail symmetry.

In both cases, implicit is an axiom of *permanence* of the material element typology and such an element is considered as a system in energetic contact with the surrounding environment, but not exchanging mass with it [13], [65], [87], [38].

Refined views are possible.

- A first attempt is to consider the material element as a container of several microstructural individuals, each one described by  $\nu$  – an example is a system of linear polymeric chains, each one represented by an end-to-tail vector – and to introduce the *number* of microstructures at  $x$  characterized by  $\nu$ , that we call *microstructural numerosity* (see [66], [11]), or even the entire distribution function of microstructural elements [117]. In this case it is possible to imagine the material element as a system open to the exchange of mass due to the migration of microstructures. Fluids containing polymers are an example since the molecules are free to migrate in the surrounding liquid. Other special cases can be listed. An evolution equation for the microstructural numerosity has been derived in [66]. The result tells us that the migration of microstructures is due primarily to the *competition* of the microstructural actions between neighboring material elements. That evolution equation reduces to Cahn-Hilliard one when  $\nu$  is a scalar indicating the volume or mass fraction of one phase in a two-phase material, and the free energy is double-walled.
- Another approach accounts for the local multiplicity of microstructural elements not in statistical sense, as it occurs in the use of distribution functions. When we imagine  $r$  microstructural elements at a place  $x$  (remind: the description is multi-scale), each one described by  $\nu$ , the map  $x \mapsto \nu \in \mathcal{M}$  is  $r$ -valued over  $\mathcal{M}$ . Moreover, the multi-values of the microstructural descriptor must be determined up to permutations of the labels that we assign to the  $r$  microstructural elements in the family at  $x$ . In general, there is no reason to presume a priori a hierarchy between the elements of the microstructural family for they are identical with one another. This point of view, presented first in [33], implies a number of analytical problems:
  - although we can give meaning to the notion of differentiability for a manifold- $r$ -valued map there is no representation such that each component mapping  $x \mapsto \nu_j \in \mathcal{M}$  is differentiable, taking into account the quotient with respect to the permutations;

- even in the case in which  $\mathcal{M}$  is a smooth manifold, the set of  $r$ -valued maps over  $\mathcal{M}$  defined above is not a smooth manifold anymore, and it has to be treated as a metric space only;
- the appropriate interpretation in this setting, even extensions when it is the case, of concepts in calculus of variations, such as the notion of quasiconvexity, which can allow us to determine the existence of minimizers (ground states) for an energy depending on that type of maps and their gradients, besides the standard deformation.

Answers to these problems are in [33]. A key ingredient for them is the completeness of  $\mathcal{M}$ . Affirming that  $\mathcal{M}$  is a complete manifold means that the notion of a geodetic curve is available for it and any pair of elements of  $\mathcal{M}$  can be connected by a geodetic path.

**1.6. Comparison between microstructural descriptor maps and displacements over  $\mathcal{M}$ .** An assumption of completeness for  $\mathcal{M}$  is also appropriate when we want to define distances between different global microstructural states with the aim of giving some sense to the following question: *How far is a certain distribution of microstructures over the body from another one?*

Since we consider here the entire map  $x \mapsto \nu \in \mathcal{M}$ , not specific values of it, distances in a space of maps that we can define are *not all* equivalent, for the space they belong to is infinite-dimensional. An example including two natural distances that give results with opposite physical meaning when they are used on the same concrete situation is described in [23].

With the care suggested by these remarks, giving answer to the previous question is another possible way of describing material mutations. This view is global, however, and the selection of a distance between maps is a structural ingredient of the specific model that we construct. Local microstructural mutations can be in turn described by the amount of sudden shifts of  $\nu$  over  $\mathcal{M}$ , i.e. by non-smooth variations of the map  $x \mapsto \nu$ . Comparisons between different values of  $\nu$  can be made by assigning a metric over  $\mathcal{M}$ . When  $\mathcal{M}$  is complete the *amount of transformation* from  $\nu_1$  to  $\nu_2$  can be defined as the length of the geodetic curve connecting them. It can be interpreted as

- (i): an *amount of mutation* when the transformation produces dissipation or  
as
- (ii): a sort of *displacement length* over  $\mathcal{M}$ .

**1.7. Classification of microstructural defects.** The choice of  $\mathcal{M}$  enters the stage when we want to describe microscopic material mutations: structural changes in the microstructure, the one below the spatial scale defining the material element even implicitly. However, the possibility of selecting  $\mathcal{M}$  implies a certain microscopic order in the material, at least recurrence in the type of microscopic features that we represent through the elements of  $\mathcal{M}$ .

This way we can call *defect* in the order represented by  $\mathcal{M}$  a  $p$ -dimensional subset of the reference place  $\mathcal{B}$  where the map  $x \mapsto \nu = \tilde{\nu}(x) \in \mathcal{M}$  is *not* defined or takes as values the entire  $\mathcal{M}$ .

Such a defect is **unstable** when it is generated by a mutation which is compatible with a reversible path in the state space, meaning that the matter can re-adjust itself up to cancel the defect along some physically admissible processes, by producing dissipation and without adding material (a glue, for example). Otherwise, we call



it **stable**. The classification of both classes can be made by exploring the topological properties of  $\mathcal{M}$  (see [80]), in particular its homological and/or cohomological structures.

We can also describe at least some aspects of the alteration of the microstructural order by considering the geometry associated with the reference place  $\mathcal{B}$  of the body. An example is provided by the description of plastic changes in metals.

Consider a crystalline material: an ordered set of atoms composing crystals possibly crowded in grains. In the continuum modeling, at every point of  $\mathcal{B}$  we imagine to assign at least a crystal. Hence, in the continuum approximation we can assign to every point the *optical axes* pertaining to the crystal placed there: three linearly independent vectors that determine point by point a metric tensor  $g$ , what we call commonly *material metric*. Time evolution of  $g$  is a way to indicate that the crystalline texture changes (see details in [82]), and we could consider the occurrence of defects indirectly by changing the material metric instead of describing directly the distortions that they produce (see [122]). We shall mention other geometric options in the ensuing sections.

**1.8. Macroscopic mutations.** Material elements detach from one another: cracks may occur, voids can be nucleated, subsets of  $\mathcal{B}$  with non-vanishing volume may grow and have their own kinematics relatively to the rest of the body, as e.g. the phenomenology of biological tissues shows. All these examples are structural mutations appearing at macroscopic scale. In presence of them, the deformation map  $\tilde{u} : \mathcal{B} \rightarrow \tilde{\mathcal{E}}^3$  is no more one-to-one or loses regularity on some subset of  $\mathcal{B}$ . And the one-to-one property is a basic assumption in the standard description of deformation processes.

An instinctive way to account for these circumstances is to enlarge the functional space containing fields that can be solutions of the basic equations, with the consciousness that the selection of a function space is a constitutive choice. In fact, to belong to a space, a map must satisfy a number of properties, and they are able to describe some physical phenomena, excluding others.

Such an approach considers mutations in terms of *loss of regularity* in the maps satisfying appropriate boundary value problems. For example, let us imagine to have a certain energy depending on a material parameter and associated boundary conditions. Assume to be able to determine for a fixed value of the parameter the existence of minimizers of the energy, which will be maps depending on the parameter itself. If we allow the parameter to vary, it is possible that the family of minimizers would admit a limit into a space endowed with less regularity with respect to the initial choice at fixed parameter. The behavior could be interpreted from a physical viewpoint as a phase transition. The approach can be successful in some cases and too restrictive in others.

Another point of view can be followed. In fact, when a macroscopic defect occurs – think of a crack, for example – the current placement of a body (the region that it occupies in the Euclidean space) is no-more in one-to-one correspondence with the original reference shape  $\mathcal{B}$ , rather, at a certain instant, with another set  $\mathcal{B}$  *minus* a distinguished subset of  $\mathcal{B}$ , which is the “shadow”<sup>10</sup> over  $\mathcal{B}$  of the defect (the picture is particularly appropriate for cracked bodies). In other words, a process involving

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<sup>10</sup>I use the word *shadow* to indicate that the defect is not in  $\mathcal{B}$  but in the actual configuration of the body. A subset in  $\mathcal{B}$ , however, indicates where the deformation or the descriptors of the microstructure indicate the defects in the circumstances mentioned previously. Hence, *shadow*

nucleation and grow of macroscopic defects can be pictured by considering *multiple* reference shapes. They are distinguished one another by the pre-image of what we consider defect.

**1.9. Multiple reference shapes.** The idea of multiple reference shapes is, in a sense, old as aged is calculus of variations. There it appears when we perform the so-called *horizontal variations* (details can be found in [39]). A clear example emerges when we consider the energy of a simple elastic body undergoing large strains. It is, everybody knows,

$$\mathcal{E}(u, \mathcal{B}) := \int_{\mathcal{B}} e(x, Du(x)) dx,$$

with  $e(x, Du(x))$  the energy density,  $u$  the deformation. Minimizers for such a functional are Sobolev maps (the first theorem on their existence is in [6]), so they do not admit always tangential derivatives. For this reason, the variations of  $\mathcal{E}(u, \mathcal{B})$  can be calculated just by acting with smooth diffeomorphisms<sup>11</sup> on (1) the actual shape of the body, namely  $u(\mathcal{B})$  or (2) the reference shape  $\mathcal{B}$ . In the first case we get the *canonical balance of forces* in terms of the Cauchy stress (although in a weak form in absence of appropriate regularity of the fields involved). In the latter case – what we call horizontal variations – the result is the so-called *balance of configurational actions*, in a form free of dissipative structures such as driving forces (see [42] for details and generalizations). The conceptual independence between the two balances is known since the early stage of calculus of variations (see remarks at pages 152-153 of vol. I of [39]). In presence of appropriate regularity for the fields involved, a link between the two classes of equations can be established (see e.g. [39], [78]).

More in general, Nöther theorem in classical field theories points clearly out the rôle of horizontal variations. However, what I have mentioned in previous lines deals with conservative behavior.

A basic question then arises: *Which way could we transfer the idea implicit in the technique of horizontal variations in the dissipative setting pertaining to structural material mutations?* In other words: *What is the formal way to express the idea of having multiple reference configurations in dissipative setting?*

I list below three alternatives: they are possible views leading to answers. A preliminary remark seems, however, necessary. The horizontal variations mentioned above are determined by defining over  $\mathcal{B}$  a parameterized family of diffeomorphisms – they map  $\mathcal{B}$  onto other possible reference places – which is differentiable with respect to the parameter. When we identify the parameter with time, the derivative of these diffeomorphisms with respect to it determines a velocity field over  $\mathcal{B}$ . The way to consider it opens the list already mentioned.

- With the idea of accounting for dissipative effects, we can start directly from the assignment of a vector *velocity* field over  $\mathcal{B}$  that is *not necessarily* integrable in time, so that not always a flow is associated with it. When integrability would be assured, such a vector field would coincide with the *infinitesimal generator* of the action of the group of diffeomorphisms over  $\mathcal{B}$ , and we would come back to the standard technique of the horizontal

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means that the defect pictured in  $\mathcal{B}$  is non-material there, but it is the pre-image under the maps already mentioned of the real defect.

<sup>11</sup>A diffeomorphism is a differentiable map admitting differentiable inverse.

variations.<sup>12</sup> Such a not-necessarily-time-integrable vector field can be interpreted as a sort of infinitesimal generator of the incoming mutations: the tendency of material elements to re-organize themselves with dissipation. Having in mind time-varying reference places, Gurtin has adopted this view<sup>13</sup> in [48] for writing the power developed along structural mutations by actions – called *configurational* to remind their nature, a terminology that can be attributed to Nabarro, as Ericksen pointed out in [28] – working on the reference place along the fictitious kinematics described by the “shadow” of the defect evolution on  $\mathcal{B}$ . Along this path, configurational forces, couples, and stresses are *postulated a priori*, and identified later (at least some of them) in terms of energy and standard stresses, by using a procedure based on a requirement of invariance with respect to re-parametrization of the boundary pertaining to the region in  $\mathcal{B}$  occupied by what we are considering be a defect (see details in [47]; see also [78] for other approaches). Alternatively, I use the velocity field just mentioned in previous lines to write what I call *relative power* (see [69] for its first definition in non-conservative setting, with improvements in [71]), which is the power of canonical *external* actions on a generic part of the body augmented by what I call *power of disarrangements*, which is a functional involving energy fluxes determined by the rearrangement of matter and configurational forces and couples due to breaking of material bonds and mutation-induced anisotropy. Canonical balances of standard and microstructural actions and the ones of configurational ones follow directly by a requirement of invariance of the relative power with respect to enlarged classes of isometric changes in observers. The advantage is that we do not need to connect some configurational actions (Eshelby stress, inertia and volume terms) with energy and the canonical ones (bulk forces and stresses in the current placement of the body, and self-actions and microstresses due to microstructural rearrangements) at a *subsequent stage*, as it is necessary to do in the procedure proposed in [47]. Also, when we restrict the treatment to conservative setting, the relative power reduces to an integral expression that emerges from Nöther theorem in classical field theories – it is from there that I arrived at the idea of the relative power, interpreting a relation appearing when we include in non-linear elasticity discontinuity surfaces endowed with their own surface energy, and we try to determine the relevant Nöther theorem (specific remarks and proofs are in [23]) – and the link with classical instances is established.

- Instead of considering a vector (velocity) field over  $\mathcal{B}$ , and always with the idea of extending to dissipative setting what is hidden in the technique of horizontal variations, or better, what is implied by the idea of multiple reference shapes, we could consider local maps defined over the tangent bundle of  $\mathcal{B}$  and pushing it forward onto the ambient physical space. We take into account the dissipative nature of material mutations, in the description of the body morphology, by affirming that these tangent maps are

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<sup>12</sup>The one used by Eshelby in his seminal article [29] for determining the action on a volumetric defect in an elastic body undergoing large strain.

<sup>13</sup>Although he does not discuss questions related to the integrability in time of the rate fields defined over  $\mathcal{B}$ .

not compatible, i.e. their curl does not vanish. This is the case of the multiplicative decomposition of the deformation gradient into elastic and plastic components that we accept in traditional formulations of finite-strain plasticity (see the pioneering papers [60] and [62] and the book [115] for more recent advances). However, leaving independent the tangent maps that act at distinct points, we are not able to recognize always different reference configurations – in plasticity we cannot individualize the so-called intermediate configuration, in fact, and also we could avoid to imagine it. Such a view (it can be adopted even in conjunction with what is indicated in the previous item, as we shall see in the next sections) is not only pertinent to plasticity, with its peculiar features. The idea of different configurations reached by “virtual” tangent maps appears useful even in describing relaxation processes in materials, as suggested by Rajagopal and Srinivasa (see [103] and [104]). In both cases just mentioned, however, the use of tangent maps is a way to simulate at macroscopic level irreversible rearrangements of matter at microscopic scale, leaving invariant the geometric connection of the body. In other words, the approach does not include nucleation and subsequent grow of cracks.

- To describe the occurrence of cracks or line or point defects in solids remaining otherwise elastic, a view in terms of multiple reference shapes is also appropriate. In particular, it seems necessary to consider the set of all possible reference shapes, all occupying the same gross place  $\mathcal{B}$  and differing one another by the defect pattern. A variational principle selects both the appropriate reference shape and a standard deformation determining the current macroscopic shape of the body. To define such a principle, we need to parameterize the family of possible body gross shapes. For cracks and line defects, special measures help us: varifolds. For cracks, at every point they bring information on whether that point can be crossed by a crack and in what direction. These measures play an analogous rôle for line defects. They enter the energy that appear in the selecting variational principle and, for their nature, they introduce directly curvature terms – for elastic-brittle materials the resulting energy is a generalization of Griffith’s one (that discussed in [45]). Such an approach, introduced in [41] (see related explanations in [70]), is then particularly appropriate in cases in which curvature-dependent physical effects contribute to the energy of cracks or line defects. And the relevant cases seem to be not rare (see e.g. [116]), or better, the appropriateness of the scheme depends on whether we model intermolecular bonds as springs or beams, nothing more, essentially.

**1.10. Micro-to-macro interactions.** The choice of representing peculiar aspects of the microstructural shapes on a manifold  $\mathcal{M}$  and what we call macroscopic mutations on the reference place  $\mathcal{B}$ , attributing also to its geometrical structures (metric, torsion) the rôle of witness of microscopic features, is matter of modeling. And a mathematical model is just a *representation* of the phenomenological world, a linguistic structure on empirical data. It is addressed by data but, at the same time, overcomes them and may suggest, in turn, ways that we can follow in constructing experiments – in short, a model is not reality, rather an interpretative tale over it.

There are non-trivial interactions between microscopic events and the occurrence of macroscopic defects in a material. Examples are manifold: a visible crack

is nucleated by the coalescence of multiple ruptures of microscopic material bonds, a plastic flow (a mutation indeed, which can be considered in a sense as a phase transition, see [98]) is generated in a metal by the migration of dislocations grouping along inter-granular boundaries. We could also think of the epitaxial growth, above all when the deposition of particles is coupled with elasticity of the stepped surfaces (see [121] and also [27]). Another example is growth and remodeling of biological tissues. It is almost superfluous to remind that cellular mutations and interactions are essential in that case. In [54], Humphrey has reviewed results in biomechanics and has indicated trends on the matter (see also [5] and [92]). Non-trivial theoretical issues are involved already at the level of geometrical description of the relevant processes. To date, an essential foundational contribution to the growth and remodeling issues seems to me the one by Segev [108]. Remarkably, to avoid to repeat standard instances in plasticity (which is a remodeling of matter, indeed) just with a different nomenclature, models of growth and remodeling (the processes together) should take into account the presence of nutrients: generically, a growing body is an open system, indeed.

Without going further in the specific issues and coming back to general themes, we remind that the representations of microscopic and macroscopic events should then merge one into the other. The interaction appears already in the definition of observers and their changes. In fact, although we can decide to describe events at various spatial scales in different spaces, they occur all *together* in the physical space. Hence, we must consider this obvious aspect in our modeling, with consequent non-trivial implications.<sup>14</sup>

**1.11. A plan for the next sections.** A treatise would be perhaps necessary to furnish appropriate details on all themes sketched above. The space of a monograph would be useful not only for technical developments but also, and above all probably, for the discussion of the physical meaning of formal choices made along the path, and their consequences in terms of foundational aspects in continuum mechanics. This target is, of course, far from the limits imposed to this article. Hence, in the next sections I shall make choices, presenting just some details about questions that seem to me at least prominent in the description of material mutations. The list of references is so far (what I have quoted in previous lines) and will be in the rest of this article neither complete, nor unbiased. It suffers the limits in my knowledge of the work produced. The judgment can be also translated probably to the entire paper, a consequence of personal choices and interpretations, which aim just to be useful to the appropriate reader in underlining concepts sometimes not completely usual, which could, in principle, open questions and avenues for further developments.

**1.12. Advantages.** In constructing models of the mechanics of materials with non-standard behavior, in particular in presence of prominent microstructural events, we face two main problems: (1) the correct assessment of balance equations and (2) the assignment of appropriate constitutive relations.

In the latter case we may resort to (*i*) experimental data, (*ii*) requirements of objectivity or covariance under changes in observers (see pertinent definitions

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<sup>14</sup>Views on the representation of microstructural events on macroscopic cracks or linear defects can be found in [68], [72], [40].

in the next sections), (*iii*) identification from discrete schemes, (*iv*) more general homogenization procedures.

As regards balance equations, I am always suspicious when proposals in non-standard circumstances emerge just by analogy with what is commonly accepted in different well-known domains. The reason for my suspiciousness is that analogy is a sort of hope to hit the mark in the fog. Although such a behavior could be convenient for production, it is not obvious that it brings always us to results illuminating the real physical mechanisms. In contrast, the search of first principles may lead us to a safe derivation of balance equations.

We meet a number of alternatives. We have to select amid them with care. In fact, when we accept the principle of virtual power (or work) as a starting point, we are just prescribing a priori the weak form of balance equations and we have introduced all the ingredients pertaining to them. In the case of simple bodies, we cannot do drastically more, in a sense. However, when we involve the description of intricate microstructural events in our models, we can start from principles involving less ingredients than the ones appearing eventually in the pointwise balances. I shall come back in detail on the issue in the next sections.

Here, I just summarize some aspects of what is included in the rest of the paper that are to me advantages with respect to what is presented in different literature.

The reader finds

- a way to derive for several microstructured materials balance equations of standard (canonical), microstructural, and configurational actions from a unique source, by using a requirement of invariance from changes in observers determined by isometric variations of frames in space;
- the deduction of a version of the action-reaction principle and the Cauchy stress theorem for microstructural contact actions;
- an extension to non-conservative setting of Marsden-Hughes theorem – such a generalization allows us to derive the Cauchy stress theorem, balances of standard and configurational actions, constitutive restrictions, and the structure of the dissipation from the requirement of covariance (the meaning will be clear in the next sections) of the second law of thermodynamics, written in appropriate way; the result is presented just with reference to standard finite-strain hardening plasticity, but further generalizations of it can be rather easily obtained – and
- a description of crack nucleation and/or growth in terms of a variational principle selecting among all possible cracked or intact versions of the body considered. The principle includes a generalization of Griffith's energy to a structure including curvature effects. The procedure can be adopted also for the nucleation and/or growth of linear defects.

Comparisons with alternative proposals and reasons for considering advantages the items above are scattered through the text.

With this paper I would like just to push the reader to think of what we exactly do when we construct mathematical models of mechanical phenomena.

**1.13. Readership.** The remark above opens the question of the readership. In starting the present notes, I assumed vaguely to write for a reader rather familiar with basic structures of traditional continuum mechanics in large strain regime. After writing a first draft and discussing with some colleagues, we were in agreement

that the article could not be easily intended for absolute beginners in continuum mechanics, but each of us had a different personal opinion about the meaning of *being not a beginner*. We were also conscious that the style becomes substance eventually.

To me, the appropriate reader of this article is a person who is culturally curious, not a prejudiced rival of formal general structures. I think of a person with the patience to arrive at the end, a person who could think that there could be some aspects deserving further deeper reading when thoughts decant and our natural pre-comprehension – exerted unconsciously every time we start reading a text – becomes softer, the inapt writer notwithstanding.

## 2. MATERIAL MORPHOLOGIES AND DEFORMATIONS

**2.1. Gross shapes and macroscopic strain measures.** A canonical assumption is that a set that a body may occupy in the three-dimensional Euclidean point space  $\mathcal{E}^3$ , a placement that we can take as a reference, is a connected, regularly open region  $\mathcal{B}$ , endowed with metric<sup>15</sup>  $g$  and provided with surface-like boundary, oriented by the normal  $n$  everywhere but a finite number of corners and edges. Less canonical is the choice of an isomorphic copy of  $\mathcal{E}^3$  – write  $\tilde{\mathcal{E}}^3$  for it – that we use as ambient physical space where we describe all gross places that we consider deformed with respect to  $\mathcal{B}$ . When we assign an orientation to  $\mathcal{E}^3$ , we must presume (physical reasons will emerge below) that  $\tilde{\mathcal{E}}^3$  is oriented in the same way, and the isomorphism is then an isometry, the identification eventually.<sup>16</sup> Below,  $\tilde{g}$  will indicate a metric in  $\tilde{\mathcal{E}}^3$ . There is no reason forcing us to assume a priori that  $g$  and  $\tilde{g}$  are the same.

Actual macroscopic placements are reached from  $\mathcal{B}$  by means of **deformations**: they are differentiable, orientation preserving maps assigning to every point  $x$  in  $\mathcal{B}$  its current place  $y$  in  $\tilde{\mathcal{E}}^3$ , namely

$$x \longmapsto y := u(x) \in \tilde{\mathcal{E}}^3.$$

We shall indicate by  $\mathcal{B}_a$  the image of  $\mathcal{B}$  under  $u$ , namely  $\mathcal{B}_a := u(\mathcal{B})$ , the index  $a$  meaning *actual*.

As usual, we write  $F$  for the spatial derivative  $Du(x)$  evaluated at  $x \in \mathcal{B}$ . We call it **deformation gradient** according to the tradition.  $Du(x)$  and the gradient  $\nabla u(x)$  satisfy the relation  $\nabla u(x) = Du(x)g^{-1}$ . In other words,  $F$  is 1-contravariant, 1-covariant, while  $\nabla u(x)$  is contravariant in both components. This difference is usually not emphasized in standard continuum mechanics because we use implicitly the identification of  $\mathbb{R}^3$  with its dual  $\mathbb{R}^{3*}$ . Hence, we do not distinguish between contravariant and covariant components, the former belonging to the vector space  $\mathbb{R}^3$ , the latter to its dual. Here, I stress the difference because in the following developments we shall meet an abstract manifold – what I have already

<sup>15</sup>At  $x \in \mathcal{B}$  consider three linearly independent vectors  $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$  and define a scalar product  $\langle \cdot, \cdot \rangle_{\mathbb{R}^3}$  in  $\mathbb{R}^3$ . The components of the metric  $g(x)$  are given by  $g_{AB}(x) = \langle \mathbf{e}_A, \mathbf{e}_B \rangle_{\mathbb{R}^3}$ , with the indexes running in the set  $\{1, 2, 3\}$ .

<sup>16</sup>The distinction renders significant the standard requirement that isometric changes in observers in the ambient space leave invariant the reference place  $\mathcal{B}$ , although they alter the frame (the atlas, more in general) assigned to the whole space. Moreover, the distinction between  $\mathcal{E}^3$  and  $\tilde{\mathcal{E}}^3$  can be accepted for it is not necessary that  $\mathcal{B}$  be occupied by the body we are thinking of along any motion. It is just a geometric environment where we measure how lengths, volumes, and surfaces change under deformations, and we use it to make the comparisons defining what we can call defects, at least at macroscopic scale.

mentioned, calling it *manifold of microstructural shapes* – with finite dimension and for it the natural simplifications in  $\mathbb{R}^3$  are in general not available, unless we embed the manifold in a linear space, a circumstance that I try to avoid for reasons already explained. As a consequence, to maintain a parallelism in the treatment, I distinguish explicitly between contravariant and covariant components even in cases, like the one of  $F$ , where it could be not strictly necessary. This way the advantage is a rather clear construction of mathematical structures, paying formal clearness, which help us in connecting mathematical representations and physical meaning, with the need of being careful to the geometric nature of some *objects*. Of course, the reader could have a different opinion.

At  $x \in \mathcal{B}$ , consider the three linearly independent vectors  $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ . They are a basis in the tangent space<sup>17</sup>  $T_x\mathcal{B}$ . Correspondingly, there is another basis, indicated by  $\{\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3\}$  in the dual space to  $T_x\mathcal{B}$ , namely the cotangent space  $T_x\mathcal{B}^*$ . Moreover, take other three linearly independent vectors at  $y = u(x)$ , say  $\{\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2, \tilde{\mathbf{e}}_3\}$ . They constitute a basis in the tangent space  $T_y\mathcal{B}_a$ . With respect to  $\{\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3\}$  and  $\{\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2, \tilde{\mathbf{e}}_3\}$ , and by adopting here once and for all summation over repeated indexes, we have  $F = F_A^i \mathbf{e}^A \otimes \tilde{\mathbf{e}}_i = \frac{\partial u^i(x)}{\partial x^A} \mathbf{e}^A \otimes \tilde{\mathbf{e}}_i$ . Lower case indexes refer to coordinates on  $\mathcal{B}_a$  while capital indexes label coordinates over  $\mathcal{B}$ .

By reminding the relation between  $F$  and  $\nabla u$ , written previously, in components we then have  $(\nabla u^i(x))^B = F_A^i g^{AB}$ . By definition,  $F$  is a linear operator mapping the tangent space to  $\mathcal{B}$  at  $x$ , namely  $T_x\mathcal{B}$ , to  $T_y\mathcal{B}_a$ , so we write shortly  $F \in \text{Hom}(T_x\mathcal{B}, T_y\mathcal{B}_a)$ .<sup>18</sup> Different is the behavior of  $\nabla u(x)$  which maps covectors over  $\mathcal{B}$ , namely elements of  $T_x\mathcal{B}^*$ , onto vectors over the actual shape  $\mathcal{B}_a$ . The standard identification of  $F$  with  $\nabla u(x)$  is motivated by the common choice of an orthogonal metric in  $\mathcal{B}$ , the second-rank covariant identity  $I = \delta_{AB} \mathbf{e}^A \otimes \mathbf{e}^B$ , with  $\delta_{AB}$  the standard Kronecker delta. Here, more in general,  $g$  does not coincide necessarily with  $\tilde{g}$ .

Two linear operators are naturally associated with  $F$ : the **formal adjoint**  $F^*$ , which maps elements of the cotangent space  $T_y^*\mathcal{B}_a$  to elements of  $T_x^*\mathcal{B}$ , and the **transpose**  $F^T$ , a linear map from  $T_y\mathcal{B}_a$  to  $T_x\mathcal{B}$ . An operational definition of them requires (1) the use of the scalar product into  $\mathbb{R}^3$ , namely  $\langle \cdot, \cdot \rangle_{\mathbb{R}^3}$ , and the analogous product in its isomorphic copy<sup>19</sup>  $\hat{\mathbb{R}}^3$ , namely  $\langle \cdot, \cdot \rangle_{\hat{\mathbb{R}}^3}$ , and (2) the duality pairing between a linear space and its dual. For such a pairing I shall use a dot in the rest of this paper.<sup>20</sup> Specifically, given a generic element  $v$  of a linear space  $\text{Lin}$ , formally  $v \in \text{Lin}$ , and another element  $b \in \text{Lin}^*$  –  $b$  is a linear function over  $\text{Lin}$  –

<sup>17</sup>At a point  $x \in \mathcal{B}$ , consider a smooth curve crossing  $x$  and evaluate at  $x$  its first derivative with respect to the arc length. The result is a vector that is tangent to  $\mathcal{B}$  at  $x$ . Take then three linearly independent tangent vectors at  $x \in \mathcal{B}$ : they are a basis of the tangent space to  $\mathcal{B}$  at  $x$ , a linear space coinciding with  $\mathbb{R}^3$ . Further details are included in subsequent footnotes.

<sup>18</sup>Previous remarks on the orientation of  $\mathcal{E}^3$  and its isomorphic copy  $\tilde{\mathcal{E}}^3$  are strictly necessary to give meaning to the evaluation of the determinant of  $F$ .

<sup>19</sup>Both spaces pertain to (they are constructed over)  $\mathcal{E}^3$  and its isomorphic copy  $\tilde{\mathcal{E}}^3$ , as introduced previously.

<sup>20</sup>The notation will be adopted below also for tensors – and we shall write, for example,  $A \cdot B$ , with  $A$  and  $B$  two tensors with the same rank – meaning that every covariant component of the first tensor appearing in the product acts on the companion contravariant component of the second tensor (in a common jargon we can say that every component of  $A$  is *saturated by* a component of  $B$ ), provided that the two tensors belong one to the dual space of the other, an implicit assumption every time we shall write something like  $A \cdot B$ .



we shall indicate by  $b \cdot v$  the value  $b(v)$ . In particular, for  $v_1, v_2 \in \mathbb{R}^3$ , we have by definition  $\langle v_1, v_2 \rangle = gv_1 \cdot v_2$ , with  $gv_1 \in \mathbb{R}^{3*}$ . Hence,  $F^T$  is defined as the unique linear operator such that, for every pair  $v \in \mathbb{R}^3$  and  $\bar{v} \in \tilde{\mathbb{R}}^3$ ,  $\langle Fv, \bar{v} \rangle_{\tilde{\mathbb{R}}^3} = \langle v, F^T \bar{v} \rangle_{\mathbb{R}^3}$ , while  $F^*$  is such that, for every pair  $v \in \mathbb{R}^3$  and  $b \in \tilde{\mathbb{R}}^{3*}$ ,  $b \cdot Fv = F^*b \cdot v$ .

**Proposition 1.**  $F^T = g^{-1}F^*\tilde{g}$ .

*Proof.* By direct calculation, we get  $\langle Fv, \bar{v} \rangle_{\tilde{\mathbb{R}}^3} = Fv \cdot \tilde{g}\bar{v} = v \cdot F^*\tilde{g}\bar{v} = \langle v, g^{-1}F^*\tilde{g}\bar{v} \rangle_{\mathbb{R}^3}$ .

On the other hand, by definition  $\langle Fv, \bar{v} \rangle_{\tilde{\mathbb{R}}^3} = \langle v, F^T \bar{v} \rangle_{\mathbb{R}^3}$ . By comparing the two expressions, we get the result.  $\square$

The orientation preserving condition for the deformation map  $u$  writes formally – it is well known –  $\det F > 0$ .<sup>21</sup> It assures then the existence of other two linear operators: the **inverse**  $F^{-1}$  of  $F$ , namely  $F^{-1} \in \text{Hom}(T_y\mathcal{B}_a, T_x\mathcal{B})$  and its formal adjoint  $F^{-*} \in \text{Hom}(T_x^*\mathcal{B}, T_y^*\mathcal{B}_a)$ .

To measure strain, we compare lengths, angles, surfaces, volumes in the reference place with the ones in the actual configuration. We must select then an ambient for the comparison of related quantities, once they are measured in the same frame to make significant the operation. The procedure is well known. When we select, for example, the reference place  $\mathcal{B}$  as an ambient for the comparison and pull-back in it *objects* pertaining to the actual place, we find primarily two versions of the strain tensor: The one that we immediately meet by direct calculation is given by  $E := \frac{1}{2}(C - g)$ , where the second-rank tensor  $C = F^*\tilde{g}F$ , with components  $C_{AB} = F_A^i \tilde{g}_{ij} F_B^j$ , is the fully covariant version of the **right Cauchy-Green tensor**, the pull-back of the spatial metric  $\tilde{g}$  in the reference place, so that  $E$  is a difference between two metric tensors. The second version of the strain tensor is  $\tilde{E} := \frac{1}{2}(\tilde{C} - \tilde{I})$ , where  $\tilde{C}$  is the 1–contravariant, 1–covariant version of the right Cauchy-Green tensor, namely  $\tilde{C} := g^{-1}C$  with components  $\tilde{C}_B^A = g^{AC}C_{CB}$ , and  $\tilde{I} := g^{-1}g = \delta_B^A \mathbf{e}^B \otimes \mathbf{e}_A$ .  $\tilde{E}$  has the meaning of a *relative* difference between metric tensors, the emphasized adjective being justified by the pre-multiplication of  $E$  by the inverse, namely  $g^{-1}$  of the metric in the reference place.

**2.2. Maps describing the inner morphology.** As anticipated above, information on the structure of matter at finer spatial scales can be attributed in beginning the construction of a mechanical model by assigning to every point  $x \in \mathcal{B}$  a variable – say  $\nu$  – that describe the microstructure. In general, to construct basic structures of a mechanical model it suffices to affirm that  $\nu$  is an element of a differentiable

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<sup>21</sup>We could drop, in principle, such an assumption, requiring just that  $F$  is non-singular, i.e.  $\det F \neq 0$ , as Noll did in his fundamental paper [93] (see also Šilhavý’s treatise [112]). However, I prefer to maintain it, for it is appropriate for a number of physical situations I shall discuss here.

manifold<sup>22</sup>  $\mathcal{M}$ . Hence, we have a map

$$x \longmapsto \nu := \tilde{\nu}(x) \in \mathcal{M}.$$

The following assumptions apply:

1.  $\mathcal{M}$  is finite-dimensional and such that every cover of it, made of open sets<sup>23</sup>, contains a sub-cover such that every point of  $\mathcal{M}$  has a neighborhood that meets only a finite number of the elements of the sub-cover.<sup>24</sup>
2. In principle  $\mathcal{M}$  is *not embedded* in any linear space. In special cases, however, physics may suggest us to select  $\mathcal{M}$  as a linear space per se (for example when  $\nu$  is a generic second-rank tensor or a stretchable vector, etc.).
3. The map  $\tilde{\nu}$  is differentiable.<sup>25</sup>

The notions of tangent and cotangent spaces to  $\mathcal{M}$  at  $\nu$ , indicated respectively by  $T_\nu\mathcal{M}$  and  $T_\nu^*\mathcal{M}$ , are available.<sup>26</sup> We do not introduce further geometric structures over  $\mathcal{M}$ , as anticipated in the first section, maintaining  $\mathcal{M}$  as abstract as possible in order to construct a framework sufficiently flexible to cover the special cases that

<sup>22</sup>Consider a set  $\mathcal{M}$  endowed with a topology, i.e. a family  $\mathcal{Y}$  of subsets of  $\mathcal{M}$  including the empty set and  $\mathcal{M}$  itself such that the union of any collection of elements of  $\mathcal{Y}$  is in  $\mathcal{Y}$ , as the intersection of any pair of elements of it is also in  $\mathcal{Y}$ . Assume that for any pair  $\nu_1, \nu_2 \in \mathcal{M}$  it is possible to find two non-intersecting sets in  $\mathcal{Y}$  containing  $\nu_1$  and  $\nu_2$ , respectively. We can summarize these properties by affirming that  $\mathcal{M}$  is a Hausdorff topological space – the topology is  $\mathcal{Y}$ . We say that  $\mathcal{M}$  is *locally Euclidean* with dimension  $\bar{m}$  when, for every  $\nu \in \mathcal{M}$ , there is a neighborhood  $\mathcal{X} \in \mathcal{Y}$  of  $\nu$  and a one-to-one map  $\varphi : \mathcal{X} \rightarrow \mathcal{Y}$ , with  $\mathcal{Y}$  an open subset of  $\mathbb{R}^{\bar{m}}$ . We call *chart* the pair  $((\mathcal{X}, \varphi))$  because  $\varphi$  induces a coordinate system over  $\mathcal{X}$  and the component  $\nu^\alpha$  makes sense with respect to a chart, namely  $\nu^\alpha := \varphi^\alpha(\nu)$ , with  $\varphi^\alpha(\nu)$  the  $\alpha$ -th components of  $\varphi(\nu) \in \mathbb{R}^{\bar{m}}$ . We call *atlas* a system of charts covering the whole  $\mathcal{M}$ . Consider one such atlas – say  $\mathfrak{F} := \{(\mathcal{X}_i, \varphi_i)\}$ , with  $i$  in some indexing set  $K$  – and imagine that it be such that (i) for all  $i, j \in K$  the maps  $\varphi_i \circ \varphi_j^{-1} : \mathcal{X}_i \cap \mathcal{X}_j \rightarrow \mathcal{Y}_i \cap \mathcal{Y}_j \subseteq \mathbb{R}^{\bar{m}}$  are of class  $C^k$ , with  $1 \leq k < +\infty$  and (ii) any other chart  $(\mathcal{X}, \varphi)$  such that  $\varphi_i \circ \varphi^{-1}$  and  $\varphi \circ \varphi_i^{-1}$  are of class  $C^k$  for all  $i \in K$  be in  $\mathfrak{F}$ . When these conditions are satisfied, we affirm that  $\mathcal{M}$  is endowed with a *differentiable structure* of class  $C^k$ . It is just the presence of  $\mathfrak{F}$  that gives to  $\mathcal{M}$  the structure of a *differentiable manifold of class  $C^k$* . When the regularity class  $C^k$  is not specified, the differentiable structure is intended to be smooth. Hence, even the reference place  $\mathcal{B}$  is a manifold when we assign over it an atlas with appropriate regularity.

<sup>23</sup> $\mathcal{M}$  is endowed with a topology so that for it the notion of open subset makes sense.

<sup>24</sup>This last property assures that  $\mathcal{M}$  admits partitions of unity for any open cover, with consequent technical advantages. Also, the assumption does not restrict the generality of the physical meaning of the developments presented later and referred to what we know in the mechanics of materials in terms of classical field theories.

<sup>25</sup>We affirm that a map  $\tilde{\nu}$  taking values on a manifold is differentiable at  $\nu$  (or in a neighborhood of  $\nu$ ) when in some chart  $\{(\mathcal{X}, \varphi)\}$  around  $\nu$  the map  $\tilde{\nu} \circ \varphi$  is differentiable in the standard sense adopted in  $\mathbb{R}^{\bar{m}}$ .

<sup>26</sup>Consider non-intersecting differentiable curves over  $\mathcal{M}$ , namely differentiable maps of the type  $\phi : (-\bar{s}, \bar{s}) \rightarrow \mathcal{M}$ , with  $\bar{s} > 0$ . We affirm that two such curves, say  $\phi$  and  $\tilde{\phi}$ , agree at  $\nu := \phi(0)$  when  $\phi(0) = \tilde{\phi}(0)$  and  $\frac{d\phi}{ds}|_{s=0} = \frac{d\tilde{\phi}}{ds}|_{s=0}$ . Hence, we call *tangent vector* to  $\mathcal{M}$  at  $\nu$  (and indicate it by  $\dot{\nu}$ , leaving implicit that it is referred to a specific  $\nu$ ) the equivalence class of curves over  $\mathcal{M}$  agreeing at  $\nu$  – it not the sole way to define the tangent vector to a manifold at a point. All these vectors at  $\nu$  form a linear space with the usual operations of componentwise addition and multiplication by a scalar. This space is what we indicate by  $T_\nu\mathcal{M}$  and call the *tangent space*. It has dimension equal to the one of  $\mathcal{M}$ . Its dual (i.e. the linear space of linear forms over  $T_\nu\mathcal{M}$ ) is what we call *cotangent space* to  $\mathcal{M}$  at  $\nu$ . The disjoint union  $T\mathcal{M} := \cup_{\nu \in \mathcal{M}} T_\nu\mathcal{M}$  is the *tangent bundle* to  $\mathcal{M}$ . Its dimension is twice the one of  $\mathcal{M}$ . Elements of  $T\mathcal{M}$  are, in fact, pairs  $(\nu, \dot{\nu})$ . Although  $T_\nu\mathcal{M}$  is a linear space,  $T\mathcal{M}$  does not, unless  $\mathcal{M}$  is embedded in a linear space.

we know and to constitute a tool for stipulating further models of specific material classes.

The spatial derivative of the map  $\tilde{\nu}$  is indicated by  $N$ , namely  $N := D\tilde{\nu}(x)$ . It is a linear operator from the tangent space to  $\mathcal{B}$  at  $x$  onto  $T_\nu\mathcal{M}$ . In short, we write  $N \in \text{Hom}(T_x\mathcal{B}, T_{\tilde{\nu}(x)}\mathcal{M})$ .

When we assign a unique  $\mathcal{M}$  to the whole body, we are presuming in a sense that the *typology* of microstructures is uniform, or better, that we choose to describe microstructural features of the *same type* at every point. We are tacitly adopting the already mentioned axiom of permanence of the material element for we presume implicitly that the microstructure is *always* adequately represented by  $\nu \in \mathcal{M}$  along motions. Of course, the choice limits the description of some classes of possible material mutations.

**2.3. Additional remarks on strain measures.** Having constructed so far an enriched description of the body morphology, a question is whether the traditional deformation measures, i.e.  $E$  or the right Cauchy-Green tensor  $C$  or their Eulerian counterparts (not rendered explicit here but matter of standard textbooks) are sufficient to evaluate completely the strain. An example motivating the question can be found in the special case of micromorphic media (see [87]). For them, in fact,  $\nu$  is a second-rank symmetric tensor and represents a microscopic strain: every material element is considered as a cell able to deform independently of its neighbors.<sup>27</sup> Hence, it is possible to think of a relative strain (see [87]): it is the macroscopic one deprived by the microscopic part, a type of strain measure, indeed. Another example is in the theory of the Cosserat brothers [19]; there  $\mathcal{M}$  coincides with the special orthogonal group<sup>28</sup>  $SO(3)$  or, alternatively, with the unit sphere  $S^2$ ; in other words, the material element is considered as a *small* rigid body<sup>29</sup> able to rotate independently of the neighboring elements.

To answer the previous question on the extension of strain measures, the key point is the specific nature of  $\nu$ . In fact, when  $\nu$  represents an independent micro-strain or a rotation, or else a micro-displacement, it is possible to define strain measures involving  $\nu$  and/or its spatial derivative  $N$ . In contrast, when  $\nu$  describes something like the volume fraction of a phase or the spontaneous polarization in ferroelectrics, etc., the common strain tensor in Lagrangian or Eulerian representation is sufficient to measure strain.

In general, what I can say is that we could imagine to define a second-rank symmetric tensor – let us say  $G$  – depending on  $F$ , the spatial metric  $\tilde{g}$ ,  $\nu$ , and  $N$ , which is a metric on  $\mathcal{B}$  and reduces to the right Cauchy-Green tensor  $C$  when  $\nu$  does

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<sup>27</sup>The scheme can be appropriate for composites made of polymers scattered in a softer matrix. It has also a role in explaining how the scheme that we are discussing here includes also the one of second-grade elasticity and enrichments of it (see [12] for a decisive result on this point).

<sup>28</sup> $Q \in SO(3)$  means that  $Q$  is a second-rank tensor such that  $\det Q = 1$  and  $Q^{-1} = Q^T$ . Incidentally,  $SO(3)$  is a manifold with the algebraic structure of a group, given by the standard multiplication between matrices. Hence,  $SO(3)$  is, by definition, a Lie group for being both a group and a smooth manifold such that the operations defining the group structure (i.e. multiplication and inversion) are smooth mappings.  $SO(3)$  is a subgroup of the orthogonal group  $O(3)$  with elements having determinant  $+1$  or  $-1$ . The elements with determinant equal to  $-1$  describe reflections. In particular,  $SO(3)$  is the connected component of the identity of  $O(3)$ .

<sup>29</sup>Smallness makes sense time to time as a structural ingredient of the specific model where Cosserat's scheme is adopted.

not describe a deformation-type property. This way we could have a generalized deformation tensor  $\hat{E}$ , defined by  $\hat{E} := \frac{1}{2}(\mathbf{G} - g)$ .

Another question is the possible comparison between microstructural states. The paragon between  $\nu$  and  $\nu_1$ , values at  $x$  of two different maps, say  $\tilde{\nu}$  and  $\tilde{\nu}_1$ , is not the sole point. We could require a comparison between the two derivatives at  $x$ , namely  $N := D\tilde{\nu}(x)$  and  $N_1 := D\tilde{\nu}_1(x)$ , or even the two maps  $\tilde{\nu}$  and  $\tilde{\nu}_1$ . To this aim, we need to define additional geometric structures over  $\mathcal{M}$  and/or to impose that  $\mathcal{M}$  is a complete manifold, as already mentioned in the introduction. Further details are in [23].

**2.4. Motions.** In the standard format of continuum mechanics, **motions** are time-parameterized families of deformations, namely  $(x, t) \mapsto y := u(x, t) \in \tilde{\mathcal{E}}^3$ , with  $t$  the time running in some interval of the real line. We assume that  $u$  is at least twice piecewise differentiable with respect to time, and we write  $\dot{y}$  for the velocity  $\frac{du}{dt}(x, t)$ , considered as a field over  $\mathcal{B}$ , taking values in  $T_y\mathcal{B}_a$ , and  $v := \tilde{v}(y, t)$  for the same velocity viewed now as the value in  $T_y\mathcal{B}_a$  of a field over the actual place  $\mathcal{B}_a := u(\mathcal{B}, t)$  – the latter is the Euclidean representation of the velocity while the former is the Lagrangian one. The second derivative of  $u$  with respect to time, evaluated at  $x$  and  $t$ , and indicated by  $\ddot{y}$ , defines the acceleration in Lagrangian description. Its Eulerian version  $a(y, t)$  is given by  $a := \frac{\partial v}{\partial t} + D_y v$ , where  $D_y$  is the derivative with respect to  $y$ .

The scheme presented so far, however, includes the description of the geometry of the finer scale material texture. Hence, we have to intend motions as pairs of time-parameterized families of deformations *and* descriptors of the material morphology at micro-scales in space. In addition to  $u(x, t)$  we consider maps  $(x, t) \mapsto \nu := \tilde{\nu}(x, t) \in T_\nu\mathcal{M}$  and indicate by  $\dot{\nu}$  the rate of change of the finer scale morphology in Lagrangian representation, namely  $\dot{\nu} := \frac{d\tilde{\nu}}{dt}(x, t)$ .

We can also have an Eulerian view on the rate of microstructural shapes by defining a map  $\tilde{\nu}_a := u^{-1} \circ \tilde{\nu}$ , the Eulerian version of  $\tilde{\nu}$ , and a field  $(y, t) \mapsto v := \tilde{v}(y, t) \in T_{\tilde{\nu}_a(y, t)}\mathcal{M}$ . While  $\dot{y} = v$ , we do not get identity between  $\dot{\nu}$  and its Eulerian version.

**2.5. Further geometric notes**<sup>30</sup>. Consider a vector  $a \in \mathbb{R}^3$  at  $x \in \mathcal{B}$ . Its image under the deformation  $u$  is  $\tilde{a} = Fa$ , with  $F$  given by  $Du(x)$ . I am repeating here what is written above just to remind that  $F$  governs how line elements change from the reference to the current shape of the body – they are stretched and rotated. The way in which oriented areas change is described by Nanson formula: in it the key rôle is played by the cofactor  $\text{cof}F$ . Finally, the determinant  $\det F$  is the factor linking a volume in  $\mathcal{B}$  with its counterpart in the actual shape  $\mathcal{B}_a$ . These three aspects of the way in which a body deforms can be collected in a unique geometric entity, a **3–vector** indicated by  $M(F)$ . It is a third-rank, skew-symmetric tensor, with all contravariant components. It is defined by using the wedge product  $\wedge$ .<sup>31</sup>

<sup>30</sup>In principle, the reader could jump such a section during a first reading, coming back to it just before beginning the last section.

<sup>31</sup>Let  $\mathcal{L}$  be a linear space, with basis  $(\mathbf{e}_1, \dots, \mathbf{e}_m)$ . The symbol  $\wedge$  indicates a map  $\wedge : \mathcal{L} \times \mathcal{L} \rightarrow \text{Skw}(\mathcal{L}^*, \mathcal{L})$ , with  $\text{Skw}(\mathcal{L}^*, \mathcal{L})$  the space of skew-symmetric tensors from the dual of  $\mathcal{L}$ , indicated by  $\mathcal{L}^*$ , to  $\mathcal{L}$ . The linear space  $\mathcal{L}^*$  is endowed with basis  $(\mathbf{e}^1, \dots, \mathbf{e}^m)$ . The space of skew-symmetric tensors of type  $(k, 0)$ , namely tensor with  $k$  contravariant components, also called  **$k$ -vectors**, is then indicated by  $\Lambda_k(\mathcal{L})$ . It is a linear space. Its dual,  $\Lambda^k(\mathcal{L})$ , the space of linear maps over  $\Lambda_k(\mathcal{L})$ , is linear too.

To construct  $M(F)$ , select linearly independent vectors  $a_1, a_2$ , and  $a_3$  at a point  $x$  in  $\mathcal{B}$  and consider maps of the type

$$\begin{aligned} a_1 \wedge a_2 \wedge a_3 &\longmapsto Fa_1 \wedge a_2 \wedge a_3, \\ a_1 \wedge a_2 \wedge a_3 &\longmapsto Fa_1 \wedge Fa_2 \wedge a_3, \\ a_1 \wedge a_2 \wedge a_3 &\longmapsto Fa_1 \wedge Fa_2 \wedge Fa_3, \end{aligned}$$

obtained by pushing forward by means of  $F$  one or more vectors from  $\mathcal{E}^3$  to  $\tilde{\mathcal{E}}^3$ . The values of these three maps are linearly independent and are all third-rank, skew-symmetric contravariant tensors. We then define  $M(F)$  as the third-rank, skew-symmetric contravariant tensor given by

$$\begin{aligned} M(F) &:= a_1 \wedge a_2 \wedge a_3 + \\ &+ Fa_1 \wedge a_2 \wedge a_3 + a_1 \wedge Fa_2 \wedge a_3 + a_1 \wedge a_2 \wedge Fa_3 + \\ &+ Fa_1 \wedge Fa_2 \wedge a_3 + Fa_1 \wedge a_2 \wedge Fa_3 + a_1 \wedge Fa_2 \wedge Fa_3 + \\ &+ Fa_1 \wedge Fa_2 \wedge Fa_3 = \\ &= (a_1, Fa_1) \wedge (a_2, Fa_2) \wedge (a_3, Fa_3). \end{aligned}$$

Its components are the number 1, and all the entries of  $F$  (in the terms where  $F$  acts on just one vector),  $\text{cof}F$  (where  $F$  is applied to two vectors),  $\det F$  (the last term).

In deriving the standard strain measures, we have in mind that  $F := Du(x)$ , while we can construct  $M(F)$  even in case of incompatible strain, that is when the map  $x \mapsto F(x)$  is such that  $\text{curl}F \neq 0$ , then  $F \neq Du(x)$ .  $M(F)$  belongs to  $\Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$  (see previous footnote) but not all elements of  $\Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$  are of the type  $M(F)$ . In other words, not all 3-vectors are generated by only one linear operator, as  $M(F)$  is by construction. Two constants, say  $\zeta$  and  $\mathbf{a}$ , and two independent linear operators, e.g.  $H$  and  $A$  determine, in fact, a generic element  $M$  of  $\Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$ . With respect to the bases in  $\mathbb{R}^3$  and  $\tilde{\mathbb{R}}^3$  indicated above, namely  $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$  and  $(\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2, \tilde{\mathbf{e}}_3)$ , every 3-vector  $M \in \Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$  has the form

$$\begin{aligned} M &= \zeta \mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3 + \sum_{i,J}^3 (-1)^{J-1} H^{iJ} \mathbf{e}_J \wedge \tilde{\mathbf{e}}_i + \\ &+ \sum_{i,J}^3 (-1)^{i-1} A^{iJ} \mathbf{e}_J \wedge \tilde{\mathbf{e}}_i + \mathbf{a} \tilde{\mathbf{e}}_1 \wedge \tilde{\mathbf{e}}_2 \wedge \tilde{\mathbf{e}}_3, \end{aligned}$$

where  $\bar{J}$  is the complementary multi-index to  $J$  with respect to  $(1, 2, 3)$  and  $\bar{i}$  has an analogous relation with  $i$  (for example, if  $J = 1$ , then  $\bar{J} = (2, 3)$  and  $\mathbf{e}_{\bar{J}} = \mathbf{e}_2 \wedge \mathbf{e}_3$ , and the same holds for the index  $i$  and its pertinent  $\bar{i}$ ).<sup>32</sup> For the sake of conciseness we shall write  $M = (\zeta, H, A, \mathbf{a})$ . In the previous definition of  $M$  we put in evidence the algebraic signs to allow easily the identification of the coefficients in the special case  $M = M(F)$ .

$M$  coincides with  $M(F)$  when  $\zeta = 1$ ,  $H = Fg^{-1}$ ,  $A = \tilde{g}\text{cof}F$  when  $\text{cof}F$  is defined by  $(\det F)(F^{-1})^*$  or  $A = \text{cof}Fg^{-1}$  when we consider  $\text{cof}F$  as given by  $(\det F)(F^{-1})^T$ , and  $\mathbf{a} = \det F$ . In short we can write  $\mathbf{M}(F)$  for the list  $(F, \text{cof}F, \det F)$  so that, when  $M = M(F)$ , we have  $M(F) = (1, \mathbf{M}(F))$ . Remind that a special case of  $M(F)$  is when  $M = M(Du)$ .

<sup>32</sup>The construction leading to  $M(F)$  can be naturally extended to  $\mathbb{R}^m$ . A detailed treatment of the matter appears in [43]

The rôle of  $M(F)$  clearly appears when we analyze the existence of ground states in non-linear elasticity of simple bodies [42], even including a detailed description of the microstructure [75]<sup>33</sup>, as we do here, and in describing the occurrence of cracks through the measures called varifolds [41], as I shall sketch below.

### 3. OBSERVERS

In traditional continuum mechanics, an observer is a frame in the ambient space and a time scale. Changes in observers are largely used to restrict possible constitutive choices by imposing requirements of *objectivity* or *covariance*. Specifically, scalars, vectors, tensors are objective when they are altered in accord to their tensor nature under isometric changes in observers in space – in the classical approach the time scale is assumed to be invariant or to undergo an affine change, so the attention is primarily focused on space.

For example, the energy density should be invariant if we presume that it is objective – in this case physics does not suggest alternatives, and the consequence in the non-linear mechanics of simple elastic bodies undergoing large strains is the incompatibility of the objectivity of the energy with its possible convexity with respect to  $F$  (see [18]).

Another rôle played by the changes in observers appears when we realize that the inner power of actions vanishes when it is evaluated on rigid-body motions. A consequence is the invariance of the external power of actions under changes in observers (frames) governed by time parameterized families of isometries in space (rigid-body motions). Such a remark, due to Gabrio Piola, has been adopted in a reverse way, roughly speaking, by Walter Noll (see [94] and [95]) who has used in the standard setting of continuum mechanics (the one of Cauchy's bodies<sup>34</sup>) the invariance of the sole external power of actions as a first principle from which we can derive standard integral balances of actions, the existence of the stress and, finally, pointwise balance equations under appropriate regularity of the fields involved.

Due to its crucial (in the sense just specified) significance, the notion of observer has to be discussed in the enlarged setting that we are treating here.

In the standard framework, the ambient space and the time scale are the sole geometric environments where we represent motion and body morphology. Hence, I find reasonable to suggest for the enlarged setting discussed here a definition that accounts strictly for the essence of the standard approach.

**Definition 1.** *An **observer** is a collection of coordinate systems (an atlas, in short) over all the geometrical environments necessary to describe the morphology of a body and its motion.*

In the present framework, beyond the ambient space  $\tilde{\mathcal{E}}^3$ , and the time scale (an interval of the real line), the complete list would include the space  $\mathcal{E}^3$  where

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<sup>33</sup>See also [92] for another point of view, an interesting one for the inclusion of a Korn-type inequality, on the existence results in the class of micromorphic media, the case when  $\mathcal{M}$  is a space of second-rank tensors. The coercitivity condition in [75] is stronger than the one in [92]. However, the use of the weakened condition adopted in [92] takes advantage from a special expression of the energy less general than the one used in [75].

<sup>34</sup>I call *Cauchy's bodies* those described appropriately (the adverb refers to our evaluation of the effectiveness of the models that we propose) by the traditional scheme in which the material morphology is represented by the sole place occupied by the body in space and the actions are standard bulk forces and stresses.

we place the reference shape, and the manifold  $\mathcal{M}$  of microstructural shapes. In defining changes in observers, alternatives are possible. The main list follows.

**3.1. Isometry-based changes in observers.** The classes of changes in observers listed below are synchronous. Including affine changes in time would not alter the results. Moreover, more intricate changes in time would lead us toward relativistic setting that is not considered here.

*3.1.1. Class 1: leaving invariant the reference space.* Two observers  $\mathcal{O}$  and  $\mathcal{O}'$  differ in the representation of the ambient space  $\mathcal{E}^3$  by time parametrized families of isometries (rigid-body motions). Smooth maps  $t \mapsto a(t) \in \mathbb{R}^3$  and  $t \mapsto Q(t) \in SO(3)$ , with  $t \in \mathbb{R}$  the time, describe the isometries just mentioned. If  $\dot{y}$  and  $\dot{y}'$  are the velocities evaluated at  $x$  and  $t$  by  $\mathcal{O}$  and  $\mathcal{O}'$  respectively, the pull-back of  $\dot{y}'$  into the frame defining  $\mathcal{O}$ , namely  $\dot{y}^* := Q^T \dot{y}'$ , is given by

$$(3.1) \quad \dot{y}^* = \dot{y} + c(t) + q(t) \times (y - y_0),$$

where  $y_0$  is an arbitrary point in space,  $c := Q^T \dot{a} \in \mathbb{R}^3$ , and  $q$  is the axial vector of the skew-symmetric tensor  $Q^T \dot{Q}$ . The relation is standard. Since Lagrangian and Eulerian representations of the velocity coincide, i.e.  $\dot{y}(x, t) = v(y, t)$ , with  $v$  the velocity intended as a field over  $\mathcal{B}_a$  at the instant  $t$ , the Eulerian counterpart of (3.1) is given by

$$(3.2) \quad v^* = v + c(t) + q(t) \times (y - y_0).$$

The problem is now to understand how we have to interpret changes in observers on the manifold of microstructural shapes  $\mathcal{M}$ .

Picturing the morphology of bodies in the product space  $\tilde{\mathcal{E}}^3 \times \mathcal{M}$  is just a model. There are interactions between macroscopic deformation and microstructural events. In contrast, in the scheme sketched above, gross deformation and microstructural changes are described in different spaces. Also, what we define formally to be an observer is a picture of our physical observation of phenomena. In laboratory, when we change frame (and it is in the physical space), in principle we may perceive a different picture of microstructural events, according to the change, so in the continuum model we must take into account that microstructures are in fact in the physical space and that their representation over  $\mathcal{M}$  is just a convenient tool that allows us to transfer at macroscopic level information on microscopic events. We have to consider then a possible **link** between changes in observers in the ambient space  $\mathcal{E}^3$  and the ones over  $\mathcal{M}$ .

Before specifying the link, we have to define the manner in which we can change atlas over  $\mathcal{M}$ . To this aim we use smooth diffeomorphisms of  $\mathcal{M}$  onto itself. They constitute a group, indicated by  $\text{Diff}(\mathcal{M}, \mathcal{M})$ . It is not precisely necessary to consider changes on  $\mathcal{M}$  determined by any arbitrary element of  $\text{Diff}(\mathcal{M}, \mathcal{M})$ . More specifically, we can affirm that we alter  $\mathcal{M}$  by a Lie group<sup>35</sup>  $G$  which can coincide either with  $\text{Diff}(\mathcal{M}, \mathcal{M})$  or a subgroup of it and is such that its action over  $\mathcal{M}$  is non-singular.  $\mathfrak{g}$  is a common notation for its Lie algebra: the tangent space to the identity of  $G$ .

Consider a one-parameter smooth curve  $\mathbb{R}^+ \ni s \mapsto \mathfrak{g}_s \in G$  over  $G$ . The tangent vector to the curve at  $s = 0$ , namely  $\xi := \frac{d\mathfrak{g}_s}{ds} \Big|_{s=0}$  belongs to  $\mathfrak{g}$ . Its action over  $\nu \in \mathcal{M}$  is denoted by  $\xi_{\mathcal{M}}(\nu)$ . In particular, we indicate by  $\nu_{\mathfrak{g}}$  the value

<sup>35</sup>See footnote 27.

$\mathbf{g} \circ \nu = \mathbf{g}(\nu)$ . From a given  $\nu \in \mathcal{M}$ , the curve  $s \mapsto \mathbf{g}_s$  generates an orbit  $s \mapsto \nu_{\mathbf{g}_s}$  over  $\mathcal{M}$  itself, so we get  $\xi_{\mathcal{M}}(\nu) = \frac{d}{ds} \nu_{\mathbf{g}_s} |_{s=0}$ . Essentially, we can consider a field  $x \mapsto v(x) := \xi_{\mathcal{M}}(\nu(x))$  assigning to every  $x$  in  $\mathcal{B}$  an element of the tangent space of  $\mathcal{M}$  at  $\nu(x)$ , generated by the action of  $\xi_{\mathcal{M}}$ , which is essentially a virtual rate of change of the material microstructure.

With these tools, we can define the link between changes of frames in the ambient space and the ones over  $\mathcal{M}$ . Formally, it is established by the existence of a **family** of differentiable homomorphisms  $\{\lambda\}$  mapping the group of diffeomorphisms of the ambient space over  $G$ , namely  $\{\lambda : \text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3) \rightarrow G\}$ . Changes in the ambient space governed by  $h \in \text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3)$  imply changes  $\nu \mapsto \nu_h := \mathbf{g}_h(\nu)$  on  $\mathcal{M}$ , with  $\mathbf{g}_h = \lambda(h)$ . When  $\{\lambda\}$  is not empty, any smooth curve  $t \mapsto h(t) \in \text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3)$  induces, consequently, a related curve  $t \mapsto \nu_h(t)$  over  $\mathcal{M}$ . Differentiation at  $t = 0$  defines the relevant  $\xi_{\mathcal{M}}(\nu)$ . However, the family  $\{\lambda\}$  can be even empty in appropriate physical circumstances, and this case has also its significant consequences.

In this section, the changes in observers considered in the ambient space  $\tilde{\mathcal{E}}^3$  are isometries (two observers differ with each other by a rigid-body motion: translation  $a(t) \in \mathbb{R}^3$  and rotation  $Q(t) \in SO(3)$ , indeed). Hence, the homomorphisms in  $\{\lambda\}$  must account *just* for the effect of frame rotation in the physical space on the representation of microstructures on  $\mathcal{M}$ , which is not altered by a rigid translation of the whole body. Formally,  $\{\lambda\}$  reduces to  $\{\lambda : SO(3) \rightarrow G\}$ . The consequent analysis distinguishes two different cases: (1)  $SO(3)$  is a subgroup of  $\text{Diff}(\mathcal{M}, \mathcal{M})$ , (2)  $SO(3)$  is not included in  $\text{Diff}(\mathcal{M}, \mathcal{M})$ .

In both cases the rule governing how  $\dot{\nu}$  is altered under changes in observers is

$$(3.3) \quad \dot{\nu}^* = \dot{\nu} + \mathcal{A}(\nu)q,$$

with  $q$  the vector of rotational speed in (3.1) and, at any  $t$  in the time interval under scrutiny,  $\mathcal{A}(\nu) \in \text{Hom}(\mathbb{R}^3, T_\nu \mathcal{M})$ .

What changes from case 1 to case 2 is the meaning of the linear operator  $\mathcal{A}(\nu)$ .

When  $SO(3)$  is a subgroup of  $\text{Diff}(\mathcal{M}, \mathcal{M})$  and the family  $\{\lambda\}$  is not empty,  $\mathcal{A}(\nu)$  is the infinitesimal generator of the action of  $SO(3)$  over  $\mathcal{M}$  – in analogous way the rigid velocity in (3.1) is given by the action of the Euclidean group (the one of rigid-body motions, once again a Lie group) over the ambient space  $\tilde{\mathcal{E}}^3$ . Consider a differentiable map  $t \mapsto Q(t) = \exp(-\mathbf{e}q(t)) \in SO(3)$ , with  $\mathbf{e}$  Ricci's symbol, and  $q(t) \in \mathbb{R}^3$ . Denote by  $\nu_q$  the value of  $\nu$  after the action of  $Q$  (its specific form depends on the tensor rank of  $\nu$ ). By explicit computation of the time derivative of  $\nu_q$ , we find that the vector  $q$  in (3.3) is the rate of  $q(t)$ , namely  $q := \frac{dq(t)}{dt}$ , and we compute<sup>36</sup>

$$\mathcal{A}(\nu) = \frac{d\nu_q}{dq} |_{q=0}.$$

When  $SO(3)$  is not included in  $\text{Diff}(\mathcal{M}, \mathcal{M})$  and the set  $\{\lambda\}$  is not empty, by indicating by  $\nu_{\lambda(Q)}$  the value of  $\nu$  after the action of  $\lambda(Q) \in G$  (once again the explicit expression of  $\nu_{\lambda(Q)}$  depends on the tensor nature of  $\nu$  and  $\lambda(Q)$ ),  $\mathcal{A}(\nu)$  is given by

$$\mathcal{A}(\nu) = \frac{d\nu_{\lambda(Q)}}{d\lambda} \frac{d\lambda(Q)}{dq} |_{q=0}.$$

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<sup>36</sup>This one is the sole case treated in [13].



The expression (3.3) can be accepted, at least formally, even when we do not consider any link between changes in observers in the ambient space and on  $\mathcal{M}$ , i.e. when  $\{\lambda\}$  is empty. In this case, in formula (3.3) the vector  $q$  would not coincide with the rotation velocity vector in the ambient space  $\tilde{\mathcal{E}}^3$ .

**Example 1.** Let  $\mathcal{M}$  be the unit sphere  $S^2$ .  $\nu \in S^2$  is a unit vector (it is the case of magneto-elasticity in saturation conditions). When the physical space rotates by the action of  $Q(t) \in SO(3)$ , in this special case  $\nu$  becomes  $\nu' = Q\nu$  so that  $\dot{\nu}' = \dot{Q}\nu + Q\dot{\nu}$ . By defining  $\dot{\nu}^* := Q^T\dot{\nu}'$  – it is the pull-back of  $\dot{\nu}'$  into the frame of the first observer – we get  $\dot{\nu}^* = \dot{\nu} + Q^T Q \dot{\nu} = \dot{\nu} + q \times \nu$  so that, in this case,  $\mathcal{A}(\nu) = -\nu \times$ .

3.1.2. *Class 2: changing by isometries the reference space.* In all the ramifications of the previous class of changes in observers the reference place is left invariant<sup>37</sup>. We can have an enlarged view defining changes in observers that include alterations of frames in the reference space *in addition* to what is done in the ambient space and over  $\mathcal{M}$ .

We presume then isometry-based changes in observers in  $\tilde{\mathcal{E}}^3$  and their consequences over  $\mathcal{M}$  exactly as in the previous class. In addition we impose isometric changes of frame in the space  $\mathcal{E}^3$  where there is the reference place  $\mathcal{B}$ . Formally, consider a vector field  $x \mapsto w$  over  $\mathcal{B}$  (it is a field assigning at every  $x \in \mathcal{B}$  a vector in the tangent space to  $\mathcal{B}$  at the same point).  $w$  is what is perceived by the observer  $\mathcal{O}$ .  $w'$  is what an observer  $\mathcal{O}'$  measures. The pull-back of  $w'$  into  $\mathcal{O}$ , indicated by  $w^*$ , is given by

$$(3.4) \quad w^* = w + \bar{c}(t) + \bar{q}(t) \times (y - y_0),$$

where  $\bar{c}$  and  $\bar{q}$  are, as in Class 1, translational and rotational velocities. We impose that  $c$  differs from  $\bar{c}$  so as  $q$  from  $\bar{q}$ , a key point in the following developments.

3.2. **Diffeomorphism-based changes in observers.** In principle we can imagine that two observers may deform smoothly one with respect to the other in the representation of  $\tilde{\mathcal{E}}^3$ , with consequences on  $\mathcal{M}$  dictated by the family of homomorphisms  $\{\lambda\}$  introduced above. We can also foresee changes in observers deforming smoothly the reference space  $\mathcal{E}^3$ . This way we construct generalizations of the previous classes.

3.2.1. *Generalized class 1.*  $\mathcal{O}$  and  $\mathcal{O}'$  differ in time by smooth deformations of the ambient space  $\tilde{\mathcal{E}}^3$ . Formally, we have time parametrized families of diffeomorphisms  $t \mapsto h_t : \tilde{\mathcal{E}}^3 \rightarrow \tilde{\mathcal{E}}^3$ , with  $h_t \in \text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3)$ ,  $h_{t_0} = \text{identity}$ , which are differentiable in time,  $t_0$  the initial instant for the change in observer. A vector field  $y \mapsto \bar{v} := \frac{d}{dt}h_t|_{t=t_0}$  is then defined over  $\tilde{\mathcal{E}}^3$ , and, in particular, over the actual placement  $\mathcal{B}_a$  of the body.<sup>38</sup> Being a function of  $y \in \mathcal{B}_a$ ,  $\bar{v}$  enters directly a rule for the change in observer of the Eulerian representation  $v$  of the velocity. The rule is

$$v \longrightarrow v^\# := v + \bar{v}.$$

Precisely,  $v^\#$  is the imagine in  $\mathcal{O}$  of the Eulerian velocity evaluated by  $\mathcal{O}'$ . However, since  $\dot{y} = v$  (Lagrangian and Eulerian representations of the velocity coincide) we

<sup>37</sup>It is the basic reason pushing us to select the reference place of the body in a different space. In fact, if it would be in  $\tilde{\mathcal{E}}^3$ , we would not be able to leave it invariant by roto-translating the frame covering the entire space, as a change in observers imposes.

<sup>38</sup>It is the infinitesimal generator of the action of the group of diffeomorphisms  $\text{Diff}(\tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3)$ .

can consider  $\bar{v}$  as the value of a field defined over the reference place, so that, instead of  $v \longrightarrow v^\# := v + \bar{v}$ , we can write (with a slight abuse of notation)

$$\dot{y} \longrightarrow \dot{y}^\# := \dot{y} + \bar{v}.$$

As regards the influence that such changes in  $\tilde{\mathcal{E}}^3$  might have on the representation of the microstructural shapes on  $\mathcal{M}$ , we have to consider the family of homomorphisms  $\left\{ \lambda : \text{Diff} \left( \tilde{\mathcal{E}}^3, \tilde{\mathcal{E}}^3 \right) \rightarrow G \right\}$ . Consequently, with the notations introduced above, by indicating by  $\nu_{\lambda(h_t)}$  the value of  $\nu$  after the action of  $\lambda(h_t) : \mathcal{M} \longrightarrow \mathcal{M}$ , with  $h_t : \tilde{\mathcal{E}}^3 \longrightarrow \tilde{\mathcal{E}}^3$ ,  $h_t$  a diffeomorphism, we could then accept for changes in observers a relation of the type

$$\dot{\nu}^\# = \dot{\nu} + v + \mathcal{A}(\nu)q,$$

with  $\mathcal{A}(\nu)$  now given by

$$\mathcal{A}(\nu) := \left. \frac{d\nu_{\lambda(h_t)}}{d\lambda(h_t)} \frac{d\lambda(h_t)}{dt} \right|_{t=0},$$

$v$  a generic element of the linear space  $T_\nu \mathcal{M}$ ,  $q$  a rigid rotational velocity of the physical space.

The previous relation is, however, formal. The key point is to understand whether a change in physical space induced by a diffeomorphism  $h(t)$  alters the features of the microstructure that we represent by  $\mathcal{M}$  in the specific mechanical model that we develop. In this sense the choice of the class of changes in observers may depend on the physical situation that we have at hands.

Of course, we could just choose a general rule for changes in observers over  $\mathcal{M}$  of the type

$$\dot{\nu}^\# = \dot{\nu} + \bar{v},$$

with  $\bar{v}(x) \in T_{\nu(x)} \mathcal{M}$ , as a general compact version of the previous relation for  $\dot{\nu}^\#$ , which, in turn, puts in evidence the influence of the change in observer in the physical space on the way we represent the microstructure over  $\mathcal{M}$ . Obviously, in the case of isometric changes in observers,  $\dot{\nu}^\# = \dot{\nu}^*$ .

**3.2.2. Generalized class 2.** The generalization deals with changes in observer in the reference space induced by smooth deformations, precisely by time parameterized maps  $\hat{h}_t : \mathcal{E}^3 \longrightarrow \mathcal{E}^3$ , with  $\hat{h}_{t_0} = \text{identity}$ , which are diffeomorphisms in space and are differentiable in time – once again  $t_0$  is the initial instant of the change in observer.

A new vector field is then defined over the reference space and is  $x \longmapsto \bar{w} := \left. \frac{d}{dt} \hat{h}_t \right|_{t=t_0}$ . Hence, by indicating by  $w^\#$  the image in  $\mathcal{O}$  of the vector  $w$  evaluated by  $\mathcal{O}'$ , we get

$$(3.5) \quad w \longmapsto w^\# := w + \bar{w}.$$

In  $\tilde{\mathcal{E}}^3$  and over  $\mathcal{M}$  changes in observers are like in the generalized class 1.

### 3.3. Notes on definitions and use of changes in observers.

- Requirements of invariance under isometry-based changes in observers deal with what we call **objectivity** in the enlarged setting including  $\mathcal{M}$ . Their counterparts for the diffeomorphism-based classes are what we intend for **covariance** in the same framework.

- The diffeomorphism-based classes of changes in observers contain the relevant isometry-based versions. Then, a requirement of covariance is more stringent than the one of objectivity. At times, different choices may lead to different results, above all in the derivation of balance equations. For example, the requirement of invariance of the external power of actions under isometry-based changes in observers allows us to derive directly integral balances, while, in contrast, covariance brings us toward weak balances or pointwise balances under appropriate regularity conditions for the fields involved.
- In principle it would be possible to exclude the representation of the manifold  $\mathcal{M}$  from the definition of observer, considering  $\nu$  as an ‘entity’ insensitive to changes in observers. In this case the evolution of  $\nu$  would be represented by rules resulting independent of the observers. I shall come back on this issue.

#### 4. THE RELATIVE POWER IN CASE OF BULK MUTATIONS

**4.1. External power of standard and microstructural actions.** We call **part** any subset  $\mathfrak{b}$  of  $\mathcal{B}$  with non-null volume measure and the same geometric regularity of  $\mathcal{B}$  – in other words  $\mathfrak{b}$  is a fit region exactly as  $\mathcal{B}$  is. When we imagine to enucleate (the cut is just ideal) a generic part  $\mathfrak{b}$  of the body, we affirm commonly that  $\mathfrak{b}$  interacts with the rest of the body and the external environment by **bulk** and **contact** actions. The former ones are a consequence of the interaction with the rest of the universe. The latter actions are exerted through the boundary  $\partial\mathfrak{b}$  of  $\mathfrak{b}$ . A representation of them follows by analyzing the body and its environment as elements of a universe of parts, a set partially ordered with respect to the relation “*being part of*” in which, in addition, we define two operations: *meet* and *join*. A part  $\mathfrak{b}$  is the join of other two when it is the least envelop of them (which is still a part in the sense specified above). Also,  $\mathfrak{b}$  is the meet of other two parts when it is the greatest common part of the two factors. Meet and join assign to the set of parts of a body and its environment, a universe indeed, the structure of an algebra, once we have included the empty set and an infinite set (what is called “material all” by Noll). Bulk and contact actions are then defined as vector-valued functions over the set of pairs of disjoint parts of a given universe (see details in [95]). The extension of the procedure to the a scheme in which we include a multi-field and multi-scale description of material microstructures, as sketched in previous sections, has been proposed in [16]: that analysis requires not only a modified version of meet and join operations, but also the embedding of  $\mathcal{M}$  in a linear space, a tool not necessary in the developments presented below.

Another way of defining the actions is through the power that they develop. A **power** is a functional which is additive over disjoint parts of a body and linear with respect to the rates involved (see [107] for basic geometric issues on the matter). Among powers that we could define in principle, the one with the minimum entities involved is the power of all actions *external* to a generic part of the body.

Bulk and contact actions due to the deformation are on the actual shape of the body. For any part  $\mathfrak{b}_a$  of  $\mathcal{B}_a$ , in traditional continuum mechanics the representation of the **external power**,  $\mathcal{P}_{\mathfrak{b}_a}^{ext}(v)$ , of all actions over  $\mathfrak{b}_a$  is

$$\mathcal{P}_{\mathfrak{b}_a}^{ext}(v) := \int_{\mathfrak{b}_a} b_a^\dagger \cdot v \, dy + \int_{\partial\mathfrak{b}_a} t_a \cdot v \, d\mathcal{H}^2,$$

where  $dy$  and  $d\mathcal{H}^2$  indicate volume and “surface” measures in  $\mathcal{B}_a$ .  $b_a^\ddagger(y) \in T_y^*\mathcal{B}_a$  represents body forces, the *sum* of inertial and non-inertial components.  $\mathfrak{t}_a(y) \in T_y^*\mathcal{B}_a$  indicates the traction through the boundary of  $\mathfrak{b}_a$ . At any  $y \in \partial\mathfrak{b}_a$ , where the normal  $n_a(y)$  is defined uniquely (by assumption the condition is satisfied at all points of  $\partial\mathfrak{b}_a$  but a finite number of corners and edges, as already mentioned),  $\mathfrak{t}_a$  depends only on  $y$  and  $n_a(y)$  at every instant. This is the standard Cauchy assumption (see the discussion about it in [34]). We consider here the normal to  $\partial\mathfrak{b}_a$  as a covector, i.e. the normalized derivative of the function defining  $\partial\mathfrak{b}_a$  through the locus of its zeros. The presumed regularity of  $\partial\mathfrak{b}_a$  allows us such an interpretation.

An essential requirement for  $\mathcal{P}_{\mathfrak{b}_a}^{ext}(v)$ , an axiom indeed (see [95]), is its *invariance under isometry-based changes in observers of class 1*. Formally, we impose

$$\mathcal{P}_{\mathfrak{b}_a}^{ext}(v) = \mathcal{P}_{\mathfrak{b}_a}^{ext}(v^*)$$

for any translational ( $c(t)$ ) and rotational ( $q(t)$ ) velocities appearing in (3.2), and for any  $\mathfrak{b}_a$ . The assumption that the fields  $x \mapsto b_a^\ddagger(y)$  and  $x \mapsto \mathfrak{t}_a(y)$  are integrable and the invariance condition imply the validity of the balance of forces,

$$\int_{\mathfrak{b}_a} b_a^\ddagger dy + \int_{\partial\mathfrak{b}_a} \mathfrak{t}_a d\mathcal{H}^2 = 0,$$

and couples,

$$\int_{\mathfrak{b}_a} (y - y_0) \times b_a^\ddagger dy + \int_{\partial\mathfrak{b}_a} (y - y_0) \times \mathfrak{t}_a d\mathcal{H}^2 = 0.$$

If we assume that  $b_a^\ddagger$  is bounded and  $\mathfrak{t}_a$  is continuous with respect to  $y$ , the integral balance of forces implies the action-reaction principle, namely

$$\mathfrak{t}_a(y, n_a) = -\mathfrak{t}_a(y, -n_a),$$

and the Cauchy theorem, i.e. the linearity of  $\mathfrak{t}_a$  with respect to  $n_a$ , namely

$$\mathfrak{t}_a(y, n_a) = \sigma(y) n_a,$$

at every instant, that follows by the standard tetrahedron argument (see, e.g. [118]), and we have

$$\sigma(y) = \sum_{i=1}^3 \mathfrak{t}_a(y, \tilde{e}_i) \otimes \tilde{e}_i,$$

with  $\tilde{e}_i$  the  $i$ -th vector of a basis in a neighborhood of  $y$ . The assumption of continuity for  $\mathfrak{t}_a(\cdot, n_a)$  has been variously weakened (see [111] and [113]), and we have also at disposal notions of stress over manifolds (see [107], [109], [110]). Here, we accept the stronger version for the sake of simplicity. We just remark that the essence of the Cauchy theorem is that  $\sigma$  is independent of  $n_a$ . The stress  $\sigma$  is a linear operator mapping covectors (normals in the interpretation above) to covectors, the traction  $\mathfrak{t}_a$  indeed, so it is of the form  $\sigma(y) = \sigma_j^i(y) \tilde{e}_j \otimes \tilde{e}^i$ , where  $\tilde{e}^i$  is the  $i$ -th vector of the dual basis in a neighborhood of  $y$  – such a basis is defined to be such that  $\tilde{e}^i \cdot \tilde{e}_j = \delta_j^i$ , with  $\delta_j^i$  the Kronecker index. We summarize this remark writing simply  $\sigma(y) \in \text{Hom}(T_y^*\mathcal{B}_a, T_y^*\mathcal{B}_a)$ .

The standard use of the Piola transform furnishes the Lagrangian representation of the balance equations in terms of (1) the first Piola-Kirchhoff stress  $P(x) \in$

$\text{Hom}\left(T_x^*\mathcal{B}, T_{u(x)}^*\mathcal{B}_a\right)$ , obtained by pulling back into the reference place  $\mathcal{B}$  the second component of  $\sigma$ , namely

$$P = (\det F) \sigma F^{-*},$$

where  $F^{-*} := (F^{-1})^*$ , and (2) the referential bulk actions

$$b^\ddagger := (\det F) b_a^\ddagger.$$

Should we consider the normal as a vector instead of a covector, as above, in the definition of the first Piola-Kirchhoff stress the adjoint of  $F$  should be substituted by the transpose.

Alternatively, we could consider bulk and contact actions as the values over the cotangent bundle of  $\mathcal{B}_a$ , namely  $T^*\mathcal{B}_a$ , of fields defined over the reference place  $\mathcal{B}$ , accepting from the beginning the Lagrangian description. In this case the expression of the **external power** reads

$$\mathcal{P}_b^{ext}(\dot{y}) := \int_b b^\ddagger \cdot \dot{y} \, dx + \int_{\partial b} \mathfrak{t} \cdot \dot{y} \, d\mathcal{H}^2,$$

where now, at every instant, we have fields  $x \mapsto b^\ddagger(x) \in T_{u(x)}^*\mathcal{B}_a$  and  $x \mapsto \mathfrak{t}(x, n(x)) \in T_{u(x)}^*\mathcal{B}_a$  – assumed to be integrable over their domains – with  $n$  the normal to  $\partial b$  in all points to within a finite number of corners and edges. Of course, we have

$$\mathfrak{t}(x, n(x)) = \mathfrak{t}_a(u(x), n_a(u(x))).$$

The requirement of *invariance under isometry-based changes in observers of class 1* writes now

$$\mathcal{P}_b^{ext}(\dot{y}) = \mathcal{P}_b^{ext}(\dot{y}^*)$$

for any translational ( $c(t)$ ) and rotational ( $q(t)$ ) velocities appearing in (3.1), and for any  $b$ . Its immediate consequence is the validity of the integral balances of forces,

$$(4.1) \quad \int_b b^\ddagger \, dx + \int_{\partial b} \mathfrak{t} \, d\mathcal{H}^2 = 0,$$

and couples,

$$(4.2) \quad \int_b (y - y_0) \times b^\ddagger \, dx + \int_{\partial b} (y - y_0) \times \mathfrak{t} \, d\mathcal{H}^2 = 0,$$

in Lagrangian representation.

Under conditions of boundedness for  $b^\ddagger$  and continuity for  $\mathfrak{t}$  – not the weakest ones, indeed – we can use the balance of forces (4.1) to prove once again the action-reaction principle and the linearity of  $\mathfrak{t}(x, n)$  with respect to  $n$ , namely the relation

$$\mathfrak{t}(x, n) = P(x) n,$$

which is in components

$$\mathfrak{t}_i(x, n) = P_i^A(x) n_A.$$

We now have

$$P(x) = \sum_{K=1}^3 \mathfrak{t}(x, e_K) \otimes e_K,$$

with  $e_K$  the  $K$ -th vector of a basis in a neighborhood of  $x$ .

When we want to include the actions that develop power in the microstructural time rates, we may presume that they are subdivided into bulk and contact actions,

exactly like the standard ones, accepting for example the Lagrangian representation, we write an extended expression of  $\mathcal{P}_b^{ext}(\dot{y})$ , namely  $\mathcal{P}_b^{ext}(\dot{y}, \dot{\nu})$ , defined by

$$\mathcal{P}_b^{ext}(\dot{y}, \dot{\nu}) := \int_b \left( b^\ddagger \cdot \dot{y} + \beta^\ddagger \cdot \dot{\nu} \right) dx + \int_{\partial b} (\mathfrak{t} \cdot \dot{y} + \tau \cdot \dot{\nu}) d\mathcal{H}^2,$$

where  $\tau(x) \in T_{\tilde{\nu}(x)}^* \mathcal{M}$  indicates microstructural contact actions, and  $\beta^\ddagger(x) \in T_{\tilde{\nu}(x)}^* \mathcal{M}$  represents external bulk actions over the microstructure alone.<sup>39</sup> The microstructural contact actions  $\tau$  are due to non-homogeneous microstructural changes across the boundary  $\partial b$ .

We require *invariance of  $\mathcal{P}_b^{ext}(\dot{y}, \dot{\nu})$  with respect to isometry-based changes in observers in class 1*, i.e. we impose

$$\mathcal{P}_b^{ext}(\dot{y}, \dot{\nu}) = \mathcal{P}_b^{ext}(\dot{y}^*, \dot{\nu}^*)$$

for any choice of  $c$  and  $q$  in (3.1) and (3.3), and for any part  $b$ . we get first (4.1) and a varied version of (4.2), namely

$$\int_b \left( (y - y_0) \times b^\ddagger + \mathcal{A}^* \beta^\ddagger \right) dx + \int_{\partial b} \left( (y - y_0) \times \mathfrak{t} + \mathcal{A}^* \tau \right) d\mathcal{H}^2 = 0$$

(see also [15] and [65]).

**4.2. Cauchy's theorem for microstructural contact actions.** We assume that  $\tau$  is function of the point  $x$  and the normal  $n$  to  $\partial b$  in all points where the normal itself is uniquely defined and at every instant. In other words we presume the validity of Cauchy's postulate for the microstructural contact actions.

A question is then whether we can prove the Cauchy theorem for  $\tau$ .

A proof is in [16] but there the microstructure is represented in a Euclidean space, with undoubtable advantages. Here we want to maintain the representation of the microstructure in a manifold as abstract as possible, avoiding even the embedding of  $\mathcal{M}$  into a linear space for it is not unique (a question already discussed in the introduction).

We then follow another path sketched below.

First imagine to freeze the macroscopic motion and to allow just the microstructure to vary in time. In other words: select  $\dot{y} = 0$ . The requirement of invariance of  $\mathcal{P}_b^{ext}(0, \dot{\nu})$  implies just the validity of the integral balance

$$(4.3) \quad \int_b \mathcal{A}^* \beta^\ddagger dx + \int_{\partial b} \mathcal{A}^* \tau d\mathcal{H}^2 = 0.$$

It has two main advantages:

- (1): The linear operator  $\mathcal{A}^*$  projects both  $\beta^\ddagger$  and  $\tau$  into  $\mathbb{R}^3$  from  $T^* \mathcal{M}$ , which is in general a non-linear space.
- (2):  $\mathcal{A}$  does not depend on  $n$ . It is a function of  $\tilde{\nu}(x)$  alone at every instant  $t$ .

These two aspects allow us to use the integral balance (4.3) in the standard way leading to Cauchy's theorem.

We presume first that both  $\mathcal{A}^*(\tilde{\nu}(\cdot)) \beta^\ddagger(\cdot)$  and  $\mathcal{A}^*(\tilde{\nu}(\cdot)) \tau(\cdot, n)$  are essentially bounded.<sup>40</sup> By the standard technique leading to the action-reaction principle (see

<sup>39</sup>An example for  $\beta^\ddagger$  is given by the action of an electromagnetic field on the polarization of a ferroelectric material.

<sup>40</sup>It means that the integral over  $b$  of the bulk actions is bounded by the volume of  $b$  and the integral of the contact actions is bounded by the area of  $\partial b$ .

e.g. [118]) we can then prove that

$$\mathcal{A}^*(\tilde{\nu}(x))\tau(x, n) = -\mathcal{A}^*(\tilde{\nu}(x))\tau(x, -n),$$

which is

$$\mathcal{A}^*(\tau(x, n) + \tau(x, -n)) = 0,$$

i.e. the sum  $\tau(x, n) + \tau(x, -n)$  belongs to the kernel of the linear operator  $\mathcal{A}^*$ . That sum is well defined: since  $\tilde{\nu}(\cdot)$  is continuous and single-valued, as assumed from the beginning, we have at  $x$  a unique value  $\nu$  so that both  $\tau(x, n)$  and  $\tau(x, -n)$  belong to the same cotangent space  $T_\nu^*\mathcal{M}$ , which is a linear space.<sup>41</sup>

**Example 2.** Consider  $\nu$  as a 3D real vector. It is, for example, the case of quasicrystals, where  $\nu$  collects inner degrees of freedom exploited for the atomic rearrangements determining the quasi-periodic structure of the lattice. In this case we compute  $\mathcal{A} = -\nu \times$ . Consequently, at a given  $\nu$  the kernel of  $\mathcal{A}^*$  is the 1D-space parallel to  $\nu$ . Hence, the action-reaction principle deduced above prescribes that the sum  $\tau(x, n) + \tau(x, -n)$  is a vector parallel to  $\nu$ , which reduces to zero when it is projected on the physical space. Such a vector is powerless on any “rigid” rate of  $\nu$ , i.e. a rate of the type  $\mathcal{A}q$ , with  $q$  the rotation velocity vector in the physical space.

Let now assume that  $\mathcal{A}^*(\tilde{\nu}(\cdot))\tau(\cdot, n)$  is continuous.

We can exploit then the integral balance (4.3) reproducing the standard tetrahedron argument or exploiting just two linearly independent vectors in space as in [118]. What we find is that  $\mathcal{A}^*\tau(x, n) = \mathcal{A}^*\mathcal{S}(x)n$ , i.e. at  $x$  there is a linear operator mapping  $n$  into the cotangent space  $T_{\tilde{\nu}(x)}^*\mathcal{M}$  (we write in short  $\mathcal{S}(x) \in \text{Hom}(T_x^*\mathcal{B}, T_{\tilde{\nu}(x)}^*\mathcal{M})$ ) such that

$$(4.4) \quad \tau(x, n) = \mathcal{S}(x)n$$

with  $\mathcal{S}(x) \in \text{Hom}(T_x^*\mathcal{B}, T_{\tilde{\nu}(x)}^*\mathcal{M})$ . Precisely, we get

$$\mathcal{S}(x) := \sum_{K=1}^3 \tau(x, e_A) \otimes e_A,$$

where, as above,  $e_A$  is the  $A$ -th vector of a basis in a neighborhood of  $x$ . In components we have

$$\tau_\alpha(x, n(x)) = \mathcal{S}_\alpha^A(x)n_A(x),$$

where Greek indices indicate components over  $\mathcal{M}$ . We call  $\mathcal{S}$  **microstress** to recall its rôle analogous to the standard stress and its microstructural origin.

Refinements seem possible:

- the construction of a framework determining the need of Cauchy’s postulate for  $\tau$  (I refer to the appropriate generalization of the Hamel-Noll theorem, see [118]), and
- the weakening of the continuity assumption along the guidelines indicated in [111] and [113].

Difficulties arise when we consider  $\tilde{\nu}(\cdot)$  as a multi-valued function over  $\mathcal{M}$ , with values determined modulo a permutation, as proposed for a refined description of material complexity in [33], where the conditions for the existence of the ground states for the relevant elastic energy are determined in this case.

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<sup>41</sup>The cotangent bundle  $T^*\mathcal{M} := \cup_{\nu \in \mathcal{M}} T_\nu^*\mathcal{M}$  is in general non-linear.

**4.3. The relative power: a definition.** In the expressions of the power discussed above, the reference place  $\mathcal{B}$  is presumed fixed once and for all. In presence of bulk mutations in the matter we can resort to the idea of having multiple reference shapes interpreted in one of the ways described in the introduction. Here the attention is on the definition of the vector field  $x \mapsto w(x) \in T_x\mathcal{B}$ , that we presume to be differentiable, a *virtual* velocity mimicking the incoming rearrangements of material elements that determine the mutation. In this case we can think of writing the external power *relatively* to  $w$ . Moreover, since the vector field  $w(\cdot)$  represents *material* mutations, we have to consider that along these mutations we have

- (i): changes in the energetic landscape and
- (ii): actions in  $\mathcal{B}$  power conjugated with the rupture of existing material bonds and/or the formation of new ones, and mutation-induced anisotropy.

In principle, in both cases we can have energy fluxes across boundaries inside the body and consequent emergence of anisotropies in the distribution of the energy itself. However, *although we mention energy at this stage, we are not referring to specific constitutive classes*. We need just to affirm that there is the free energy  $\psi$  and it changes in space and time when material mutations occur, nothing more. In particular, we write

$$\psi = \tilde{\psi}(x, t, \varsigma),$$

with  $\varsigma$  the list of state variables that we *do not specify*. They have to be rendered explicit in discussing constitutive issues, not here. Moreover, in addition to standard and microstructural actions we should include the ones not associated with deformation or microstructural events described by  $\dot{\nu}$  (see item (ii) in the list above). A way to maintain distinct these new actions is to represent them as covector fields over  $\mathcal{B}$  (vectors if we use the standard identification of  $\mathbb{R}^3$  with its dual) of forces  $f$  and couples  $\mu$  developing power on  $w$  and its curl, respectively. Further assumptions apply.

- (1)  $f$  may have just dissipative nature. It vanishes when the mechanical process is conservative.
- (2)  $\mu$  has dissipative and conservative components, the latter appearing when the material mutations produce anisotropy without breaking and/or reforming material bonds.

By taking into account the representation of the contact actions in terms of stress and microstress in Lagrangian configuration, I define the **relative power**, writing  $\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w)$  for it, as the sum of the **relative power of actions**, indicated by  $\mathcal{P}_b^{rel-a}(\dot{y}, \dot{\nu}, w)$ , and another functional that I call **power of disarrangements**,  $\mathcal{P}_b^{dis}(w)$ , determined by the energy fluxes and the configurational forces  $f$  and  $\mu$  listed above. Precisely,  $\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w)$  has the following form:

$$\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w) := \mathcal{P}_b^{rel-a}(\dot{y}, \dot{\nu}, w) + \mathcal{P}_b^{dis}(w)$$

with

$$\begin{aligned} \mathcal{P}_b^{rel-a}(\dot{y}, \dot{\nu}, w) &: = \int_b b^\ddagger \cdot (\dot{y} - Fw) \, dx + \int_{\partial b} Pn \cdot (\dot{y} - Fw) \, d\mathcal{H}^2 + \\ &+ \int_b \beta^\ddagger \cdot (\dot{\nu} - Nw) \, dx + \int_{\partial b} \mathcal{S}n \cdot (\dot{\nu} - Nw) \, d\mathcal{H}^2 \end{aligned}$$



and

$$\mathcal{P}_b^{dis}(w) := \int_{\partial b} (n \cdot w) \psi \, d\mathcal{H}^2 - \int_b (\partial_x \psi + f) \cdot w \, dx + \int_b \mu \cdot \operatorname{curl} w \, dx.$$

In the previous expressions,  $\partial_x \psi$  is the **explicit derivative** of  $\tilde{\psi}(x, t, \varsigma)$  with respect to  $x$ , holding fixed all the other entries of the energy. It is an indicator of the loss of homogeneity in the energy landscape, altered by the mutation. The term  $(n \cdot w) \psi$  is the energy density flux across the boundary  $\partial b$ , due to the mutation itself.

- When  $w = 0$  at every point (the body does not undergo bulk macroscopic mutations),  $\mathcal{P}_b^{dis}(w)$  vanishes and  $\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w)$  reduces to the external power  $\mathcal{P}_b^{ext}(\dot{y}, \dot{\nu})$ .
- $\mathcal{P}_b^{dis}(w)$  accounts for macroscopic mutations. The microscopic ones pertain to the terms

$$\int_b \beta^\ddagger \cdot \dot{\nu} \, dx + \int_{\partial b} \mathcal{S} n \cdot \dot{\nu} \, d\mathcal{H}^2$$

in  $\mathcal{P}_b^{rel-a}(\dot{y}, \dot{\nu}, w)$ . There is micro-to-macro interaction. It appears in the pointwise balance equations and the constitutive issues.

- When we do not consider a multi-field and multi-scale representation of material microstructures and describe bodies in the standard format, the relative power obviously reduces to

$$\mathcal{P}_b^{rel}(\dot{y}, w) := \mathcal{P}_b^{rel-a}(\dot{y}, w) + \mathcal{P}_b^{dis}(w)$$

where  $\mathcal{P}_b^{rel-a}(\dot{y}, w)$  is derived by  $\mathcal{P}_b^{rel-a}(\dot{y}, \dot{\nu}, w)$  by cancelling microstructural actions and is

$$\mathcal{P}_b^{rel-a}(\dot{y}, w) := \int_b b^\ddagger \cdot (\dot{y} - Fw) \, dx + \int_{\partial b} Pn \cdot (\dot{y} - Fw) \, d\mathcal{H}^2,$$

while  $\mathcal{P}_b^{dis}(w)$  remains the same.

Notice that I have written  $\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w)$  in terms of the first Piola-Kirchhoff stress  $P$  and the microstress  $\mathcal{S}$  taking advantage of the discussion about their existence in previous sections. However, we could write  $\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w)$  in its more primitive form including  $\mathbf{t}$  and  $\boldsymbol{\tau}$  in place of  $Pn$  and  $\mathcal{S}n$ . In this case the results below, emerging from a requirement of invariance of  $\mathcal{P}_b^{rel}(\dot{y}, \dot{\nu}, w)$  under changes in observers of class 2, would be enriched by the proof of the existence of  $P$  and  $\mathcal{S}$ , and their independence of  $n$ .

**4.4. Kinetics.** Microstructural inertia can appear for example in the case of bubbles migrating inside a liquid in motion, relatively to it, and vibrating within it (see remarks in [14]), or solids with an enormous number of cavities, each one containing a gyroscope (a case discussed in [85]).

In his book on continua with microstructure [13], Capriz writes the kinetic energy in a multi-field and multi-scale representation of bodies as the sum of the standard macroscopic kinetic energy and a microscopic component. By indicating with  $b$  in apex position a covector corresponding to the vector decorated by the apex, we rewrite explicitly the sum as

$$k(\dot{y}^b, \nu, \dot{\nu}^b) := \frac{1}{2} \rho \dot{y}^b \cdot \dot{y} + \kappa(\nu, \dot{\nu}^b),$$

where  $\kappa$  is such that  $\kappa(\nu, 0) = 0$  and it admits second derivative with respect to  $\dot{\nu}^b$ , which is positive defined, namely

$$\frac{\partial \kappa(\nu, \dot{\nu}^b)}{\partial \dot{\nu}^b \partial \dot{\nu}^b} \cdot (\dot{\nu}^b \otimes \dot{\nu}^b) \geq 0.$$

The equality sign holds when  $\dot{\nu}^b = 0$ .

In contrast with [13], I presume that the dependence of  $\kappa(\nu, \dot{\nu}^b)$  must be considered deprived by the effects of macroscopic rigid-body motion. Microstructural inertia appears, should it exist, as a local microscopic fluctuation with respect to the macroscopic motion. Hence, we may consider  $\kappa$  as a function

$$\kappa(\nu, \dot{\nu}^b) = \mathfrak{h}(\nu, \dot{\nu}^b - (\mathcal{A}q)^b).$$

The choice prevents an incongruence that would occur, in contrast, when  $\kappa$  is quadratic with respect to  $\dot{\nu}^b$  and we calculate the total kinetic energy of the body along a rigid-body motion – an unjustified extra inertia moment would appear if we do not use a form like  $\mathfrak{h}$  (details are in [65]).

A standard assumption used below is that both  $b^\ddagger$  and  $\beta^\ddagger$  admit additive decompositions into inertial ( $b^{in}$  and  $\beta^{in}$ ) and non-inertial ( $b$  and  $\beta$ ) components:

$$b^\ddagger = b^{in} + b, \quad \beta^\ddagger = \beta^{in} + \beta.$$

**4.5. Invariance of the relative power under isometry-based changes in observers.** Here I refer to changes in observers of class 2. The velocity  $w$  is defined on  $\mathcal{B}$  (precisely, the map  $x \mapsto w(x) \in T_x \mathcal{B}$  is a section of the tangent bundle to  $\mathcal{B}$ ), so we have to use the rule (3.4) in the changes in observers.

Along the path, I shall assume that some fields are piecewise differentiable over  $\mathcal{B}$  (in short we say that they are of class  $PC^1$ ) with bounded discontinuities over a surface  $\Sigma$ , oriented locally by the normal  $m$ , and not moving relatively to  $\mathcal{B}$  itself. For any field  $x \mapsto a(x)$  of this type, taking values in a linear space, the limits  $a^\pm(x) := \lim_{\epsilon \downarrow 0} a(x \pm \epsilon n)$ ,  $x \in \Sigma$ , define the **jump**  $[a]$  of  $a$ , as the difference  $[a] := a^+ - a^-$ , and the **average**  $\langle a \rangle$  as  $\langle a \rangle := \frac{1}{2}(a^+ + a^-)$ . Given two fields  $x \mapsto a_1(x)$  and  $x \mapsto a_2(x)$  taking values in a linear space and such that a product  $a_1 a_2$  between them, distributive with respect to the sum, can be defined, we get the identity  $[a_1 a_2] := [a_1] \langle a_2 \rangle + \langle a_1 \rangle [a_2]$ .

The definition of  $[a]$  underlines the need of having a field taking values in a linear space. If it would be not so, in fact, the difference would possibly be not defined. For this reason, in what follows, I shall consider the field  $x \mapsto \nu$  continuous across  $\Sigma$ . In fact, since  $\mathcal{M}$  is here in general non-linear, the jump  $[\nu]$  of  $\nu$  could not make sense. In contrast, the jump of  $\dot{\nu}$  and the one of  $\mathcal{S}$  are always defined, being both in linear spaces at every  $x \in \mathcal{B}$ .

I presume also that the derivatives of the map  $x \mapsto \nu$  suffer bounded discontinuities across  $\Sigma$ . Also,  $\Sigma$  is here unstructured: it means that it cannot sustain its own surface standard and microstructural tractions; in other words it is not endowed with its own surface energy.

**Axiom 1.**  $\mathcal{P}_6^{rel}(\dot{y}, \dot{\nu}, w)$  is invariant under isometry-based changes in observers in class 2 for any choice of  $\mathfrak{b}$  and the rates involved.

**Axiom 2.** *The bulk actions admit additive decompositions into inertial and non-inertial parts and the inertial components are determined by the integral balance*

$$\frac{d}{dt} \int_{\mathfrak{b}} k(\dot{y}, \nu, \dot{\nu}) \, dx + \int_{\mathfrak{b}} (b^{in} \cdot \dot{y} + \beta^{in} \cdot \dot{\nu}) \, dx = 0,$$

which holds for any choice of the part  $\mathfrak{b}$  and the velocity field, with the kinetic energy satisfying the structure assumptions presented above.

**Theorem 1.** *The following assertions hold true.*

(1): *The integral balances below hold, provided that the fields involved are integrable:*

$$(4.5) \quad \int_{\mathfrak{b}} b^{\ddagger} \, dx + \int_{\partial \mathfrak{b}} Pn \, d\mathcal{H}^2 = 0,$$

$$(4.6) \quad \int_{\mathfrak{b}} \left( (y - y_0) \times b^{\ddagger} + \mathcal{A}^* \beta^{\ddagger} \right) \, dx + \int_{\partial \mathfrak{b}} \left( (y - y_0) \times Pn + \mathcal{A}^* \mathcal{S}n \right) \, d\mathcal{H}^2 = 0,$$

$$(4.7) \quad \int_{\partial \mathfrak{b}} \mathbb{P}n \, d\mathcal{H}^2 - \int_{\mathfrak{b}} \left( F^* b^{\ddagger} + N^* \beta^{\ddagger} \right) \, dx - \int_{\mathfrak{b}} (\partial_x \psi + f) \, dx = 0,$$

$$(4.8) \quad \int_{\partial \mathfrak{b}} (x - x_0) \times \mathbb{P}n \, d\mathcal{H}^2 - \int_{\mathfrak{b}} (x - x_0) \times \left( F^* b^{\ddagger} + N^* \beta^{\ddagger} \right) \, dx - \\ - \int_{\mathfrak{b}} (x - x_0) \times (\partial_x \psi + f) \, dx + \int_{\mathfrak{b}} 2\mu \, dx = 0.$$

where  $P := \psi I - F^* P - N^* S$ , with  $I$  the second-rank unit tensor.

(2): *If the fields  $x \mapsto P$  and  $x \mapsto P$  are of class  $PC^1(\mathcal{B}) \cap C^0(\bar{\mathcal{B}})$  with discontinuity set the surface  $\Sigma$  described above, and the fields  $x \mapsto b$ ,  $x \mapsto F^* b$ ,  $x \mapsto f$ , and  $x \mapsto \partial_x \psi$  are continuous over  $B$ , we get in  $B$*

$$(4.9) \quad \text{Div} P + b^{\ddagger} = 0,$$

and a field  $x \mapsto z(x) \in T_{\nu(x)}^* M$ , with  $z = z_1 + z_2$ ,  $z_2 \in \text{Ker} A^*$ , exists and is such that

$$(4.10) \quad \text{Div} \mathcal{S} + \beta^{\ddagger} - z = 0$$

and

$$(4.11) \quad \text{Skw} P F^* = \frac{1}{2} \mathbf{e} (\mathcal{A}^* z + (D\mathcal{A}^*) \mathcal{S}),$$

moreover

$$(4.12) \quad \text{Div} \mathbb{P} - F^* b^{\ddagger} - N^* \beta^{\ddagger} + \partial_x \psi = f,$$

$$(4.13) \quad \text{Skw}(g^{-1} \mathbb{P}) = -2\bar{\mathbf{e}}\mu,$$

with  $\bar{\mathbf{e}}$  Ricci's symbol with all contravariant components, namely  $\bar{\mathbf{e}}^{ABC}$ . Across  $\Sigma$  we get

$$(4.14) \quad [P]m = 0,$$

$$(4.15) \quad [\mathcal{S}]m = 0,$$

$$(4.16) \quad [\mathbb{P}]m = 0.$$

**(3):** The inertial components of the body actions are given by

$$b^{in} = -\rho\ddot{y}$$

and

$$\beta^{in} = \frac{d}{dt} \frac{\partial \chi(\nu, \dot{\nu})}{\partial \dot{\nu}} - \frac{\partial \chi(\nu, \dot{\nu})}{\partial \nu},$$

with

$$\chi : \mathcal{TM} \longrightarrow \mathbb{R}^+$$

a  $C^1$  function such that

$$\kappa(\nu, \dot{\nu}^b) := \frac{\partial \chi(\nu, \dot{\nu})}{\partial \dot{\nu}} \cdot \dot{\nu} - \chi(\nu, \dot{\nu}),$$

at any  $\dot{\nu}$ .

**(4):** If the material is homogeneous, no driving force is present, and  $\mu = 0$ , then  $P$  is symmetric and, in absence of body forces,

$$\int_{\partial \mathfrak{b}} \mathbb{P} n \, d\mathcal{H}^2 = 0,$$

for any part  $\mathfrak{b}$ .

**(5):** An extended version of the virtual power principle holds. It reads

$$\mathcal{P}_{\mathfrak{b}}^{rel}(\dot{y}, \dot{\nu}, w) = \mathcal{P}_{\mathfrak{b}}^{rel-int}(\dot{y}, \dot{\nu}, w),$$

where

$$\begin{aligned} \mathcal{P}_{\mathfrak{b}}^{rel-int}(\dot{y}, \dot{\nu}, w) & : = \int_{\mathfrak{b}} \left( P \cdot \dot{F} + z \cdot \dot{\nu} + \mathcal{S} \cdot \dot{N} + \mathbb{P} \cdot Dw + \mu \cdot \operatorname{curl} w \right) dx + \\ & + \int_{\mathfrak{b} \cap \Sigma} (\langle P \rangle m \cdot [\dot{y}] + \langle \mathcal{S} \rangle m \cdot [\dot{\nu}] + \langle \mathbb{P} \rangle m \cdot [w]) \, d\mathcal{H}^2, \end{aligned}$$

with the obvious simplification when  $w$  is continuous across  $\Sigma$  and/or  $\dot{y}$  and  $\dot{\nu}$  are continuous too.<sup>42</sup>

- Invariance of the relative power with respect to translations in  $\tilde{\mathcal{E}}^3$  furnishes the integral balance of forces. We do not have the integral balance of micro-actions (or micro-forces if you want to use the term *force* in an extended sense) because translations are not available over  $\mathcal{M}$  unless it is a priori selected as a linear space. Even in that case, however, if we accept changes in observers in class 2 (or class 1 in absence of material mutations), a translation over  $\mathcal{M}$  is not accounted for.
- The integral balance of couples (4.6) includes the micro-actions. However, it does not mean that  $\mathcal{S}$  and  $\beta^\ddagger$  are couples for they appear multiplied by the adjoint of the linear operator  $\mathcal{A}$ , which projects over the reference space their component over  $\mathcal{M}$ .
- In principle, we could abandon the procedure based on the invariance of the relative power, or the external power alone, deciding to postulate the integral form of balance equations. We would be then pushed to postulate an integral balance of microstructural actions, declaring it as “our first principle”. This way we would face the basic difficulty that in this case such a balance would be not defined in general for we take  $\mathcal{M}$  as a manifold not necessarily coincident with a linear space. In fact, when  $\mathcal{M}$  is a non-linear

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<sup>42</sup>The choice that  $w$  is continuous is rather natural, since  $w$  is arbitrary. A bit more delicate is the treatment when  $\Sigma$  moves relatively to the rest of the body.

manifold, the integrals in that balance would be not defined because the fields  $x \mapsto \beta^\dagger$  and  $x \mapsto \mathcal{S}n$  take values in the cotangent bundle of  $\mathcal{M}$ , a non-linear target space, indeed. A balance of microstructural actions could be formally defined only when  $\mathcal{M}$  is a linear space. However, in any case its choice would introduce an assumption, namely the structure of that integral balance, which is not necessary, as shown by previous theorem (its proof can be developed by direct calculation). Moreover, if we would presume such an integral balance a priori when  $\mathcal{M}$  is linear, we should postulate the existence of the self-action  $z$ , which has been, in contrast, *deduced* with the procedure used in the previous theorem.

- Another option could be a virtual power approach. We could assume the identity

$$\mathcal{P}_{\mathcal{B}}^{rel}(\dot{y}, \dot{\nu}, w) = \mathcal{P}_{\mathcal{B}}^{rel-int}(\dot{y}, \dot{\nu}, w),$$

as a first principle, presuming its validity for any choice of (compactly supported) rate fields.<sup>43</sup> Such assumption, however, is a way to affirm that we are postulating a priori the weak form of the pointwise balances of actions. We should then presume the existence of all ingredients appearing in the balance equations, having already in mind their structure. The difference between a procedure requiring the invariance of external power and the virtual power approach is not particularly appreciable in the standard setting for the elements appearing in the inner power are already present in the external one. In contrast, in the enriched setting discussed here, in postulating the inner power we should introduce a priori the self-action  $z$  without showing the need of its existence.

- There is an indeterminacy in the pointwise balance of micro-actions (4.10). In fact, any element  $z'$  belonging to  $\text{Ker } \mathcal{A}^*$  satisfies (4.11). Hence, it would appear in (4.10)<sup>44</sup>. The indeterminacy can be eliminated by covariance techniques (see [23]), i.e. by requiring at least invariance with respect to the generalized class 1. If we require such an invariance for the external power or the relative one, however, we do not obtain an appreciable result. Covariance requirements need the use of the balance of energy or the second law of thermodynamics.<sup>45</sup> In this case, however, energy is involved, and the specification of the list of state variables is required. This way we would

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<sup>43</sup>If we cancel  $w$ ,  $\mathcal{P}_{\mathcal{B}}^{rel}(\dot{y}, \dot{\nu}, w)$  reduces to  $\mathcal{P}_{\mathcal{B}}^{ext}(\dot{y}, \dot{\nu})$ , already defined above, and  $\mathcal{P}_{\mathcal{B}}^{rel-int}(\dot{y}, \dot{\nu}, w)$  becomes

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

If we would start taking as a first principle (the principle of virtual power) the identity

$$\mathcal{P}_{\mathcal{B}}^{ext}(\dot{y}, \dot{\nu}) = \mathcal{P}_{\mathcal{B}}^{int}(\dot{y}, \dot{\nu}),$$

presuming that it holds for any pair of (compactly supported) velocity fields, we should introduce a-priori the self-action  $z$ , as proposed by Germain in [38] in the case in which  $\mathcal{M}$  is a linear space, instead of proving the need of its existence as it occurs along the path that we follow here.

<sup>44</sup>An elementary example: Consider  $\mathcal{M}$  to be coincident with  $\mathbb{R}^3$ . At  $r \in \mathbb{R}^3$ ,  $\mathcal{A}(r) = -r \times$ , the kernel of  $\mathcal{A}^*$  coincides with the linear space of vectors parallel to  $r$ . As a consequence,  $z'$  in this case is of the type  $\lambda r^\flat$ , with  $r^\flat$  the covector naturally associated with  $r$ , and  $\lambda$  a real number.

<sup>45</sup>Consequences of the covariance of the balance of energy of elastic simple bodies are discussed in [77] while for the covariance of the second law of thermodynamics, in the case of elastic-plastic materials, the first theorem published is in [73].

pay the use of a more stringent invariance requirement by loosing the hierarchical distinction between the derivation of balance equations and the discussion of constitutive issues, the former determined without the need of the latter.

- Invariance of the relative power with respect to translations and rotations in the reference space  $\mathcal{E}^3$  determines integral balances of configurational forces and couples, the ones governing the bulk mutation. Hence, we are not forced to introduce a priori a stress  $\mathbb{P}$  and bulk configurational forces and then to identify them with  $\psi I - F^*P - N^*S$  and  $-F^*b^\ddagger - N^*\beta^\ddagger$  by means of an additional procedure, the one described in [47] and [48].
- The assumption that  $f$  is solely dissipative reduces to the inequality  $f \cdot w \geq 0$ , the equality sign valid only when  $w = 0$ , which implies that  $f$  is a linear function of  $w$ , with a positive coefficient. The result changes (4.12) into an evolution equation.

#### 4.6. And if we leave $\mathcal{M}$ a part?

- In principle we could consider  $\nu$  to be observer-independent. In this case the invariance of the external power or the relative one with respect to isometry-based changes in observer would not lead (under appropriate regularity) to the pointwise balances of microstructural actions (4.10) and (4.11), as it is obvious from the procedure sketched above. Hence,  $\nu$  would play a parametric rôle at equilibrium and its evolution should be prescribed a part, with the sole proviso of satisfying the second law of thermodynamics. This way we would enter the scheme of internal variables, intended just as entities describing the removal from thermodynamical equilibrium (see [24] for a standard treatise on the matter, from the point of view of non-equilibrium thermodynamics, above all with reference to chemical processes). The approach has been coupled with deformations in [17], [52], with a subsequent rich literature, in the majority of cases related with plasticity and/or damage (see e.g. the treatise [59]). The balance of microstructural actions can be reduced to the evolution equation that appears in internal variable schemes in absence of external body actions (including even possible rotational microstructural inertia), microstress and when the self-action is the sum of conservative and dissipative components (see [65] for details). However, the relation is just formal: the difference in the use of the notion of observer continues to distinguish the two approaches.
- When there is no link between changes of frames in  $\tilde{\mathcal{E}}^3$  and changes of atlas on  $\mathcal{M}$ , i.e. when  $\{\lambda\}$  is empty, the invariance procedure leading to the previous theorem would lead to a splitting of (4.6) into two integral balances:

$$\int_{\mathfrak{b}} (y - y_0) \times b^\ddagger \, dx + \int_{\partial \mathfrak{b}} (y - y_0) \times Pn \, d\mathcal{H}^2 = 0,$$

and

$$\int_{\mathfrak{b}} \mathcal{A}^* \beta^\ddagger \, dx + \int_{\partial \mathfrak{b}} \mathcal{A}^* S_n \, d\mathcal{H}^2 = 0.$$

The first one is the standard balance of couples leading to the symmetry of  $PF^*$  under the regularity condition listed in the theorem above. The

second balance would produce once again (4.10) and

$$\mathcal{A}^* z + (D\mathcal{A}^*) \mathcal{S} = 0.$$

The circumstance stresses the rôle played in this setting by the notion of observer and its changes.

#### 4.7. Perspectives: low-dimensional defects, strain-gradient materials, covariance of the second law.

- In presence of structured discontinuity surfaces, those endowed with their own surface energy for they are able to sustain surface standard and microstructural actions (it is a reasonable mathematical scheme for thin transition layers between phases, for example), the expression of the relative power has to be extended with the addition of two contributions: (1) the **relative power of surface actions**, (2) the **surface power of disarrangements** containing fluxes of the surface energy and the surface counterparts of  $f$  and  $\mu$ . The list of surface actions includes the standard surface stress and surface microstress and self-actions – the existence of the last actions has been proven in [65]. The definition of the relative power in this case and the results emerging from the requirement of its invariance are in [74]. However, a special case of that extended expression of the relative power in conservative case emerges from the extension of Nöther's theorem, presented in [23], to the elasticity of complex materials endowed with structured discontinuity surfaces. Different approaches can be followed to analyze the mechanics of structured discontinuity surfaces, with other assumptions and different procedures (see [48], [51], [79], [114]). The reader will be able to distinguish the procedure requiring the smallest number of assumptions, a peculiarity allowing it to be a flexible tool to tackle non-standard situations.
- Analogous generalizations can be obtained in presence of line defects endowed with their own line energy. This one is a scheme that we can adopt for example for the description of the dislocation core in metals. In this case, an expression of relative power in a setting where dissipation is essentially attributed to the counterparts of  $f$  and  $\mu$  and to the self-action is in [72].
- We can define the relative power even for strain-gradient materials, including the microstress. When we focus the attention on the actions in the bulk alone, in the conservative setting of strain-gradient elasticity an expression of the relative power can be derived from the Nöther theorem (for it see [58]). The extension of the Nöther theorem to the case in which structured discontinuity surfaces appear in strain-gradient elasticity (for example think of two strain-gradient elastic materials glued with each other) has been proven in [67], where the surface hyperstress has been introduced first. In the dissipative setting, the appropriate expression of the relative power including bulk and surface hyperstress is in [74].
- Besides issues concerning low-dimensional defects endowed with their own energy in single-gradient or second-gradient field theories, another perspective deals with covariance in dissipative setting. In fact, we can write a version of the second law of thermodynamics including the relative power and impose invariance under diffeomorphism-based changes in observers.

The procedure requires *(i)* the specification of the list of state variables (it includes the metric in the reference place) and *(ii)* a rule satisfied by the rate of the free energy under changes in observers (it affirms essentially that the energy changes tensorially, as assumed in elasticity in [77]). This way we deduce (1) the existence of the stresses, (2) the pointwise balances in the previous theorem, (3) the constitutive restrictions (among them we find that the conservative part of the Eshelby stress is the derivative of the free energy with respect to the material metric), (4) the structure of the dissipation. Details in the case of elastic-plastic hardening materials are collected in the next section.

##### 5. BALANCE EQUATIONS FROM THE SECOND LAW OF THERMODYNAMICS: THE CASE OF HARDENING PLASTICITY

In the previous section we have seen the link between isometric changes in observers and balance equations, established by the invariance of the external power or the relative one – the latter case determines even configurational balances. As anticipated above, an analogous link exists among diffeomorphism-based changes in observers, existence of the standard stress, constitutive restrictions, and even dissipation (for it the use of the second law of thermodynamics is necessary). In this sense we can affirm that the structure of pointwise balances is covariant.

The concept can be specified in different settings.

- When the environment is purely conservative, horizontal and vertical first variations – the latter involving the actual shape  $\mathcal{B}_a$  of the body – of the total energy or a Lagrangian determine balance equations in weak or pointwise form, depending on the regularity of the fields involved (for non-linear elasticity of simple bodies see [42]). In this setting, by taking into account the way in which they are defined, horizontal and vertical variations play the rôle of (can be interpreted as) diffeomorphism-based changes in observers.
- Another setting is established by Marsden-Hughes theorem [77], which enlarges the purely conservative case to include non-conservative body forces. The theorem deals with the standard format of continuum mechanics (Cauchy's bodies). It is based on a requirement of invariance of the first law of thermodynamics, written with respect to the actual place  $\mathcal{B}_a$ , under changes in observers governed by the action of diffeomorphisms altering the physical ambient space  $\tilde{\mathcal{E}}^3$  where we evaluate the actual places  $\mathcal{B}_a$ . Ancillary but not less fundamental assumptions are (1) the dependence of the internal energy on the metric in  $\tilde{\mathcal{E}}^3$ , and (2) that the energy density behaves tensorially, as the density of a volume form, under diffeomorphism-based changes in observers. The results are *(i)* the derivation of the existence of the Cauchy stress tensor, *(ii)* the pointwise balance equations of forces and couples, and *(iii)* the constitutive restriction linking the Cauchy stress to the derivative of the energy with respect to the spatial metric (Doyle-Ericksen formula). The basic limitation of the theorem and the one of its possible generalizations involving the description of microstructures and/or the relative power is that the use of the first law of thermodynamics excludes the possible presence of dissipative stresses, like the non-conservative part of the Piola-Kirchhoff stress in viscoelasticity. Hence, it does not furnish the expression of the dissipation in presence of plastic effects.



- To go beyond the point of view of Marsden-Hughes theorem, with the aim of including dissipation, we need to ask *covariance to the second law of thermodynamics*. This idea appeared first in [73] with reference to the description of elastic-perfectly-plastic bodies.<sup>46</sup> Here, I refer once again to plastic behavior for the discussion allows me to put together diffeomorphism-based changes in observers with the notion of independent tangent maps, mentioned in the introduction as one of the possible approaches to the description of the mutations in solids. I present a mild generalization of the result in [73] to the case of traditional representation of hardening, without adding proofs, for they are exactly like the ones in [73] to within an addendum that needs just a little care to be managed.
- The setting, also, allows the reader to think once again of analogies and differences between the framework discussed in previous sections for describing micro-to-macro interactions in solids and the scheme of internal variables that appears useful at times when we describe phenomena far from thermodynamic equilibrium.

To express clearly the result, recalling some notions can be expedient.

**5.1. Multiplicative decomposition of  $F$ .** Plasticity is the macroscopic emergence of the cooperation of microscopic structural changes in the matter. In this sense the phenomenon is a mutation.

There are various manners of interpreting plastic phenomena. In this sense we can speak of *theories* of plasticity instead of a unique format.

A traditional approach is based on a multiplicative decomposition of the deformation gradient,  $F$ , into *elastic*,  $F^e$ , and *plastic*,  $F^p$ , factors:

$$F = F^e F^p.$$

For  $F^p$  we presume that

- $\det F^p > 0$  at all  $x$  in  $\mathcal{B}$ , where  $F^p$  is defined,
- the field  $x \mapsto F^p(x)$  is differentiable,
- $\text{curl} F^p \neq 0$ .

With the last assumption we affirm that  $F^p$  is not intended as the spatial derivative of any deformation.  $F^p$  is only a linear operator that maps the tangent space to  $\mathcal{B}$  at  $x$  onto another linear space that we *imagine* (and in this setting we cannot do more than imagining) as the tangent space to what is commonly called *intermediate configuration*, determined by the structural changes in the material. This way we are factorizing the elastic-plastic process. The choice appears fictitious for elastic and plastic changes in the matter cooperate. However, the factorization of elastic and plastic phenomena seem to have microscopic justification at least in the case of crystals even without calling upon explicitly a notion of intermediate configuration. Parry has shown, in fact, in [101] that, for crystal lattices, a view based on the dislocation tensor and other elastic invariants<sup>47</sup> leads to a decomposition of the type  $F = F_1^e F^p F_2^e$ , which obviously reduces to the traditional one when

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<sup>46</sup>There is no restriction to apply the idea also to visco-elasticity with and without microstructures.

<sup>47</sup>It is possible to establish a basis for them [102].

$F_2^e$  coincides with the identity. Another justification constructed by considering deformations as *SBV* ( $\mathcal{B}$ ) maps<sup>48</sup> appears in [106].

When we accept the multiplicative decomposition  $F = F^e F^p$ , the right Cauchy-Green tensor in its version with both covariant components writes

$$C = F^{p*} F^{e*} \tilde{g} F^e F^p = F^{p*} C^e F^p,$$

with  $C^e = F^{e*} \tilde{g} F^e$ . The second-rank tensor  $C^e$ , endowed with positive determinant, is the so-called **elastic right Cauchy-Green tensor**. Its components are covariant. Precisely,  $C^e$  is the pull-back of the spatial metric  $\tilde{g}$  through  $F^e$ .

The 1-contravariant, 1-covariant versions of  $C^e$  and  $C$  read, respectively,  $\tilde{C}^e = F^{eT} F^e$  and  $\tilde{C} = F^{pT} \tilde{C}^e F^p$ . Also, the push-forward by  $F^p$  of the material metric, namely the second-rank tensor  $\bar{g} := F^{p-*} g F^{p-1}$  is *independent* of any change of frame on  $\mathcal{B}$ , induced by diffeomorphisms of the reference space onto itself. The proof is elementary and can be found in [73]. Notice that  $\tilde{C}^e = \tilde{g}^{-1} C^e$  and  $\tilde{C} = \tilde{g}^{-1} C$ .

The plastic factor of the deformation gradient maps the tangent spaces to  $\mathcal{B}$  at different points onto distinct linear spaces. We do not have any information assuring us that we can glue together all the linear spaces obtained by means of  $F^p$ , varying  $x$  in  $\mathcal{B}$ , to construct the tangent bundle of a manifold that could be a fit region of the type  $\mathcal{B}$ , identified with what we call intermediate configuration.

This one is another way to interpret the assumption  $\text{curl} F^p \neq 0$ , which excludes the possibility to individualize such a configuration that remains fictitious. In principle, it is even not necessary to imagine an intermediate (global) configuration, as I have already affirmed, although, point by point, the factorization  $F^e F^p$  implies a mapping from  $T_x^* \mathcal{B}$  onto an unknown linear space determined by  $F^p$ . The linear spaces determined by  $F^p$  varying  $x$  in  $\mathcal{B}$  could be interpreted as the tangent spaces of different configurations. Such an interpretation brings us back to the notes in the introduction dealing with virtual tangent spaces and multiple reference configurations.

**5.2. Factorization of changes in observers.** Consider changes in observers in the *generalized class 2* presented previously, excluding what is pertinent to  $\mathcal{M}$ , which does not appear in this section. The velocity field  $\bar{v}$  in the relation

$$\dot{y} \longrightarrow \dot{y}^\# := \dot{y} + \bar{v}$$

is function of  $x$  through  $y := u(x)$ , so that we write  $D\bar{v} = D_y \bar{v} F$ . For  $D\bar{v}$ , according to [73], I assume a multiplicative decomposition of the type

$$(5.1) \quad D\bar{v} = \overline{H^e F^p}.$$

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<sup>48</sup>We say that an integrable function  $u$  over an open set  $\Omega$  in  $\mathbb{R}^N$  is a function of bounded variation, in short  $u \in BV(\Omega)$  if

$$\int_{\Omega} u \frac{\partial \phi}{\partial x^i} dx = - \int_{\Omega} \phi dD_i u$$

for any  $\phi \in C_0^\infty(\Omega)$ , for some  $\mathbb{R}^N$ -valued measure  $Du = (D_1 u \dots D_N u)$  in  $\Omega$ . In particular, we say that  $u$  belongs to the space of *special functions of bounded variation*, and write  $u \in SBV(\Omega)$ , when  $Du$  is decomposed in the sum of two terms: the first one is absolutely continuous with respect to the volume measure, namely  $\nabla u \mathcal{L}^N$ , with  $\mathcal{L}^N$  the  $N$ -dimensional Lebesgue measure, the second term is a  $(N-1)$ -rectifiable measure. In other words, when  $u \in SBV(\Omega)$  its singular set does not contain isolated points so that  $Du$  can be recovered from the approximate differential  $\nabla u$ , the limits  $u^+$  and  $u^-$  to the jump set, together with the relevant normal to the set itself.

The presence of  $F^p$  does not reduce the generality of  $D\bar{v}$ , due to the arbitrariness of  $H^e$ , a linear operator from the linear space individuated by  $F^p$  to the translation space over  $\tilde{\mathcal{E}}^3$ . Although it has no effects on the generality of changes in observers, the previous factorization of  $D\bar{v}$  is crucial for the result on hardening plasticity presented here.

A relation is useful below. To get it, define

$$L_H^e := \dot{H}^e F^{e-1}, \quad L^p := \dot{F}^p F^{p-1},$$

and use the identity  $D\bar{v} = D_y \bar{v} F$  and (5.1). By computing  $D_y \bar{v}$ , we get<sup>49</sup>

$$D_y \bar{v} = \overline{H^e F^p} F^{-1} = \text{Sym} L_H^e + \text{Skw} L_H^e + H^e L^p F^{e-1}.$$

**5.3. A version of the second law of thermodynamics involving the relative power.** According to [73], I use here an isothermal version of the second law of thermodynamics (a mechanical dissipation inequality) reading, for any part  $\mathfrak{b}$  of  $\mathcal{B}$  and any choice of the velocity fields,

$$(5.2) \quad \mathfrak{E}(\dot{y}, w; \psi, \mathfrak{b}) := \frac{d}{dt} \int_{\mathfrak{b}} \psi \, dx - \mathcal{P}_{\mathfrak{b}}^{rel}(\dot{y}, w) \leq 0,$$

where, we recall,  $\psi$  is the free energy.

- The common expression of the mechanical dissipation inequality involves the external power alone. Here, we include the relative power, extending in this sense the standard inequality to account for the remodeling of the material structure induced by the plastic phenomena.
- When it is the case – not here, however – the inequality can be further generalized by including the expression of the relative power that involves microstructural actions or hyperstresses in the presence of strain-gradient effects.

A direct description of the microstructures does not appear in this section for we are restricting the treatment to the standard framework of hardening plasticity just to exemplify how some general ideas discussed here work on a well-known ground.

**5.4. Specific constitutive assumptions.** The assumptions listed below apply.

**(H1):** The state variables pertaining to the generic material element are  $F$ ,  $F^p$ , and the hardening parameter  $\alpha$ , a second-rank tensor taking into account hardening anisotropy and measuring how much along the plastic process the material goes far from equilibrium where  $\alpha$  plays *only* a parametric rôle, being considered an *observer-independent internal variable*. Hence, the free energy is of the form

$$\psi = \hat{\psi}(x, F, F^p, \alpha).$$

It satisfies further assumptions:

**(H1.a):** For any linear operator  $G \in \text{Hom}(\mathbb{R}^3, \mathbb{R}^3)$  with  $\det G = 1$ ,

$$\hat{\psi}(x, F, F^p) = \hat{\psi}(x, FG, F^p G, \alpha).$$

**(H1.b):** The free energy is *objective*. The requirement emerges naturally from the isotropy of the three-dimensional Euclidean space: if we rotate rigidly a frame in the physical space, the free energy of a material should not change. Elements of the orthogonal group  $SO(3)$  describe rotations, we recall.

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<sup>49</sup>See [73] for details on the derivation of (??).

- H1.a is completely standard (see e.g. [84] and [99]). It implies that

$$\hat{\psi}(x, F, F^p, \alpha) = \bar{\psi}(x, F^e, \bar{g}, \alpha),$$

where  $\bar{g} := F^{p-*}gF^{p-1}$  and we adopt the multiplicative decomposition of  $F$ . The previous restriction on the structure of the energy enlarges the common use of the invariance under the action of  $G$ , as described above, interpreted as a constraint leading to a structure of the free energy of the type  $\hat{\psi}(F, F^p) = \bar{\psi}(F^e)$  alone, not considering  $\bar{g}$ , which plays in contrast a rôle here, as we shall see below.

- For any  $Q \in SO(3)$  that rotates frames in the space where the actual places are determined, since  $\bar{g}$  has no components in that space and  $\alpha$  is considered here observer-independent, just to follow the standard view on hardening, objectivity writes formally

$$\bar{\psi}(x, F^e, \bar{g}, \alpha) = \bar{\psi}(x, QF^e, \bar{g}, \alpha),$$

which implies

$$\bar{\psi}(x, F^e, \bar{g}, \alpha) = \check{\psi}(x, \tilde{C}^e, \bar{g}, \alpha).$$

Since  $\tilde{C}^e = \bar{g}^{-1}C^e$ , we can write

$$\check{\psi}(x, \tilde{C}^e, \bar{g}, \alpha) = \tilde{\psi}(x, C^e, \bar{g}, \alpha).$$

**(H2):** Under diffeomorphism-based changes in observers acting on both the ambient space and the reference one (it is the generalized class 2 in which we do not consider  $\mathcal{M}$ ), we get

$$\frac{d\psi^\#}{dt} = \frac{d\psi}{dt} + \frac{\partial\psi}{\partial C^e} \Big|_{\downarrow\#} \cdot 2\text{Sym}L_H^e + \frac{\partial\psi}{\partial \bar{g}} \Big|_* \cdot \mathcal{L}_{\bar{w}}g + \frac{\partial\psi}{\partial \alpha} \cdot \dot{\alpha},$$

where  $(\cdot) \Big|_*$  indicates the pull-back in the reference place of  $(\cdot)$  while  $(\cdot) \Big|_{\downarrow\#}$  is the push-forward of  $(\cdot)$  in the current configuration with the additional lowering of the first index.<sup>50</sup>

<sup>50</sup>In Marsden-Hughes theorem, the energy density – the elastic one  $e$  in that case – is referred to the actual place and is function of the sole metric in space, besides  $y$  and  $t$ . Under the action of parameterized families of diffeomorphisms  $h_\epsilon : \mathcal{E}^3 \rightarrow \mathcal{E}^3$ , the tensoriality requirement reads  $e(h_\epsilon(y), t) = e(y, t, h_\epsilon^* \circ \bar{g})$ , where  $h_\epsilon^*$  indicates pull-back. In fact, deformation is a relative concept: a shape of a body is deformed *with respect to* another one that we consider ‘undeformed’. Hence, in writing the energy with respect to the actual place as a function of the spatial metric, we do not have an immediate paragon (the reference place) to speak about deformation. Consequently, to mimic such a paragon, we can evaluate the energy over a varied metric, namely  $h_\epsilon^* \circ \bar{g}$  – that is a varied way to measure lengths, so to indicate an incoming deformation superposed to the place that we are considering. When we want to transfer such a viewpoint in the setting that we are considering here, we should have to require ‘tensoriality’ of the free energy with respect to changes of atlas in both ambient and reference spaces. First we have to remind that  $C^e$  is a function of  $F^e$  and  $\tilde{g}$ , while  $\bar{g}$  is a function of the reference metric  $g$  and  $F^p$ . Hence, by considering both  $h_\epsilon : \mathcal{E}^3 \rightarrow \mathcal{E}^3$  and  $\hat{h}_\epsilon : \mathcal{E}^3 \rightarrow \mathcal{E}^3$ , as defined in generalized class 2, we should require

$$\psi^\# = \tilde{\psi}(x, C^e(F^e, h_\epsilon^* \circ \bar{g}), \bar{g}(F^p, \hat{h}_\epsilon^* \circ g, \alpha(\hat{h}_\epsilon^*(x))).$$

In computing the derivative with respect to  $\epsilon$  (we distinguish here between the parameter in  $h$  and  $\hat{h}^*$  and the time  $t$ , for  $F^e$  and  $F^p$  depend themselves on time, then, after calculating the derivative of  $\psi$ , we identify  $\epsilon$  with  $t$ ), the term  $\hat{h}_\epsilon^* \circ g$  generates the Lie derivative  $\mathcal{L}_{\bar{w}}g$  which is twice the symmetric part of  $gD\bar{w}$ . An analogous reasoning should be applied when we handle the term  $h_\epsilon^* \circ \bar{g}$ . However, in that case we have to be addressed by physics. In fact, due to the decomposition (??), the symmetric part of  $D_y \bar{v}$  would include contributions of the plastic strain which does not affect neither  $h_\epsilon^* \circ \bar{g}$  nor  $C^e$ . This is the reasoning leading to the presence of the

- The push-forward of  $(\cdot)$  in the current configuration, with the additional lowering of the first index, is given explicitly by

$$\frac{\partial\psi}{\partial C^e}|_{\downarrow\#} = \tilde{g}F^e \frac{\partial\psi}{\partial C^e} F^{e*},$$

which is, in components,

$$\left(\frac{\partial\psi}{\partial C^e}|_{\downarrow\#}\right)_i^j = \tilde{g}_{ik} (F^e)_\alpha^k \left(\frac{\partial\psi}{\partial C^e}\right)^{\alpha\beta} (F^{e*})_\beta^j.$$

$\frac{\partial\psi}{\partial C^e}|_{\downarrow\#}$  is then a 1-contravariant, 1-covariant tensor in the current place, an element of the dual space of  $SymL_H^e$ .

- The pull-back in the reference place of  $(\cdot)$  is given by

$$\frac{\partial\psi}{\partial \tilde{g}}|_* = F^{pT} \frac{\partial\psi}{\partial \tilde{g}} F^{p-*},$$

which is, in components,

$$\left(\frac{\partial\psi}{\partial \tilde{g}}|_*\right)^{ij} = (F^{pT})_\alpha^i \left(\frac{\partial\psi}{\partial \tilde{g}}\right)^{\alpha\beta} (F^{p-*})_\beta^j.$$

- The term  $\mathcal{L}_{\bar{w}}g$  indicates that the (virtual) velocity  $\bar{w}$  alters the material metric  $g$ , dragging it. Indirectly, then,  $\bar{w}$  induces changes in the metric  $\tilde{g}$  on the intermediate configuration, since  $\tilde{g}$  is the push-forward of  $g$  induced by  $F^p$ . Hence, instead of writing  $(\partial\psi \setminus \partial\tilde{g})|_* \cdot \mathcal{L}_{\bar{w}}g$ , we could consider the push-forward of  $\mathcal{L}_{\bar{w}}g$  through  $F^p$ , multiplying it by  $\partial\psi \setminus \partial\tilde{g}$ , which would conceptually be the same thing.
- The spatial metric  $\tilde{g}$  can suffer alterations when it is dragged along the (virtual) velocity  $\bar{v}$ . There is then an effect on  $\psi$  through  $C^e$ , the pull back through  $F^e$  of  $\tilde{g}$  into the linear space determined by  $F^p$  and coinciding with  $F^{pT} \mathcal{B}$ . This one is the reason justifying the introduction of the term  $(\partial\psi / \partial C^e)|_{\downarrow\#}$  in H2.
- In H2 the factor  $\mathcal{L}_{\bar{w}}g$  has no counterpart  $\mathcal{L}_{\bar{v}}\tilde{g}$  in the current place because  $H^e$  is not the spatial derivative of any vector field. This aspect justifies the presence of the factor  $SymL_H^e$ .

**(H3):** Contact actions depend on the same state variables entering the energy.<sup>51</sup>

**5.5. The covariance principle in dissipative setting.** Independently of the use of external, relative, or internal power, the isothermal version of the second law of thermodynamics is a certain expression lesser or equal to zero, say  $B \leq 0$ . Another observer  $\mathcal{O}'$  evaluates always an inequality, say  $B' \leq 0$ , with  $B \neq B'$ , in general.

Thanks to H2 and the linearity of the relative power with respect to the velocities  $\dot{y}$  and  $w$ , the pull-back of  $B'$  into  $\mathcal{O}$  gives rise to an inequality of the type  $B^* \leq 0$ , with  $B^* = B + B^\dagger$ . The addendum  $B^\dagger$  involves the velocity fields  $\bar{v}$  and  $\bar{w}$ , entering

term  $SymL_H^e$  in H2. Finally, since  $\alpha$  is considered an observer-independent internal variable, we do not consider changes in the atlas pertaining to the space it belongs to. We just evaluate it in the new place determined by  $h_\epsilon$ . The choice justifies the term  $\frac{\partial\psi}{\partial \alpha} \cdot \dot{\alpha}$ .

<sup>51</sup>In presence of viscous effects such an assumption does not hold, obviously, because we have to add the dependence of the contact actions on the rate of deformation gradient, presuming also the additive decomposition of the same actions into conservative and dissipative components. In that case H3 should be restricted to the sole conservative components of the contact actions.

the rules of changes in observers. Conversely, if we push forward  $B$  to the frames defining the observer  $\mathcal{O}'$ , we find an inequality of the type  $B' + B^\ddagger \leq 0$  because now, the change in observer  $\mathcal{O}' \rightarrow \mathcal{O}$  is governed by the inverse of the previous maps, namely  $h^{-1}$  and  $\hat{h}^{-1}$ . Hence,  $B^\ddagger$  is in principle different from  $B^\ddagger$ .

Previous remarks suggest a principle.

**Proposition 2. Covariance principle in dissipative setting** [73]. *In any change in observer in the generalized class 2 (defined previously), when we project the mechanical dissipation inequality evaluated by an observer into the frame defining the other, the additional term arising in the process is always non positive.*

Essentially, the principle affirms that the dissipative nature of a process is indifferent to changes in observers.

**5.6. The covariance result for standard hardening plasticity.** The covariance principle in dissipative setting is the key ingredient for proving the following theorem. It shows the covariant structure of the equations governing the standard description of hardening plasticity in finite strain regime.

**Theorem 2.** *If we adopt for (5.2) the covariance principle in dissipative setting, under assumptions H1, H2, and H3, the expression of the contact actions in terms of stress follows and if the fields  $x \mapsto P$  and  $x \mapsto \mathbb{P} := \psi I - F^*P$ , with  $I$  the identity the space of second-rank 1-contravariant, 1-covariant tensors<sup>52</sup>, are continuous and differentiable everywhere in  $\mathcal{B}$ , except a (fixed and free of its own energy) smooth surface  $\Sigma$ , oriented by the normal  $m$ , where they suffer bounded jumps, and the fields  $x \mapsto b$ ,  $x \mapsto F^*b$ , and  $x \mapsto \partial_x \psi$  are integrable over  $\mathcal{B}$ , the local balance equations*

$$(5.3) \quad \text{Div} P + b^\ddagger = 0,$$

$$(5.4) \quad \text{Skw} (PF^*) = 0,$$

$$(5.5) \quad \text{Div} \mathbb{P} - F^*b^\ddagger - \partial_x \psi = f,$$

$$(5.6) \quad \text{Skw} (g^{-1}\mathbb{P}) = -2\bar{e}\mu,$$

with  $\bar{e}$  Ricci's symbol with all contravariant components, namely  $\bar{e}^{ABC}$ , hold in the bulk, while

$$(5.7) \quad [P]m = 0, \quad [\mathbb{P}]m = 0$$

are valid along  $\Sigma$ . Moreover, we get

$$(5.8) \quad P = 2\bar{g}F^e \frac{\partial \tilde{\psi}(x, C^e, \bar{g}, \alpha)}{\partial C^e} F^{p-*},$$

$$(5.9) \quad \bar{\mathbb{P}} = 2F^{pT} \frac{\partial \tilde{\psi}(x, C^e, \bar{g}, \alpha)}{\partial \bar{g}} \bar{g} F^{p-T},$$

with  $\bar{\mathbb{P}} := g^{-1}\mathbb{P}g$ , and the local mechanical dissipation inequality

$$(5.10) \quad P \cdot F^e \dot{F}^p + \pi \cdot \dot{\alpha} \geq 0,$$

<sup>52</sup>With  $\{e_1, e_2, e_3\}$  a vector basis in a neighborhood of  $x \in \mathcal{B}$ , and  $\{e^1, e^2, e^3\}$  its dual counterpart, tensor  $I$  is of the type  $I = \delta_B^A e^B \otimes e_A$ .

where  $\pi$  is the thermodynamic flux  $\pi := -\frac{\partial \tilde{\psi}}{\partial \alpha}$  conjugated with  $\dot{\alpha}$  in terms of dissipation production.

The proof of this theorem can be developed by reproducing the analogous proof in [73], with the minor variations required by the presence of  $\alpha$ . It is left to the reader. Notice that with respect to what is presented in [73], the assumption H2 is varied by the insertion of the factor 2, which appears then in (5.8).

Evolution equations for  $\dot{F}^p$  and  $\dot{\alpha}$  can be derived by accepting the maximum dissipation principle. This is a standard view determining associate plasticity [115], while completely non-standard is the previous theorem.

To state the maximum dissipation principle we need first to introduce an admissibility criterion, as it is well known. It can be expressed in terms of stress or strain. Here we adopt a standard representation in terms of stress  $P$  and thermodynamics flux  $\pi$  and write  $f(P, \pi) \leq 0$  for such a criterion, considering admissible the pairs  $(P, \pi)$  for which  $f$  satisfies the previous inequality.

The **principle of maximum dissipation**<sup>53</sup> prescribes that *among all possible pairs  $(P, \pi)$  satisfying the admissibility criterion, the one that is physically realized maximizes the dissipation.*

The expression of the dissipation here is (5.10). Maximizing it among admissible pairs  $(P, \pi)$  is tantamount to minimize the Lagrangian

$$\mathfrak{L} := -(P \cdot F^e \dot{F}^p + \pi \cdot \dot{\alpha}) + \lambda f(P, \pi)$$

with respect to  $P$  and  $\pi$ . When  $f$  is differentiable we get

$$\dot{F}^p = \lambda F^{e-1} \frac{\partial f(P, \pi)}{\partial P} = \lambda F^p F^{-1} \frac{\partial f(P, \pi)}{\partial P}$$

and

$$\dot{\alpha} = \lambda \frac{\partial f(P, \pi)}{\partial \pi},$$

with  $\lambda \geq 0$ , so that we can identify the Lagrange multiplier  $\lambda$  with the rate of the plastic shift (see [77]), and we have first  $\lambda f(P, \pi) = 0$ , then we can prove the consistency condition  $\lambda \dot{f}(P, \pi) = 0$  (see [115] for the proof).

Another way of determining evolution laws for  $\dot{F}^p$  and  $\dot{\alpha}$  is, obviously, to prescribe them. The choice depends on the specific case that we are handling.

**5.7. Doyle-Ericksen formula in hardening plasticity.** The relation (5.8) allows us to show that Doyle-Ericksen formula, commonly derived and discussed in finite strain elasticity (see [?]), holds also for elastic-plastic materials with hardening.

First, consider that (5.8) can be written as

$$P = 2\rho \tilde{g} F^e \frac{\partial \tilde{\psi}^\diamond(x, C^e, \bar{g}, \alpha)}{\partial C^e} F^{p-*},$$

after defining  $\tilde{\psi}^\diamond(x, C^e, \bar{g})$  as the free energy per unit mass, namely

$$\tilde{\psi}(x, C^e, \bar{g}, \alpha) = 2\rho \tilde{\psi}^\diamond(x, C^e, \bar{g}, \alpha),$$

being  $\rho$  the density of mass in the reference configuration.

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<sup>53</sup>It seems that the first scholar who has discussed this principle has been Richard von Mises (1883-1953) in 1928.

Write  $\rho_a$  for the density of mass in the actual configuration. When mass is preserved, we have (it is well known)  $\rho = \rho_a \det F$ .

**Proposition 3.** *In finite-strain (traditional) hardening plasticity, in the assumptions satisfying the covariance theorem above, if the mass is conserved, Doyle-Ericksen formula*

$$\sigma = 2\rho_a \tilde{g} \frac{\partial \psi}{\partial \tilde{g}}$$

holds true.

*Proof.* Since by definition the right elastic Cauchy-Green tensor with all covariant components is defined by  $C^e := F^{e*} \tilde{g} F^e$ , namely  $C_{\alpha\beta}^e = (F^{e*})_{\alpha}^i \tilde{g}_{ij} (F^e)^j_{\beta}$ , we can consider  $C^e$  as a function of  $F^e$  and  $\tilde{g}$ , namely  $C^e = \tilde{C}^e(F^e, \tilde{g})$ . Since  $\psi = \tilde{\psi}(x, C^e, \tilde{g})$ , as a result of  $G$ -invariance and objectivity requirements, we then have

$$\frac{\partial \psi}{\partial \tilde{g}} = F^e \frac{\partial \tilde{\psi}(x, \tilde{C}^e(F^e, \tilde{g}), \tilde{g}, \alpha)}{\partial C^e} F^{e*},$$

so that

$$\frac{\partial \tilde{\psi}(x, C^e, \tilde{g}, \alpha)}{\partial C^e} = F^{e-1} \frac{\partial \psi}{\partial \tilde{g}} F^{e-*}.$$

From the definition of the first Piola-Kirchhoff stress, it then follows that

$$\begin{aligned} \sigma &= \frac{1}{\det F} P F^* = \frac{2\rho}{\det F} \tilde{g} F^e \frac{\partial \tilde{\psi}^{\diamond}(x, C^e, \tilde{g}, \alpha)}{\partial C^e} F^{p-*} F^* \\ &= 2\rho_a \tilde{g} \frac{\partial \psi}{\partial \tilde{g}} F^{e-*} F^{p-*} F^* = 2\rho_a \tilde{g} \frac{\partial \psi}{\partial \tilde{g}} F^{-*} F^*, \end{aligned}$$

which completes the proof.  $\square$

### 5.8. Remarks and perspectives.

- $\pi$  does not appear in the power as an action conjugated with  $\dot{\alpha}$ , with an eventual identification with  $-\frac{\partial \tilde{\psi}}{\partial \alpha}$ . For this reason  $\pi$  does not contribute to any balance equation. Hence,  $\alpha$  is an internal variable in the sense of non-equilibrium thermodynamics (see, e.g. [24] and [14]).
- Previous remark inspires naturally (at least to me) another question: *Can plasticity be described in the sense of the framework discussed in previous sections?* In other words, can we associate to the plastic phenomena microstructural interactions satisfying their own balance equations? The approach would be in contrast with the choice of  $\alpha$  that is an unknown parameter useful just to measure the trend far from the neighborhood of thermodynamical equilibrium where the mechanical behavior ceases to be elastic. In principle there is no obstacle to an affirmative answer. Of course it is matter of modeling because many choice of the nature of  $\nu$  can be done, depending on the specific mechanism that we want to describe. An approach that connects the evolution of micro-defects leading to plasticity with micro-actions satisfying their own balance is in [25]. The micromorphic scheme, the case when  $\nu$  is a second-rank tensor (see [81] for the linear case and also [44] and [119] for the non-linear setting), has been adapted to plasticity in [31] and references therein. Another example pertaining specifically to plasticity is given in [49] where  $\nu$  is identified with the slip



velocity in single crystals. The subsequent pertinent literature is rather wide (see for example [50], [56], [46], [105]), and a specific essay could be dedicated to review it. The proposed models seem adequate (even particularly in certain cases) to capture various aspects of plastic phenomena and are often evidently useful to develop computations that may solve practical problems. And essentially the balance equations involving both macroscopic and microscopic actions (the latter associated with the mechanisms that the authors believe are essential to the description of specific aspects of the plastic flows) are in the most general cases deduced by resorting to the principle of virtual power as a basic source. To me this choice involves a foundational problem. In fact, when we start from the virtual power principle to find balance equations for a certain model, morally we have already in mind the exact structure of these balances. And I have already stressed the point speaking in general about microstructures in previous sections. Proposing a virtual power principle is tantamount to assign a priori the weak form of balance equations. Essentially, it could be the same to declare candidly in pointwise form the balances that one believes to be necessary for the analysis at hands. The question pertains the internal actions appearing in these balances. When we assign the expression of the virtual power, we are postulating the existence of such inner actions (see e.g. [50] and references therein). It could be perhaps useful to find that these actions are necessary, by means of some invariance procedure, for example from the external power alone, as it appears in previous sections. Hence, to me a rather interesting question is the following: *For what available models of plastic phenomena, based on balances of micro-actions, it is possible to prove the need of the existence of the inner actions that they involve (when they do it), by means of some invariance procedure accepted as a first principle, without postulating such actions?* An answer could help in discriminating among models of the same phenomena, probably.

- Beyond the question of the emergence of self-actions in the balance equations involving micro-actions, another issue to be discussed is the choice of  $\nu$  to represent adequately plastic mechanisms. The issue could appear volatile when considered in full generality, for an answer depends on the specific material or phenomenon under analysis. However, in the case of crystalline materials, some details can be done. For crystal lattices, Parry and Šilhavý have determined in [102] a basis for elastic invariants (see also [20] for their definition). In a discussion we had in September 2001 at Taormina, Parry and I were in agreement that generic functions of the elastic invariants could be adequate candidate for  $\nu$ , but we neither prosecuted our discussion nor wrote something about. If we accept our remark and want to follow it, however, we have to handle it with care. In fact, a minimalistic choice for  $\nu$  could be the dislocation density tensor, even without considering its gradient. The choice could be also appealing for it can be associated with geometric properties of the body manifold (its torsion). However, the same choice could be criticized. At the end of a 2001 paper on “Benefits and shortcomings of the continuous theory of dislocations”, Kröner wrote (page 1132) what follows: “The greatest shortcoming is that the dislocation density tensor  $\alpha$ , no matter whether introduced through

differential geometry or in the conventional way, measures the *average* dislocation density only and, therefore, regards the internal mechanical state utmost incompletely. In principle, this shortcoming could be overcome by reorientation of dislocation theory towards a statistical theory, but only with highest expenditure of computations." The remark suggests at least prudence in selecting a candidate for  $\nu$ .

- Viewing plasticity in terms of the general framework of multi-scale and multi-field representations of material complexities, as introduced in previous sections, opens the way to models of strain gradient effects in plastic phenomena. The necessity of the extension has been pointed out by crucial experiments [32], which have evidenced the effects due to the grain size in the torsion of thin metallic wires. These effects can be interpreted in terms of strain gradients. As a consequence, a number of related models of strain gradient plasticity has been developed. Some of them have been quoted in the previous items, all times we have discussed the possibility of interpreting plastic phenomena in terms of a framework involving the balance of micro-actions due to microstructural events. A question is then the origin of the link between the analysis of the strain-gradient effects and the multi-field setting. To give an adequate answer, we have to refer to a basic 1995 paper by Gianfranco Capriz [12], with a preamble concerning a contemporary work by J. E. Dunn and James Serrin [26], who showed that the presence of the spatial derivatives of strain in the list of constitutive variables, defining the state of a material point, is compatible with the second law of thermodynamics when the standard inner power density  $P \cdot \dot{F}$  is augmented by an addendum that depends on the same spatial derivatives of strain appearing in the list of state variables, decided from the beginning (such a description is rough, however it is sufficient to explaining our argument here). Dunn and Serrin called such an addendum *interstitial working*, to remind the pioneering use of gradients of density made by Korteweg to describe capillary effects. However, notwithstanding the clear indication of the way to be followed to consider correctly strain gradient effects, they did not go inside the nature of the interstitial working with the aim of linking it with microstructural events. The link was established explicitly by Capriz in [12] for second-grade elasticity, i.e. in the case in which we consider the first derivative of  $F$  in the list of state variables. His remark is simple but with deep consequences. Let us consider the multi-field and multi-scale model-building framework discussed in previous sections. Imagine also that external bulk actions on the microstructure are absent, i.e.  $\beta = 0$ . If there is some physical reason to imagine an internal constraint of the type  $\nu = \hat{\nu}(F)$ , in conservative setting, the multi-field and multi-scale scheme accounting for material complexity reduces to second grade elasticity and the necessary interstitial working is no more than the power of the micro-actions. Of course, without considering the multi-field framework used in [12], for second-grade elasticity we could introduce directly a hyperstress, a third-rank stress performing inner power in the spatial derivative of  $\dot{F}$ , developing then the relevant mechanical structures. Such a stress emerges naturally in conservative setting when we consider an elastic energy depending on  $F$  and  $DF$ , and we evaluate the first variation of it

around minimizers, after proving their existence. In non-conservative case, the existence of a hyperstress should be established, e.g., by a Cauchy-type theorem – an issue tackled, but not yet closed (the reader can find basic remarks in [96], [90], [34]). With respect to the actual state of the art, the interpretation in [12] establishes a direct link between higher-order stresses and microstructural events, whatever they be.

- The general multi-field and multi-scale framework for the mechanics of microstructures appears clearly useful when we address our attention to strain gradient plasticity and identify  $\nu$  with  $F^p$  (the literature in this sense is rather wide – see remarks in [50] and references therein) or even with the plastic part of the small-strain tensor (see also [31]). In accepting the identification of  $\nu$  with  $F^p$  and going along the guidelines proposed in previous sections, we would face the problem of interpreting changes in observers over  $\mathcal{M}$ , now the set including  $F^p$ , because  $F^p$  is a factor of the macroscopic deformation gradient  $F$ . The question deserves further investigations not yet developed.

## 6. PARAMETERIZED FAMILIES OF REFERENCE SHAPES: A TOOL FOR DESCRIBING CRACK NUCLEATION

Besides the notion of relative power and the use of virtual tangent maps appearing in the description of plasticity when we adopt the multiplicative decomposition, another possible way to account for multiple reference shapes is to consider a large class of them, all covering the set  $\mathcal{B}$  and differing one another by possible defect patterns. I have already sketched this point of view in the introduction. Here, before describing the formal structure of the approach, I find expedient to recall some disparate notions that delineate the scenario.

**6.1. A remark on standard finite-strain elasticity.** Consider the energy of an elastic simple body in large strain regime, neglecting body forces for the sake of simplicity:

$$\mathcal{E}(u, \mathcal{B}) := \int_{\mathcal{B}} e(x, Du(x)) \, dx.$$

A result by Coleman and Noll (see [18]) formalizes the physical incompatibility between the objectivity of the elastic energy density  $e(x, F)$  and its convexity with respect to  $F$ . In essence it implies loss of uniqueness of equilibrium configurations under prescribed boundary conditions.

A requirement of polyconvexity of  $e$  with respect to  $F$  (the dependence suggested in [6]) reconciles analytical and physical instances. Polyconvexity means that we have to consider the elastic energy density as a convex function of the triple constituted by  $F$ ,  $\text{cof}F$  and  $\det F$ . Also, when we take a polyconvex elastic energy and try to determine its minimizers, the minimizing sequences of  $F$ ,  $\text{cof}F$ , and  $\det F$  are independent with each other. This procedure implies the possibility to cross even incompatible strains, compatibility being recovered in the limit.

In discussing strain measures, we have already pointed out that  $\det F$  and the entries of  $F$  and  $\text{cof}F$  can be put all together in a unique geometric entity, the 3–vector  $M(F) \in \Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$ , with components the ones in the list  $(1, F, \text{cof}F, \det F)$ . Hence, we can consider the energy density as a convex function of  $M(F)$ , as indicated in [42].

I have already remarked that not always  $M(F)$  coincides with  $M(Du)$ . The identity is assured only when the strain is compatible. Considering  $e$  as a convex function of  $M(F)$  would then correspond to extend it even to incompatible strain states, a circumstance in agreement with the previous remark on minimizing sequences. Even in this case compatibility is recovered at the end of the minimizing procedure.

There is something more, however. In fact, the map  $F \mapsto M(F)$  is not convex, so is the subset of  $\Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$  containing elements of the type  $M(F)$  – write  $\Sigma_{1,+}$  for it. Hence, if we want to define a convex function of  $M(F)$ , we must consider the convex hull of  $\Sigma_{1,+}$ , namely

$$\Sigma_{1,+} := \left\{ M \in \Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3) \mid M = (1, H, A, \mathbf{a}), \mathbf{a} > 0 \right\},$$

with  $H$  and  $A$  the tensors defined in Section 2.5, and  $\mathbf{a}$  the scalar coinciding with  $\det F$  when  $M = M(F)$ . Once we have defined the energy density as a convex function over  $\Sigma_{1,+}$ , we add to it further conditions dictated by physics: the energy density blows up to infinity when  $\det F$  goes to zero or  $|M(F)|$  tends to infinity – infinite energy has to be paid for shrinking to a point a volume or to stretch at infinity a string. These requirements imply an analytical property: the energy is coercive. It is crucial in determining the existence of equilibrium states (the ones reached by a requirement of minimality for the energy). Previous conditions imply also that the energy is even coercive when evaluated over the inverse map, that is when it is referred to the actual shape of the body.

When we accept

$$e(x, F) = \tilde{e}(x, M(F)),$$

the first Piola-Kirchhoff stress

$$P = \frac{\partial e(x, F)}{\partial F}$$

becomes

$$P = \frac{\partial \tilde{e}(x, M(F))}{\partial M(F)} \frac{dM(F)}{dF}.$$

Since, by definition,  $M(F)$  is a third-rank, skew-symmetric tensor with all contravariant components (see Section 2.5), the components of the third-rank, skew-symmetric tensor

$$\omega := \frac{\partial \tilde{e}(x, M(F))}{\partial M(F)}$$

are all covariant, so that  $\omega$  is dual to  $M(F)$  and the product  $\omega \cdot M(F)$  is well defined in terms of duality pairing (see Section 2). Formally, we write  $M(F) \in \Lambda_3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$  and  $\omega \in \Lambda^3(\mathbb{R}^3 \times \tilde{\mathbb{R}}^3)$ . The map  $x \mapsto \omega(x)$  is then what is called a **3-form** over  $\mathcal{B}$ .

## 6.2. The current of a map and the inner work of elastic simple bodies.

In Lagrangian representation, consider the inner power of an elastic simple body undergoing large strains, namely

$$\int_{\mathcal{B}} P \cdot \dot{F} \, dx.$$

By taking into account the expressions in the previous section, we can write

$$\begin{aligned} \int_{\mathcal{B}} P \cdot \dot{F} \, dx &= \int_{\mathcal{B}} \omega \frac{dM(F)}{dF} \cdot \dot{F} \, dx = \int_{\mathcal{B}} \omega \cdot \frac{dM(F)}{dF} \dot{F} \, dx = \\ &= \int_{\mathcal{B}} \omega \cdot \frac{dM(F)}{dF} \dot{F} \, dx = \int_{\mathcal{B}} \omega \cdot \dot{M}(F) \, dx, \end{aligned}$$

and, in case of strain compatibility,

$$\int_{\mathcal{B}} P \cdot \dot{F} \, dx = \int_{\mathcal{B}} \omega \cdot \dot{M}(Du) \, dx.$$

Since  $\omega \cdot \dot{M}(Du)$  is an inner power density, the integral

$$\int_{\mathcal{B}} \omega \cdot M(Du) \, dx$$

has the meaning of **inner work**.

Once we fix  $u$ , we can allow  $\omega$  to vary arbitrarily. The physical significance of such a choice is the one of a virtual inner work obtained by testing over a given deformation virtual stresses. The remark clarifies the physical meaning of the functional  $G_u$  defined on smooth forms compactly supported over  $\mathcal{B} \times \tilde{\mathbb{R}}^3$  by

$$G_u(\omega) := \int_{\mathcal{B}} \omega(x, u(x)) \cdot M(Du(x)) \, dx$$

and commonly called **current** of  $u$  in geometric functional analysis (see the treatise [43]). For any second-rank skew-symmetric tensor-valued map  $x \mapsto \bar{\omega}(x)$ , we define another functional,  $\partial G_u$ , by

$$\partial G_u(\bar{\omega}) = G_u(d\bar{\omega}),$$

with  $d$  the exterior derivative.  $\partial G_u$  is commonly called **boundary** of  $G_u$ .

Summable maps  $u$  over  $\mathcal{B}$  with summable first distributional derivative, specifically elements of  $W^{1,1}(\mathcal{B}, \tilde{\mathbb{R}}^3)$ , such that

- $\det Du(x) > 0$  for almost every  $x \in \mathcal{B}$ ,
- the map assigning to every  $x$  the modulus (intended in the standard sense of modulus of tensors)  $|M(Du(x))|$  is summable too,
- $\partial G_u = 0$  on smooth, compactly supported 2-forms over  $\mathcal{B} \times \tilde{\mathbb{R}}^3$ ,
- for any  $\tilde{f} \in C_c^\infty(\mathcal{B} \times \tilde{\mathbb{R}}^d)$

$$(6.1) \quad \int_{\mathcal{B}} \tilde{f}(x, u(x)) \det Du(x) \, dx \leq \int_{\tilde{\mathbb{R}}^3} \sup_{x \in \mathcal{B}} \tilde{f}(x, r) \, dr,$$

are called **weak diffeomorphisms** [42].

Under the conditions assuring coercivity, minimizers of the elastic energy in finite strain regime are found in a subclass of the space of weak diffeomorphisms with summability  $p > 1$ , as shown in [42].

The integral inequality (6.1) allows self-contact of the body boundary along the deformation and prevents self-penetration. The constraint  $\partial G_u(\bar{\omega}) = 0$  is stable when we superpose to  $u$  any other smooth deformation. It excludes formation of holes and/or fractures. When such a condition is satisfied,  $u$  cannot be multi-valued in any part of its domain, as it occurs, for example, when a crack is nucleated and, eventually, opens and/or close along a deformation. In other words, the graph of  $u$  is free of vertical components – verticality refers to the reference placement  $\mathcal{B}$  in

the six-dimensional space  $\mathbb{R}^3 \times \tilde{\mathbb{R}}^3$ , the first factor referred to the 3D point space containing  $\mathcal{B}$ .

In this framework, if we want to model elastic-brittle behavior, we need to enlarge the functional setting at least weakening the constraint  $\partial G_u(\bar{\omega}) = 0$ .

**6.3. Griffith's energy.** When a fracture occurs in a body, energy is dissipated but also energy is localized along the crack margins, to assure the stability of the matter. It was Josiah Willard Gibbs who insisted on the assignment of positive surface energy to interfaces to assure stability of condensed matter structure. For fractures, in his pioneer work [45], Alan Arnold Griffith presumed that the surface energy is just *proportional* to the area of the crack margins. Hence, for an elastic-brittle solid undergoing bulk deformations, when a fracture occurs, Griffith's energy,  $\mathfrak{E}(u, \mathcal{B}, \mathcal{C})$ , writes

$$\mathfrak{E}(u, \mathcal{B}, \mathcal{C}) := \int_{\mathcal{B}} e(x, Du(x)) \, dx + \int_{\mathcal{C}} \phi \, d\mathcal{H}^2,$$

where  $\mathcal{C}$  is the image in the reference place of the crack occurring in the actual place, and  $\phi$  is the constant surface energy.

Such an expression has been used by Gilles Francfort and Jean-Jacques Marigo in [35] to propose a variational approach to fracture processes. In their view *at each instant*  $t \in [0, \bar{t}]$  *of a cracking process the pair*  $(\mathcal{C}, u)$  *should realize a minimum of the global energy*  $\mathfrak{E}$  with  $\mathcal{C}$  an admissible crack, i.e. a rectifiable set (the image of a countable number of Lipschitz maps) with zero volume measure.

Formally, instead of considering continuous time variation, the interval of time is discretized and minimality is required at time steps. Various analytical problems appear even so. The essential difficulty deals with the control in three dimensions of minimizing sequences of surfaces leading to the image  $\mathcal{C}$  in the reference place of the possible actual crack.

By taking into account that  $\mathcal{C}$  coincides with the jump set of the deformation  $u$  when the entire crack is open, a convenient simplification of the model is the identification of cracks with such a set. In accepting this point of view, bounded variation ( $BV$ ) or special bounded variation ( $SBV$ ) functions can be involved as candidates to be minimizers of the elastic energy. This way, and thinking always of elastic-brittle bodies, the energy that we can consider is the one of an elastic simple body (I have written it previously) and minimizers are sought in a space of maps including candidates to be reasonable descriptors of the elastic-brittle behavior. The approach stresses once again that the choice of function spaces where we search minimizers of some energy has constitutive nature. Along this path, essential results have been proven (see [21], [36], [20]).

Further difficulties emerge, however. Theorems allowing the selection of fields with discontinuity sets describing reasonable (physically significant) crack patterns seem to be not yet available (see [10] for a review of the current literature). Also, the identification of the crack with the discontinuity set of the deformation does not account for partially opened cracks. In the time-discretized procedure mentioned above, along a loading program described by time-dependent boundary conditions, in fact, it could happen that a crack nucleated at the  $i$ -th instant might close even partially, and then re-open at subsequent time steps. Along the closed margins the deformation is continuous, *but* the material bonds are broken in the actual place.

Once the minimizing problem has been successfully tackled, when a crack is identified with the discontinuity set of the deformation, stronger regularity assumptions on the geometry of the crack pattern are necessary to obtain balance equations (see once again [10], [21], [36], [20]).

**6.4. Aspects of a geometric view leading to an extension of Griffith's energy.** We can have another view on the description of cracks. It has been proposed in [41], [70] and extended in [40]. The items below contain its peculiar features.

- We distinguish between a crack pattern and the jump set of  $u$ , as in [35], by considering the latter set constrained to be contained in the crack pattern. This way we can describe circumstances in which parts of the crack margins are in contact but the material bonds are broken there.
- In contrast with all previous proposals, we describe the crack pattern through measures giving information about points in  $\mathcal{B}$  that can cracked directions that the fracture can have in passing through that points. Such measures are those called **curvature varifolds** for a generalized notion of curvature can be associated with them and is an indicator, in a precise sense, of how much a crack pattern is *curved* at a point, or better in a neighborhood of it.
- The energy resulting in the description of cracks in terms of varifolds differs from Griffith's one by the presence of the generalized curvature in the surface energy and the one along the tip in three dimensions. In this sense the model is an evolution of Griffith's scheme.
- We require then minimality of the energy in terms of pairs of deformations and curvature varifolds. The curvature-dependence of the surface energy has analytical advantages and permits the control of minimizing sequences. The proof of the existence of minimizers for the extended Griffith's energy in appropriate measure and function spaces is in [41].
- In the existence result the emerging crack pattern is a rectifiable set with zero volume measure. Although it can be very irregular, it has the features that our intuition assigns to a fracture.
- In contrast with previous proposals already mentioned, the balance equations can be derived in weak form from the first variation of the extended Griffith's energy, even for a crack that is a *generic* rectifiable set.

Details clarifying these items follow below.

**6.5. Cracks in terms of stratified curvature varifolds.** If a two-dimensional crack appears in the deformed configuration  $\mathcal{B}_a := u(\mathcal{B})$  and crosses a generic point  $u(x)$ ,  $x \in \mathcal{B}$ , its "direction" is locally described by the tangent plane to the crack at  $u(x)$ , when the crack is smooth. When the crack margins have a corner at  $u(x)$ , a cone of planes has to be considered. Crack patterns can be however very irregular. We could accept a set as a representative of a crack pattern when it is just rectifiable, as mentioned hitherto, for we should have at disposal an approximate notion of tangent plane, as prescribed in geometric measure theory (see [30]). Such planes can be even described in  $\mathcal{B}$ : we can take a plane crossing  $x$  as the imagine in  $\mathcal{B}$  of the one representing the crack "direction" at  $u(x)$ . In other words, we can consider in  $\mathcal{B}$  a set that is the pre-image of the crack pattern with the related approximate tangent planes.

Given a two-dimensional plane or a straight line in  $\mathcal{B}$ , the symbol  $\Pi$  indicates here the orthogonal projection over the plane or the line.  $\Pi$  is a 1-contravariant, 1-covariant tensor. The pair  $(x, \Pi)$  gives in  $\mathcal{B}$  local information on the geometry of the crack crossing possibly  $u(x)$ . In principle, any  $\Pi$  pertaining to the elements of the star of planes at  $x$  can be a candidate to describe locally the direction of a possible crack pattern. We can consider the pair  $(x, \Pi)$  as a point in a manifold  $\mathcal{G}_k(\mathcal{B})$ ,  $k = 1, 2$ , constructed by attaching at every  $x \in \mathcal{B}$  the manifold  $\mathcal{G}_{k,3}$  of  $2D$ -planes or straight lines on  $\mathcal{B}$ . This manifold is the so-called Grassmanian associated with  $\mathcal{B}$ . From a geometric viewpoint,  $\mathcal{G}_k(\mathcal{B})$  is a fiber bundle with natural projector  $\pi : \mathcal{G}_k(\mathcal{B}) \rightarrow \mathcal{B}$  and typical fiber  $\pi^{-1}(x) = \mathcal{G}_{k,3}$ .

A  $k$ -**varifold** over  $\mathcal{B}$  is a non-negative Radon measure<sup>54</sup>  $V$  over  $\mathcal{G}_k(\mathcal{B})$  (see [2], [3], [4], [55], [64]). It has a projection over  $\mathcal{B}$ , which is a measure indicated by  $\mu_V$ , used to define the so-called *mass*  $\mathbf{M}(V) := \mu_V(\mathcal{B})$  of the varifold itself.

In particular, we are interested in defining varifolds over subsets which can adequately describe crack patterns. Such sets, write  $\mathcal{C}$  for them, are measurable with respect to the  $k$ -dimensional Hausdorff measure<sup>55</sup> in  $\mathbb{R}^3$ ,  $k = 1, 2$ , and admit approximate tangent  $k$ -space (one-dimensional or two-dimensional). For  $\theta$  a summable function over  $\mathcal{C}$ , we say that  $V_{\mathcal{C},\theta}$  is a **rectifiable varifold** of density  $\theta$ ,

<sup>54</sup>A collection  $\Sigma$  of subsets of  $\mathbb{R}^m$  is called a  $\sigma$ -algebra on  $\mathbb{R}^m$  when  $\Sigma$  satisfies the following conditions: (i)  $\mathbb{R}^m \in \Sigma$ . (ii) If  $A \in \Sigma$ , its complement in  $\mathbb{R}^m$ , namely  $\mathbb{R}^m \setminus A$  is also in  $\Sigma$ . (iii) If  $A_k \in \Sigma$ , with  $k = 1, 2, 3, \dots$ , we get that the union of the sets  $A_k$ , varying  $k$  from 1 to infinity, is also in  $\Sigma$ , namely  $\bigcup_{k=1}^{\infty} A_k \in \Sigma$ .

The smallest  $\sigma$ -algebra containing all open subsets of  $\mathbb{R}^m$  is what we call the *Borel  $\sigma$ -algebra*. We call also its elements the *Borel sets*.

A *measure*  $\mu$  on  $\Sigma$  is a function  $\mu : \Sigma \rightarrow \mathbb{R}^+ \cup \{\infty\}$  such that

$$\mu \left( \bigcup_{k=1}^{\infty} A_k \right) = \sum_{k=1}^{\infty} \mu(A_k)$$

for any collection of mutually disjoint elements (i.e.  $A_r \cap A_s = \emptyset$  for  $r \neq s$ ) of  $\Sigma$  (in short we say that  $\mu$  is countably additive or  $\sigma$ -additive). We call  $\mu$  a *Borel measure* when it is defined on a Borel  $\sigma$ -algebra. We call a *Radon measure* a Borel measure such that  $\mu(K) < \infty$  for every compact  $K \subset \mathbb{R}^m$  and  $\mu(B) = \sup \{ \mu(K) \mid K \subset B, K \text{ compact} \}$  for every Borel set  $B$ .

<sup>55</sup>For  $k \geq 0$  and  $B \subset \mathbb{R}^m$ , we write  $\mathcal{H}^k(B)$  for the  $k$ -dimensional Hausdorff measure of  $B$  defined by

$$\mathcal{H}^k(B) = \sup_{\delta > 0} \mathcal{H}_{\delta}^k(B),$$

where, with  $0 < \delta \leq +\infty$ ,  $\mathcal{H}_{\delta}^k(B)$  is defined by

$$\mathcal{H}_{\delta}^k(B) = \frac{\omega_k}{2^k} \inf \left\{ \sum_{i \in \mathcal{I}} (\text{diam}(B_i))^k \mid \text{diam}(B_i) < \delta, B \subset \bigcup_{i \in \mathcal{I}} B_i \right\},$$

with  $\mathcal{I}$  some index set and the constant  $\omega_k$  is given by

$$\omega_k = \frac{\pi^{\frac{k}{2}}}{\Gamma\left(1 + \frac{k}{2}\right)},$$

being

$$\Gamma(t) := \int_0^{\infty} s^{t-1} \exp(-s) ds$$

the Euler  $\Gamma$ -function.

$\mathcal{H}^k$  vanishes identically for  $k > m$  and coincides with the measure counting points for  $k = 0$ . The reason for calling upon such measures is that their definition is totally independent of local parameterizations of sets and is valid even for irregular sets.  $\mathcal{H}^k$  is not  $\sigma$ -additive on all parts of  $\mathbb{R}^m$ .



associated with  $\mathcal{C}$ , when it is a measure over  $\mathcal{G}_k(\mathcal{B})$  satisfying the relation

$$\int_{\mathcal{G}_k(\mathcal{B})} \varphi(x, \Pi) dV_{\mathcal{C}, \theta}(x, \Pi) = \int_{\mathcal{C}} \theta(x) \varphi(x, \Pi) d\mathcal{H}^k,$$

for any  $\varphi \in C^0(\mathcal{G}_k(\mathcal{B}))$ .

Rectifiable sets can be considered a sort of generalized surfaces [2]. A subclass of them admits a notion of generalized mean curvature vector [3], [4]. For elements of such a subclass (not all), a notion of second fundamental form can be defined [55]. Here the attention is on varifolds admitting density  $\theta$  with integer values, the so-called **integer rectifiable varifolds**. For them, a third-rank tensor field  $(x, \Pi) \mapsto \mathbf{A}(x, \Pi)$  with components  $A_B^{HK}$  plays the rôle of a **generalized curvature**.

A varifold  $V$  is called a **curvature  $k$ -varifold with boundary** if (i)  $V$  is an integer, rectifiable  $k$ -varifold  $V_{\mathcal{C}, \theta}$  associated with  $\mathcal{C}$ , and (ii) there exists a summable function  $\mathbf{A}(x, \Pi)$  and a vector Radon measure  $\partial V$  such that, for every  $\varphi \in C_c^\infty(\mathcal{G}_k(\mathcal{B}))$ , we get

$$\int_{\mathcal{G}_k(\mathcal{B})} \left( \Pi_B^A D_{x^B} \varphi + A_B^{AK} D_{\Pi_B^K} \varphi + A_B^{AB} \varphi \right) dV(x, \Pi) = - \int_{\mathcal{G}_k(\mathcal{B})} \varphi d\partial V^A(x, \Pi).$$

The vector measure  $\partial V$  is called **varifold boundary measure** [64]. The subclass of varifolds with generalized curvature  $\mathbf{A}$  with summable  $p^{th}$ -power is indicated here by  $CV_k^p(\mathcal{B})$ . If  $V = V_{\mathcal{C}, \theta} \in CV_k^p(\mathcal{B})$ , with  $p > k$ ,  $V$  is locally the graph of a multi-valued function of class  $C^{1, \alpha}$ ,  $\alpha = 1 - \frac{p}{k}$ , far from  $\partial V$  (for the proof see [55]).

Reasons for selecting curvature varifolds with boundary as geometric descriptors of cracks can be listed.

- The set  $\mathcal{C}$  has the minimal geometrical properties of an admissible crack, at least in the sense to be a rectifiable set with zero volume measure (see [35]).
- The density  $\theta$  furnishes information on its possible faceted shape. If in a neighborhood of  $x$  there is a smooth surface,  $\theta = 1$ , when there is a net fold,  $\theta = 2$ , etc.
- The local orientation of the crack pattern is indicated by  $\Pi$ .
- The curvature of the crack is considered, although in the generalized (weak) form specified above. Its contribution does not appear in Griffith's original choice of the crack energy (remind: there the surface energy is just a constant and in subsequent cohesive models of fracture the crack curvature does not appear also – the surface energy is in that case a function of the deformation jump).
- The boundary of the crack – it includes the tip – is described by the boundary of the varifold.
- The use of varifolds allows one to account for different energetic contributions of the crack portions – the tip can have in principle a different energy from that of the crack margins. Specifically, a two-dimensional varifold  $V_2$  describes the crack, its boundary measure  $\partial V_2$  is supported by the entire boundary of the crack itself. To represent separately the crack tip, a one-dimensional varifold  $V_1$ , supported by the tip alone, has to be inserted. Its boundary describes possible corners along the tip and the points determining the intersection of the tip with the external boundary of the body  $\partial \mathcal{B}$ . The insertion of  $V_1$  allows one to assign peculiar energy to the tip of the crack.

- To capture the intuitive structure of the geometry under scrutiny, the varifolds  $V_2$  and  $V_1$  have to satisfy a certain link: the projection of the variation  $|\partial V_2|$  is bounded by  $\mu_{V_1}$ , as shown in [41].
- The framework allows us to consider not only two-dimensional cracks with the relative tips but also additional linear defects: very thin tubes along which material bonds are broken or even dislocations even emanating from a crack tip.

**6.6. Generalizing Griffith's energy.** With the previous (rather intricate) geometric premises, in the varifold-based description of the crack patterns the energy for a three-dimensional elastic-brittle simple body as proposed in [41] is

$$\begin{aligned} \mathcal{E}(u, \{V_k\}, \mathcal{B}) & : = \int_{\mathcal{B}} e(x, u(x), Du(x)) \, dx + \sum_{k=1}^2 \alpha_k \int_{\mathcal{G}_k(\mathcal{B})} |\mathbf{A}_{(k)}|^{p_k} \, dV_k + \\ & + \sum_{k=1}^2 \beta_k \mathbf{M}(V_k) + \gamma \mathbf{M}(\partial V_1), \end{aligned}$$

where  $\alpha_k$ ,  $\beta_k$ ,  $\gamma$  and  $p_k$  are constitutive coefficients. In particular,  $\alpha_k$ ,  $\beta_k$ ,  $\gamma$  are positive numbers, so the contribution of the generalized curvature of the varifolds is always present, even if it can be extremely small. The density  $e(x, u, Du)$  is defined as the difference  $e(x, u, Du) := \tilde{e}(x, Du) - w(u)$  between the **bulk elastic energy**  $\tilde{e}(x, Du)$  and the **potential  $w(u)$  of external body forces**.

- $\beta_2 \mathbf{M}(V_2)$  has the rôle of the last integral in  $\mathfrak{E}(\mathcal{C}, u)$ , that is Griffith's surface energy:  $\beta_2$  has the same meaning of  $\phi$  in  $\mathfrak{E}(\mathcal{C}, u)$ .
- $\beta_1 \mathbf{M}(V_1)$  counts energy along the tip. It is proportional to the length of the tip itself.
- $\gamma \mathbf{M}(\partial V_1)$  adds possible energy concentrated at the tip corners where material bonds can be entangled in principle in a way different from the other parts of the tip.
- The two addenda

$$\alpha_2 \int_{\mathcal{G}_2(\mathcal{B})} |\mathbf{A}_{(2)}|^{p_2} \, dV_2 + \alpha_1 \int_{\mathcal{G}_1(\mathcal{B})} |\mathbf{A}_{(1)}|^{p_1} \, dV_1$$

have pure configurational nature for they are associated strictly with the crack pattern alone. The first term accounts for the (generalized) curvature of the crack surface. The second term pertains to the tip. Curvature energy<sup>56</sup> can be associated with bending effects. They appear in the current configuration  $u(\mathcal{B})$  while  $\mathbf{A}$  is defined over the reference space. However, when bending effects are involved along the material bond breaking in the actual shape, they contribute to the mutation of the body, so they have a configurational effect pictured by  $\mathbf{A}$ . In other words, with the terms including  $\mathbf{A}$  we affirm that we pay energy for curving a crack.

- Configurations have to be compared to declare that a body is cracked. If we exclude the possibility of restoring cracks by gluing the matter across crack facies, an order relation has to be considered in the comparison. It is given by the monotonicity in the crack pattern sequences: given a crack in a certain configuration, to be compared with it, a subsequent configuration

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<sup>56</sup>Influence of the crack curvature, above all in the proximity of the tip, has been recognized in [114], a work devoted to Grinfeld's instability.

should have a crack pattern that coincides with or includes the previous crack. In terms of varifolds such a point of view is expressed by affirming the existence a family of *comparison varifolds*  $\{\tilde{V}_k\}$  such that the family of varifolds  $\{V_k\}$  describing the actual crack pattern is constrained by  $\mu_{\tilde{V}_k} \leq \mu_{V_k}$  for any  $k$  and  $\tilde{V}_k \in CV_k^{pk}(\mathcal{B})$ . The assignment of  $\{\tilde{V}_k\}$  does not mean that we are always considering in a given configuration a pre-existing crack pattern for the comparison varifold family can be even empty.

In the setting described so far, assigned boundary conditions, a minimality requirement for the energy selects among all admissible deformations and measures describing crack patterns.

*Minimize  $\mathcal{E}(u, \{V_k\}, \mathcal{B})$  with  $V_k$  in  $CV_k^{pk}(\mathcal{B})$ , comparison varifolds  $\{\tilde{V}_k\}$ ,  $u$  in an appropriate function space, with assigned boundary conditions.*

Hence, it is a minimization on a class of possible bodies: every possible crack pattern represented over  $\mathcal{B}$  defines a body, together with  $\mathcal{B}$  itself. Varifolds and deformations have to be related: possible nucleation, growth and/or opening of a crack in the current configuration are consequences of the deformation. The varifolds over  $\mathcal{B}$  are representatives of what happens in the actual configuration. The choice of the function space for  $u$  is then another key point of the treatment. Remind that we have in mind maps with discontinuity sets included in  $\mathcal{C}$  or at most coinciding with it.

The extension of the space of weak diffeomorphisms introduced in [41] satisfies that requirement.

Assigned a stratified curvature varifold  $V = \{V_k\}_{k=1}^{n-1}$  with boundary, i.e.,  $V_k \in CV^{pk}$ , we affirm that a map  $x \mapsto u$  is an **extended weak diffeomorphism** (write in short  $u \in dif^{1,1}(\mathcal{B}, V, \mathbb{R}^3)$ ) if

- (i):  $u$  is summable over  $\mathcal{B}$  and is a.e. approximately differentiable,
- (ii):  $|M(Du)|$  is also summable,
- (iii):  $\det Du(x) > 0$  for almost every  $x \in \mathcal{B}$ ,
- (iv): for any  $f \in C_c^\infty(\mathcal{B} \times \mathbb{R}^3)$

$$\int_{\mathcal{B}} \bar{f}(x, u(x)) \det Du(x) \, dx \leq \int_{\mathbb{R}^3} \sup_{x \in \mathcal{B}} \bar{f}(x, w) \, dw,$$

- (v):  $\pi_{\#} |\partial G_u| \leq \sum_{j=1}^2 \mu_{V_j} + \pi_{\#} |\partial V_1|$  as measures on  $\mathcal{B}$ , where  $\pi_{\#}$  is the projection over  $\mathcal{B}$  of the measures defined over  $\mathcal{G}_k(\mathcal{B})$ .

Such a space is closed (see proofs in [41] and [40]).

With respect to the definition of weak diffeomorphisms appearing in non-linear elasticity of simple bodies, the condition  $\partial G_u = 0$  is substituted by the last one in the previous list. It allows the possibility of discontinuities of the deformation  $u$  but imposes that they could occur only within the set  $\mathcal{C}$ : the crack pattern. The minimizing process of  $\mathcal{E}(u, \{V_k\}, \mathcal{B})$  then selects a deformation and a varifold supported over a rectifiable set (the crack pattern) where  $u$  may jump. It is in this sense that the process chooses among possible bodies.

We look for minimizers of  $\mathcal{E}(u, \{V_k\}, \mathcal{B})$  in terms of integer rectifiable stratified curvature varifolds and extended weak diffeomorphisms, precisely in a more regular

subclass of it, under conditions for the energy density  $e$  that are the same of the non-linear elasticity of simple bodies.

Within the space of extended weak diffeomorphisms, we select the subclass  $\text{dif}^{p,1}(\mathcal{B}, V, \mathbb{R}^3)$  of those such that the map  $x \mapsto |M(Du(x))|^p$  is summable, namely

$$\text{dif}^{p,1}(\mathcal{B}, V, \mathbb{R}^3) := \left\{ u \in \text{dif}^{1,1}(\mathcal{B}, V, \tilde{\mathbb{R}}^3) \mid |M(Du)| \in L^p(\mathcal{B}) \right\},$$

for some  $p > 1$ . Within such a subclass, we also select those  $u$  with bounded essential supremum – formally we write  $\|u\|_{L^\infty(\mathcal{B})} \leq K$ , with  $K$  a positive finite number.  $K$  does not have constitutive nature. Bounding the supremum of  $u$  is useful just to exclude that, in case the nucleation of a crack would separate a piece of the body from the rest, the fragment could not be translated rigidly at infinity. Hence, rather than indicating a specific property of the material,  $K$  selects among possible deformations, introducing a condition of admissibility. In this sense it is even not necessary to assign for  $K$  a specific value. It is just necessary to admit its existence.

Combination with the space of varifolds determines a functional class – write  $\mathcal{A}_{q,p,K,\{\tilde{V}_k\}}(\mathcal{B})$  for it – defined by

$$\begin{aligned} \mathcal{A}_{q,p,K,\{\tilde{V}_k\}}(\mathcal{B}) & : = \left\{ (u, \{V_k\}) \mid V_k \in CV_k^{p_k}(\mathcal{B}), u \in \text{dif}^{q,1}(\mathcal{B}, V_k, \mathbb{R}^3), \right. \\ & \left. \{V_k\} \text{ is stratified, } \|u\|_{L^\infty(\mathcal{B})} \leq K, \mu_{\tilde{V}_k} \leq \mu_{V_k}, \forall k = 1, 2 \right\}, \end{aligned}$$

where  $\tilde{V}_1$  and  $\tilde{V}_2$  are comparison varifolds describing possible initial cracks. In particular, the subclass

$$\mathcal{A}_{q,p,K,\{\tilde{V}_k\}}^{u_0}(\mathcal{B}) := \left\{ (u, \{V_k\}) \in \mathcal{A}_{q,p,K,\{\tilde{V}_k\}}(\mathcal{B}) \mid u(x) = u_0(x), x \in \partial\mathcal{B}_u \right\},$$

with  $\partial\mathcal{B}_u$  the part of the boundary of the body where we prescribe the deformation, takes into account boundary conditions of Dirichlet type, the ones under which we are able to find existence of minimizers, i.e. to select among possible cracked or not cracked bodies, at least in the setting presented here.

As mentioned above, the assumptions on the behavior of the energy density are the same presumed in non-linear elasticity of simple bodies:  $e$  is continuous in  $(x, u)$  and polyconvex in  $Du$ ; it satisfied the inequality  $e(x, u, Du) \geq c_1 |M(Du)|^r$  for  $r > 1$  and  $c_1 > 0$ ; if for some  $u \in \mathbb{R}^3$  the inequality  $e(x, u, Du) < +\infty$  holds, then  $\det Du > 0$ .

Under these conditions we can prove a theorem.

**Theorem 3** ([41]). *Assume  $K > 0$ ,  $q, p_k > 1$ , and  $\tilde{V}_k \in CV_k^{p_k}(\mathcal{B})$  for any  $k$ . If there exists  $(u_0, \{V_k^0\}) \in \mathcal{A}_{q,p,K,\{\tilde{V}_k\}}^{u_0}(\mathcal{B})$  such that  $\mathcal{E}(u_0, \{V_k^0\}, \mathcal{B}) < +\infty$ , then  $\mathcal{E}(u, \{V_k\}, \mathcal{B})$  attains in that space the minimum value.*

After proving the existence of minimizers, balance equations can be derived by the first variations for crack patterns that are just rectifiable sets. Such a possibility is not assured in approaches based only on Griffith's energy without the addition of further (regularity) assumptions. Details are collected in [41].

Notice that the presence of the curvature terms in the energy does not preclude the possibility of minimizers describing straight cracks.

**6.7. The contribution of microstructures.** Examples in the mechanics of ferroelectrics (see e.g. [37], [7]), quasicrystals (see e.g. [86]), polymeric materials (see e.g. [1], [97]), etc. show the influence of microstructural events on the formation and the growth of cracks. I have presented in [68] a general treatment of the interaction between microscopic events and macroscopic fracture, *not* in the spirit of varifold-based description of cracks. Here, I just indicate how such effects can be included in the variational, varifold-based description of cracks, as depicted so far. First, we can think of extending the energy  $\mathcal{E}(u, \{V_k\}, \mathcal{B})$  up to include microstructural effects in the bulk. With the aim of taking into account different possibilities, we can suggest a general form for the energy that can be a tool for describing special cases. A proposal is in [40], where an energy  $\mathcal{E}(u, \tilde{\nu}, \{V_k\}, \mathcal{B})$  is suggested with the form

$$\begin{aligned} \mathcal{E}(u, \tilde{\nu}, \{V_k\}, \mathcal{B}) : &= \int_{\mathcal{B}} e(x, u(x), Du(x), j(\nu)) \, dx + \sum_{k=1}^2 \alpha_k \int_{\mathcal{G}_k(\mathcal{B})} |\mathbf{A}_{(k)}|^{p_k} \, dV_k + \\ &+ \sum_{k=1}^2 \beta_k \mathbf{M}(V_k) + \gamma \mathbf{M}(\partial V_1) + \mathfrak{F}(\nu). \end{aligned}$$

We presume that the map  $\tilde{\nu}$  assigning to every  $x \in \mathcal{B}$  the descriptor  $\nu$  of the pertinent material microstructure belongs to a function space  $X$ , rendered explicit just in special cases. In general we need just to assume that  $X$  can be mapped in a space of summable fields over  $\mathcal{B}$ , taking values over  $\mathcal{M}$ . The map is

$$j : X \longrightarrow L^1(\mathcal{B}, \mathcal{M}).$$

The term  $\mathfrak{F}(\nu)$  is introduced to account for possible (even non-local, as in the case of effects determined by polarization in ferroelectrics) interactions among elements of the material microstructure and/or self-actions of a single microstructural element on itself.  $\mathfrak{F}(\nu)$  is a functional  $\mathfrak{F} : X \longrightarrow \mathbb{R}$  that is assumed to be lower semicontinuous in  $L^1$  and such that, for every  $k$ , the set  $\{\nu \in X \mid \mathfrak{F}(\nu) \leq k\}$  is compact for the  $L^1$  convergence.

For example, depending on constitutive choices,  $j(\nu)$  can be either the approximate differential  $D\tilde{\nu}$  of  $\tilde{\nu} \in X$  or the  $\tilde{m}$ -vector  $M(D\tilde{\nu})$ , with  $\tilde{m}$  the dimension of  $\mathcal{M}$ . The map  $j$  is assumed to be such that  $j(\tilde{\nu}_k) \rightharpoonup j(\tilde{\nu})$  weakly in  $L^1$  if  $\sup_k \mathfrak{F}(\tilde{\nu}_k) < +\infty$  and  $\tilde{\nu}_k \longrightarrow \tilde{\nu}$  strongly in  $L^1$ . The explicit expression of  $\mathfrak{F}$  depends on the choice of  $X$ .

**Example 3.** When, for example,  $X = W^{1,p}(\mathcal{B}, \mathcal{M})$ ,  $p > 1$ , and  $\mathcal{M}$  is selected to be the unit sphere  $S^2$ ,  $\mathfrak{F}(\nu)$  can be the Dirichlet integral

$$\frac{1}{2} \int_{\mathcal{B}} |D\nu|^2 \, dx$$

or the corresponding non-local relaxed energy

$$\frac{1}{2} \int |D\nu|^2 \, dx + 4\pi L(\nu)$$

where  $L(\nu)$  is the length of the minimal connection of the singularities of  $\nu$  (see [8] and also [43]). Correspondingly, the map  $j$  is given by  $j(\nu) := D\nu$  and has the required continuity.

**Example 4.** *Another explicit example emerges when we select*

$$X = \{\tilde{\nu} \in SBV(\mathcal{B}, \mathbb{R}^N) \mid \nu(x) \in \mathcal{M} \text{ for a.e. } x \in \mathcal{B}\}.$$

*In this case*

$$\mathfrak{F}(\nu) = \int_{\mathcal{B}} \mathbf{f}(D\nu) \, dx + c\mathcal{H}^2(J_\nu) + \|\nu\|_\infty, \quad p > 1, \, c > 0,$$

*where  $\mathbf{f}$  is a convex function such that  $\mathbf{f}(\xi) \geq c_1|\xi|^p - c_2$ ,  $p > 1$ ,  $C_1 > 0$ . The constant  $c$  has constitutive nature and adjusts the physical dimensions. Even in this case  $j(\nu) := D\nu$ .*

The proof of the existence of minimizers for  $\mathcal{E}(u, \tilde{\nu}, \{V_k\}, \mathcal{B})$  is in [40]. In particular, the minimizing deformation  $u$  can be an extended weak diffeomorphism once again or it can belong to a functional class modeled over the space  $SBV$  of special bounded variation functions.

I do not add here further details (see [40] for them). My initial plan was just to indicate a non-standard way of considering the idea of multiple reference shapes in describing mutations of bodies. The point of view based on varifolds has descriptive potentialities that are better off approaches based on the standard Griffith's energy. It has its limitations for the dissipation in the nucleation of a crack is not directly evident, rather it could emerge indirectly from a gap phenomenon which is not yet explored. Also, if we use the minimizing processes just described, both in presence or absence of a direct account of microstructural events, in a time-step procedure a related question should be the evaluation of the convergence when the time intervals go to zero.

## 7. NOTES AND FURTHER PERSPECTIVES

- The previous variational description of crack nucleation could be exploited for computational analyses, including it in a time-step procedure, to account for progressive cracking.<sup>57</sup> Another question not yet explored in that specific case is the convergence of sequences of functionals  $\mathcal{E}_{t_i}(u, \tilde{\nu}, \{V_k\}, \mathcal{B})$ , referred to the instant  $t_i$  in the time discretization, when the size of the time steps goes to zero.
- For computations, the notion of relative power could be also exploited in several circumstances, even accounting for its possible enrichments in presence of structured discontinuity surfaces, linear defects, and strain-gradient effects.
- The presence of some symmetry in the material structure could address us toward specific choices of the manifold of microstructural shapes  $\mathcal{M}$ . Imagine to have provisionally chosen an habit set  $\mathbb{S}$  for the microstructural descriptors, a finite dimensional differentiable manifold once again, and write  $G$  for the symmetry group of the aspects of the microstructure

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<sup>57</sup>A key point would be the numerical approximation of the varifold, which presumably would lead us toward a phase-field description of the fractured zones. For phase-field description of the fracture processes *not* involving a varifold-based representation of the crack patterns see [83], [9], [53].

represented by the elements of  $\mathbb{S}$ . Assume that  $G$  is a (not necessarily connected) topological group<sup>58</sup> that acts transitively from the left on  $\mathbb{S}$ .<sup>59</sup> Can take a reference  $s \in \mathbb{S}$  and its **fixer group** (also called the isotropy group)  $H_s := \{a \in G \mid as = s\}$ . For any  $a \in G$ , the set of all elements in  $G$  of the form  $ah$ , with  $h$  any element of  $H_s$ , is called a **coset** of  $H_s$  in  $G$ . Two cosets in  $G$  are either identical or have no elements in common at all. Since  $G$  acts transitively on  $\mathbb{S}$ , taken  $s_1, s_2 \in \mathbb{S}$ , and  $a \in G$  such that  $s_2 = as_1$ , we get  $H_{s_2} = aH_{s_1}a^{-1}$ , intending that any  $h_2 \in H_{s_2}$  is of the form  $h_2 = ah_1a^{-1}$ ,  $h_1 \in H_{s_1}$ . Hence, what we construct with  $G$  and  $H_{s_1}$  has its counterpart on the pair  $(G, H_{s_2})$  by the inner automorphism  $G \rightarrow aGa^{-1}$ . This last transformation preserves the group-theoretic structure and is continuous, so that it keeps also the topological structure. For this reason, we can represent the microstructural morphology by using elements of the *coset space* of  $H$  in  $G$ , indicated by  $G/H$ . We do not specify the reference element associated with the isotropy group  $H$  because the choice of  $G/H$  is independent of it in the sense specified in the previous remarks.<sup>60</sup>  $G/H$  is itself a group when  $H$  is a normal subgroup<sup>61</sup>, but in general it is not so (further details are in [80]). A paradigmatic example is that of liquid crystals in nematic order. They are composed by stick molecules that are able to change one another the relative orientation along a motion. A provisional choice for a descriptor of them could then be a unit vector associated with a single molecule or a group of them depending on the view of the material element we have. In this case  $\mathbb{S}$  would coincide with the unit sphere  $S^2$  in 3D real space. The group  $SO(3)$  acts transitively on it. The choice of  $S^2$ , however, is not completely satisfactory because the liquid crystal molecules have head-to-tail symmetry: their fixer group is that of rotations about the molecular axis and  $180^\circ$  rotations about axes perpendicular to the molecular one – write  $D_\infty$  for such a group. To account for such a symmetry, we have then to accept as morphological descriptor of the nematic structure elements of the coset space  $SO(3)/D_\infty$ , which is the projective plane  $P^2$ , a space of directions without orientation that is in this case the appropriate choice for  $\mathcal{M}$ .

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<sup>58</sup>We say that  $G$  is a *topological group* when it satisfies the following conditions:

- $G$  is a group.
- $G$  is a topological space such that for any pair of distinct elements  $a$  and  $h$  in  $G$  we can select non-intersecting neighborhoods of them.
- The functions  $a \mapsto a^{-1}$  and  $(a, h) \mapsto ah$ , with  $a, h \in G$  and  $ah$  the result of the composition rule in  $G$ , are continuous, the second function with respect to the pair of variables  $a, h$ .

<sup>59</sup>It means that for any  $s_1$  and  $s_2$  in  $\mathbb{S}$  there is a transformation  $a \in G$  which takes  $s_1$  into  $s_2$ , namely  $s_2 = as_1$ . The transformation needs not be unique.

<sup>60</sup>Take  $s \in \mathbb{S}$  as a reference morphological descriptor.  $H$  is the set of elements  $h$  of  $G$  such that  $hs = s$ . For any other  $s' \in \mathbb{S}$  we can find  $a$  in  $G$  but *not* in  $H$  such that  $s' = as$  so that we can associate  $s'$  with the coset  $aH$ . The correspondence is one-to-one and continuous (see [80] for the proof). Consequently, a convergent sequence of cosets corresponds to a convergent sequence of  $s_k = a_k s$  and vice-versa.

<sup>61</sup> $H$  is a *normal subgroup* of  $G$  when it is a subgroup of  $G$  and is such that  $aH = Ha$  for any  $a \in G$ . It means that for any  $a \in G$  and  $h_1 \in H$ , we can find  $h_2 \in H$  such that  $ah_1 = h_2a$ . Of course, when  $G$  is commutative every its subgroup is normal.

- Defects in the microstructure, considered as mutations in the order allowing us to choose  $\mathcal{M}$  to be coincident with a coset space  $G/H$ , can be classified through the homotopy<sup>62</sup> properties of  $\mathcal{M}$ . Consider as a toy example the absence of microstructure in a specific place  $\tilde{x}$  in  $\mathcal{B}$ , at a certain instant  $\tilde{t}$ . In our picture, we can say that the map  $\tilde{\nu}$  is not defined at  $(\tilde{x}, \tilde{t})$ , or, alternatively, that  $\tilde{\nu}$  takes as value at  $(\tilde{x}, \tilde{t})$  the entire  $\mathcal{M}$ . Hence, at fixed  $\tilde{t}$ , if we consider a sphere centered at  $\tilde{x}$  and restrict  $\tilde{\nu}$  to the sphere, we cannot shrink to zero the sphere being able always to recognize a well-defined limit value of the map  $\tilde{\nu}$ . This is a topological obstruction to the possibility of eliminating the defect by rearranging the matter. The idea has generated the so-called *topological theory of defects*. This point of view is attributed to Lev Davidovič Landau, and investigated further by scholars in solid-state physics (the extended reviews [80], [81], and [57] furnish a clear view on the matter). The scheme has its limits. Consider, for example, a liquid crystal occupying  $\mathcal{B}$ . As we have already seen, the natural manifold of microstructural shapes is the real projective plane  $\mathbb{P}^2$  for which the first homotopy group is  $\pi_1\mathbb{P}^2 = \mathbb{Z}/2\mathbb{Z}$  and the second one  $\pi_2\mathbb{P}^2 = \mathbb{Z}$ . As a consequence, we can recognize line and point defects in a nematic order: the former ones are just of one type because the cyclic group is of order two, so that we have just two types of point defects with charges  $+$  and  $-$ . Hence, if we insert a volumetric inclusion, we are not able to recognize it as a defect in the picture just sketched. It would be like we would imagine the liquid crystal in a new space domain which is no more the whole  $\mathcal{B}$ , rather  $\mathcal{B}$  without the inclusion, with the boundary of the latter that becomes an internal phase interface. The question on whether the inclusion is a defect would depend, then, on the view that we have.
- The topological approach mentioned in the previous item is just descriptive. To evaluate the evolution, we have to make use of the balance of microstructural actions and we have to add standard balances of forces and couples in presence of macroscopic deformations. For defect nucleation, variational approaches selecting in classes of possible bodies can be also appropriate under circumstances, as we have shown for cracks.

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<sup>62</sup>We say that two paths over  $\mathcal{M}$ , namely  $\gamma_1, \gamma_2 : [0, 1] \rightarrow \mathcal{M}$ , such that  $\gamma_1(0) = \gamma_2(0) = \nu_0$  and  $\gamma_1(1) = \gamma_2(1) = \nu_1$ , are *homotopic* if there is an *homotopy* between the two, precisely a continuous mapping  $f : [0, 1] \times [0, 1] \rightarrow \mathcal{M}$  such that  $f(t, 0) = \gamma_1(t)$ ,  $f(t, 1) = \gamma_2(t)$  and for any fixed  $s \in [0, 1]$  the mapping  $f(\cdot, s) : [0, 1] \rightarrow \mathcal{M}$  specifies a path from  $\nu_0 = f(0, s)$  to  $\nu_1 = f(1, s)$ . We pay special attention to homotopy classes of closed loops. In the notations above they are such that  $\gamma(0) = \gamma(1)$ . A group structure can be given to these classes. The resulting group, indicated by  $\pi_1(\mathcal{M})$ , is called the *fundamental group* or the *first homotopy group*. We can construct higher-order homotopy groups. I mention here just the second homotopy group  $\pi_2(\mathcal{M})$  constructed by referring to “spheres” instead of paths. The same definitions apply when we consider the homotopy of loops or spheres over  $\mathcal{B}$ . The map  $\tilde{\nu} : \mathcal{B} \rightarrow \mathcal{M}$  determines a correspondence between loops in  $\mathcal{B}$  and those in  $\mathcal{M}$ . In fact, with  $\hat{\gamma} : [0, 1] \rightarrow \mathcal{B}$  a loop in  $\mathcal{B}$  we get another loop  $\tilde{\gamma} := \tilde{\nu} \circ \hat{\gamma}$  given by  $\tilde{\gamma}(t) := \tilde{\nu}(\hat{\gamma}(t))$ . Analogous reasonings can be considered for spheres, once we specify the relevant notion for  $\mathcal{M}$ .

Remind that if  $\mathcal{B}$  is two-dimensional, loops can characterize point defects: a loop surrounding a point defect – say an atomic vacancy – cannot be shrunk to a point; in other words it is not homotopic to a point. If  $\mathcal{B}$  is three-dimensional, loops can be used to individuate line defects (it is the standard way of determining the Burgers tensor for dislocations: we start considering a loop around the dislocation itself), while spheres are associated to point defects.



The matter is vast. Vistas are far reaching. Theoretical, computational, experimental and technological instances contribute to render the sector a fruitful research ground.

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